Investigation of ions hydration using molecular modeling

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Ion hydration phenomena are of great interest in the fields of physics, chemistry, biology, geochemistry and environment. However, few studies using identical calculation methods to characterize the hydration properties of ions in water and in electrolytic systems are available. Hence, it is difficult to compare the hydration properties of ions when they come from different methods. The objective of this work is, therefore, to use a unique approach to compare the hydration properties of ions in pure water and in presence of counter-ion using a quantum mechanical method, the Density Functional Theory (DFT). For this purpose, a methodology based on the decomposition of the system's energy is described and implemented in this study. In the first part, quantum mechanics calculations are used to determine the hydration properties of ions, without counter-ion, in presence of water molecules. In the second part, the hydration characteristics of solutes in systems containing ions, counter-ions and water molecules are studied. Results show that the presence of an anion (Cl^- or SO_4^{2-}) does not cause structural and energetic changes in the cation first hydration layer (Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}). Conversely, the anion first hydration layer depends on the cation of the system.

1. Introduction

Ions hydration phenomena are of great interest in the fields of physics, chemistry, biology, geochemical and environment [1–5]. The hydration phenomenon can be considered as the disrupt induced by the presence of a solute in the water network leading to the formation of a water cluster around the solute. In the vicinity of an ion, electrostatic interactions control the formation and the structure of the hydration layer. These interactions play a fundamental role in the thermodynamic behavior of the solutions [6]. For example, the addition of NaCl or LiCl in an aqueous saccharide solution reduces the water mobility, resulting in an increase in the intrinsic viscosity of the solution [7]. Hydration plays also a substantial role in the stability and recognition of ions in biological processes. For instance, the selectivity of potassium in potassium channels depends on the hydration properties of K^+ [8].

The behavior of an ion in water can be evaluated from its hydration number, which characterizes the number of water molecules disturbed by the presence of the ion. Widely different ion hydration numbers have been obtained, depending on the determination method. For example, thermodynamic modeling calculations as well as freezing point measurements use ion hydration numbers as an adjustment variable [9–14]. In liquid/liquid extraction, the ion hydration number is calculated from the water concentration increase in a phase, following the extraction of an ion [15]. Finally, in compressibility measurements, the ions hydration numbers are determined from the apparent molar compressibility at infinite dilution of the electrolytes. The hydration layer surrounding an ion is then assumed to be incompressible [16]. Thus, the diversity of methods and results makes it difficult to compare the hydration properties of ions. In fact, the different methods do not have a single definition of the hydration number and characterize the hydration of a solute by considering different hydration layer properties.

Over the year, quantum mechanical simulations have been widely used to characterize ions hydration in water, without counter-ion [17–20]. For example, Loeffler et al. [21] discussed in details the hydration structure of Li^+. Other studies have also compared the impact of using different simulation methods on the Ca^{2+} properties in water [22] or on SmI_2 [23]. Various molecular simulation works have been used to study electrolytic solutions [24–28]. In concentrated electrolyte solutions, ions pairs impact the water molecules in the first central ion coordination layer. The specific effects of ions are expected to occur mainly at high salt concentrations (>100 mM). However, they can also be found at much lower salt concentrations [29]. Ionic specificity is therefore a consequence of ionic polarizability, hydration and size [30].

Few studies using identical calculation methods to characterize ion hydration layer in water and in electrolytic solution are available. It is therefore difficult to compare the hydration properties of ions when they arise from different methods.

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The objective of this work is thus to develop a unique approach to compare the ions first hydration layer in pure water and in the presence of counter-ion in water. The work proposes to clearly define the first hydration layer of an ion, which is the ion coordination number.

For this purpose, the ions first hydration layer will be described at the molecular level using a quantum mechanical method, the Density Functional Theory (DFT). The fundamental approach proposed consists, on the one hand, in characterizing the first hydration layer of Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, SO_4^{2-} in pure water, without counter-ion. On the other hand, the study will focus on the determination of the ions first hydration layer in presence of counter-ions and water molecules in various systems (LiCl, NaCl, KCl, $MgCl_2$, $CaCl_2$ and $MgSO_4$). The determination of the hydration properties of ions, from a common method, will make it possible to study the influence of the ion on the first hydration layer of the counter-ion. Parameters such as the coordination number, the geometry of the water network of the first hydration layer, the hydration enthalpy and the distance between the ion and the coordinated water molecules will be studied.

For that, a methodology based on the decomposition of the system energy is described and implemented in this study.

2. Computational details

2.1. Ions hydration properties in water

Ions hydration properties were computed at the DFT level using the Gaussian 09 suite of program. Geometries were fully optimized in gas phase at 298.15 K and 1 atm, without symmetry constraints, employing the hybrid density functional B3PW91 [31]. Potential surfaces energy, as well as optimized geometries, do not depend on temperature and pressure. However, thermochemistry, as enthalpy and entropy, are temperature dependent.

For the Li, Na, K, Mg, Ca, H, O, Cl et S atoms, a double-zeta 6-31G [32] basis set augmented by a polarization function were used.

In our previous work, the hydration properties of ions in pure water have been studied via a stepwise solvation by adding one water molecule at a time and geometry optimizations were carried out without any symmetry constraints [33]. The water-shell around the solutes was obtained using the methodology proposed by Castro et al. [34] for mercury compounds and also by Zhao et al. [35] for samarium complexes. Solvation enthalpy of the ion $H_{ion/w}$ was calculated at 298.15 K, from the difference between the enthalpy of the complex ion + water molecules (H_{ion+W}) and those of the two separated fragments, i.e. the ion, H_{ion} and the water cluster, H_W, as described by equation (1):

$$H_{ion/W} = H_{ion+W} - H_{ion} - H_W \quad (1)$$

The ion first hydration layer is complete if the following conditions are verified:

- the derivate of the ion hydration energy as a function of the number of water molecules becomes positive, i.e. changes sign,
- the evolution of the ion hydration energy as a function of the water molecules number reaches a plateau,
- the ion coordination number remains constant as the number of water molecules increases (the number of water molecules coordinated to the ion, in its first hydration shell, remains the same as the number of water molecules increases).

When the conditions are verified, the ion first hydration shell is considered to be complete. On these structures, the ion hydration enthalpy is then calculated by averaging the energy reached at the plateau.

The ion coordination number is defined as the number of water molecules directly in interaction to the central ion, in its first solvation layer. A water molecule is considered in direct interaction with the ion, if the length of the bond is shorter than the sum of the van der Waals radii of the interacting atoms [36,37] (Table 1). In addition, in the case of anion, hydrogen bonds have to be established between the hydrogen of the water molecule and the anion, that means a donor-acceptor distance between 1 Å (covalent O—H distance) and 2.5 Å [38] (sum of the van der Waals radii of O and H, see Table 1).

Table 1
Van der Waals radii [36,37] ($r_{VdW,}$ in Å) of the studied atoms.

Atom	r_{VdW} (Å)
Li	1.90
Na	2.30
K	2.70
Mg	1.96
Ca	2.41
Cl	1.75
S	1,85
O	1.40
H	1.10

2.2. Hydration properties of ions in presence of counter-ion

The methodology is also used to estimate the interactions between species in systems containing the ion, the counter-ion and water molecules. The methodology developed is based on the same approach as the one used for ions in pure water (see Section 2.1).

In systems containing ions, counter-ions and water molecules, interactions are more complex to study, because of the presence of 3 species in solution (cation, anion and water network), which induce additional interactions of ternary type, between the cation, the anion and the water network.

Therefore, the total energy of the system arises from:

- the enthalpy of each specie: the cation (H_{C+}), the anion (H_{A-}) and the water network (H_W),
- the interaction energy of the species taken in pairs:
  - Interaction between the cation and the anion: $H_{C+/A-}$
  - Interaction between the cation and water network: $H_{C+/W}$
  - Interaction between the anion and the water network: $H_{A-/W}$
- the interaction between the cation, the anion and the water network ($H_{C+/A-/W}$).

Thus the total enthalpy, H_{Tot}, is expressed according to the relation (2):

$$H_{Tot} = H_{C+} + H_{A-} + H_W + H_{C+/A-} + H_{C+/W} + H_{A-/W} + H_{C+/A-/W} \quad (2)$$

The schematic representation (Fig. 1) enables to understand the energy decomposition given by Eq. (2).

The interaction enthalpy between 2 species is calculated using the Eq. (1), by isolating the 2 species from the system.

The ternary interaction term is then deduced from Eq. (2):

$$H_{C+/A-/W} = H_{Tot} - (H_{C+} + H_{A-} + H_W + H_{C+/A-} + H_{C+/W} + H_{A-/W}) \quad (3)$$

The salt hydration enthalpy (Fig. 2), $H_{CA/W}$ is estimated from the relation (4) by subtracting the enthalpy of the water network (H_W) and the energy of the cation + anion ($H_{(C+)+(A-)}$), from the total energy of the system (H_{Tot}).

$$H_{CA/W} = H_{Tot} - H_W - H_{(C+)} + (A-) \quad (4)$$

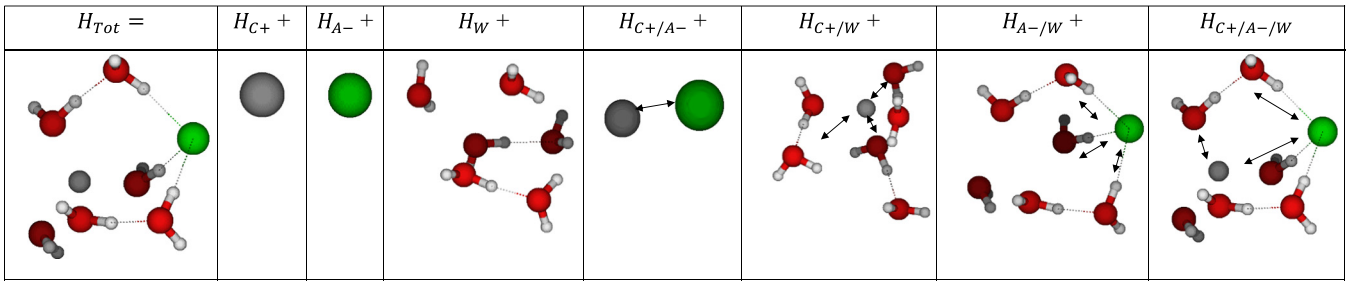


Fig. 1. Schematic representation of the energy decomposition of the system (Eq. (2)). The arrows indicate the interaction energy between species.

The evaluation of the hydration properties of the ions in systems is carried out from an iterative procedure, by adding one water molecule at a time and geometry optimizations are carried out without any symmetry constraints. For information, species coordinates are given in Electronic Supplementary information (ESI).

Regarding the hydration properties of ions, enthalpy energies (Eq. (2)) are calculated if the following conditions are satisfied:

- Ions dissociation in water is complete.

Ions are considered dissociated when the distance between cations and anions is larger than the sum of the van der Waals radii of the interacting atoms [36,37].

- The ion first hydration layer is complete,
- The interaction enthalpy between the cation and the anion, $H_{C+/A-}$, is stable.

When the dissociation of salts is complete, it is found that the hydration energy of the salt is stable.

When conditions are satisfied, the enthalpy energies of Eq. (2) are calculated. The ion hydration enthalpy is then the average of the energy reached at the plateau.

3. Results

3.1. Ions properties in pure water

In our previous work [33], an analysis of the main structural and energy characteristics of Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+} and of Cl^-, SO_4^{2-}, in pure water was carried out.

When the conditions described in II.1 are verified, the ion first hydration shell is considered to be complete.

For example, Fig. 3 shows the evolution of the hydration enthalpy of Li^+, $H_{Li+/W}$ and its derivate, $dH_{Li+/W}/dN_W$, as a function of the number of water molecules N_W, at 298.15 K.

When the first 4 water molecules are added to the system, the variation in Li^+ hydration energy is very important (about 150 $kJ.mol^{-1}.N_W^{-1}$), which shows the importance of the first 4 water molecules, necessary to stabilize the specie. These variations become lower from the 5th and 6th water molecules, about 50 $kJ.mol^{-1}.N_W^{-1}$, showing that these molecules contribute less to the stabilization of the species than the first water molecules added.

At the 7th water molecule, the $H_{Li+/W}$ derivate becomes positive, which means that the 7th water molecule has no impact on the hydration energy of the ion. Then, the ion's hydration energy continues to decrease, more slowly, showing that the added water molecules have little impact on the ion's hydration energy but rather on the stability of the water network. Each new water molecule added is used to build the water network, creating new hydrogen bonds with the first hydration layer of the species. These water molecules have less effect on the overall hydration energy of the species.

At the 8th added water molecules, the derivate of the ion hydration energy remains positive and close to zero, meaning the variation of the Li^+ hydration energy is low and positive. At the 9th water molecule, the derivate of the ion hydration energy becomes negative again (hydration energy decreases) and far from zero (higher variation of the ion hydration energy). Thus, it is considered that the first plateau of the ion hydration energy is reached between 6 and 8 water molecules (derivates of the ion hydration energy positive and close to zero). Thus, when the plateau is reached, the variation in hydration energy is lower, which is consistent with the fact that the first hydration layer is complete. Then, as the number of water molecules increases, the coordination number of Li^+ remains constant and equal to 4 (Table 2). The cation hydration

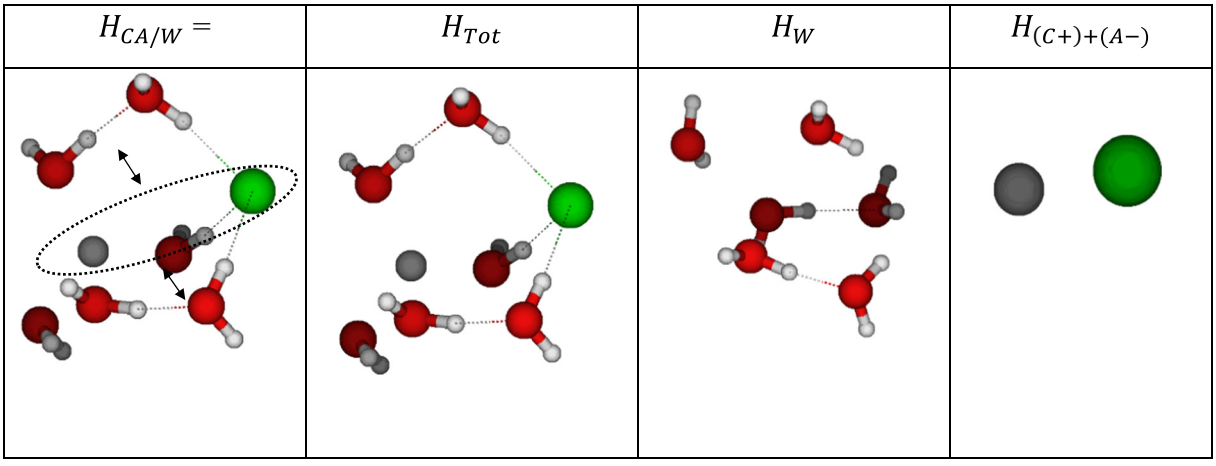


Fig. 2. Schematic representation of the salt hydration enthalpy (Eq. (4)) The arrows indicate the interaction energy between species.

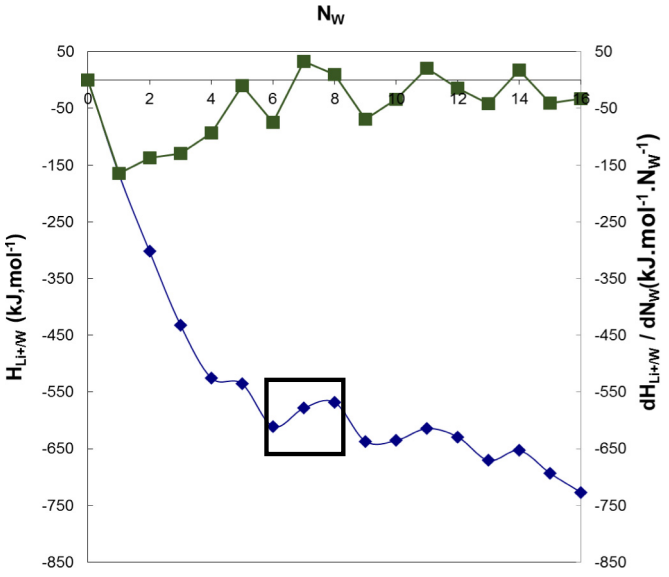


Fig. 3. Evolution of the hydration energy of Li^+, $H_{Li+/W}$ (in blue) and its derivate, $dH_{Li+/W}/dN_W$ (in green), as a function of the number of water molecules N_W, to 298.15 K.

Table 2
Li^+ hydration properties, with:
- Nw: number of water molecules in the system.
- CN: ion coordination number.
- $H_{C+/W}$: cation hydration energy.
- $dH_{C+/W}/dN_W$: derivate of the cation hydration energy with respect to the number of water molecules in the system.

N_W	CN	$H_{C+/W}$ (kJ.mol^{-1})	$dH_{C+/W}/dN_W$ (kJ.mol^{-1}.water molecule^{-1})
0	0	0	0
1	1	−165	−165
2	2	−302	−137
3	3	−432	−130
4	4	−525	−93
5	5	−536	−10
6	**4**	**−611**	**−75**
7	**4**	**−578**	**32**
8	**4**	**−568**	**10**
9	4	−637	−69
10	4	−635	−34
11	4	−614	21
12	4	−629	−15
13	4	−671	−42
14	5	−653	18
15	4	−693	−40
16	5	−727	−33

enthalpy is then calculated as the average of the hydration energy obtained for 6, 7 and 8 water molecules, i.e. −590 kJ.mol^{-1}.

The Table 3 summarizes the main structural parameters of the ions hydration shell obtained, corresponding to the ion coordination number, CN, the average distance between the central ion and the water molecules, d, the ion solvation enthalpy, $H_{ion/w}$, and the geometry of the water cluster coordinated to the ion. To validate the approach, values predicted in the present work are compared with those obtained from simulation works [21,39–41] and from experimental works [42–46] (Table 3). There is a dispersion of the simulation results, depending of the method. There is also a dispersion of the experimental values, depending on the experimental method used.

The coordination number of Li^+, estimated from the experimental data range between 3.3 and 6.5, depends strongly on the salt concentration [47]. Still, X-ray diffraction [48] and Raman spectroscopy [49,50] yields a coordination number of 4 for Li^+, which is in agreement with the value obtained in our work. The experimental hydration energy of Li^+ varies by up to 80 kJ/ mol. Hydration energy obtained in this study is a little overestimated (5%) but lies within the extremes and can therefore be considered to be in as good agreement with the experimental data.

Thus, the Li^+ ion is mainly bonded to 4 water molecules, located at a distance in between 1.99 and 2.11 Å. The geometry of Li^+, hydrated by these 4 water molecules, is tetrahedral, as shown in Fig. 4. Similar geometric shapes for Li^+ are reported from simulation works [21].

For K^+, the coordination number is in good agreement with other experimental [51] and simulation [52] works. However, the hydration enthalpy energy obtained is somewhat less satisfactory, 15% larger than experimental works. Compared to simulation works (−370 kJ.mol^{-1} [41]), −390 kJ.mol^{-1} is still rather good.

Structures of the hydration shell of Na^+ and K^+ are respectively a trigonal bipyramid and an octahedron (Figs. 5, 6 respectively). Similar geometric shapes are reported by Loeffler et al. [21] from simulation results.

Concerning Mg^{2+}, experimental [53,54] and simulation [55] works established that its coordination number includes six water molecules. The early X-ray diffraction [53] studies, Raman spectroscopy [56], and Extensive X-ray diffraction studies [54] showed that Mg^{2+} had a CN of 6 in aqueous solutions of different concentrations, containing chlorides, nitrates, perchlorates, and sulfate ions. The hydration energy of Mg^{2+} is overestimated by 10% compared to the results obtained from thermodynamic models of hydration. The water arrangement around Mg^{2+} is octahedral (Fig. 7) in line with previous simulation studies [19,57].

The coordination number of Ca^{2+}, reported from EXAFS experiments [58] in $CaCl_2$ solution is the same as the one obtained in this study, i.e. 8. Results concerning the distance between the Ca^{2+} and the water molecules (d) and the hydration energy of the ion are also in good agreement with other experimental [58] and simulation studies [59]. Finally, the water cluster around Ca^{2+} has a square antiprismatic structure (Fig. 8), in line with experimental results of Jalilehand et al. [58].

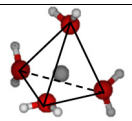
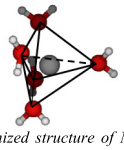
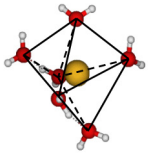
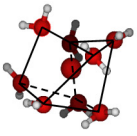
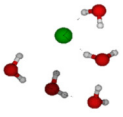
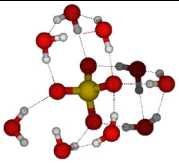
Results indicated in Table 3 show that 4, 5, 6, 6 and 8 water molecules are respectively involved in the first hydration shell of Li^+, Na^+, K^+, Ca^{2+} and Mg^{2+}.

The coordination number of the monovalent cations, CN, as well as the ion – water distance, $d_{C+/W}$, can be ranked as follow: $Li^+ < Na^+ < K^+$. Therefore, short cation-water distances imply a stronger water-cation interaction, as reflected by the stronger solvation enthalpy. For instance, Li^+ with a solvation energy of −590 kJ.mol^{-1} and a Li^+-water distance between 1.99 and 2.11 Å, has stronger interaction with water than K^+, (K^+-water distance: 2.81–2.92 Å, $H_{C+/W} = -390$ kJ.mol^{-1}).

On the other hand, the coordination number of the divalent cations can be ranked as follow: $Mg^{2+} < Ca^{2+}$. Indeed, both the coordination number of Mg^{2+} and the cation-water distance of Mg^{2+} are lower than those of Ca^{2+}.

Finally, comparing monovalent and divalent cations, for instance K^+ and Mg^{2+} that have the same coordination number, the Mg^{2+}- water interactions ($H_{C+/W} = -2150$ kJ.mol^{-1}) are stronger than the K^+-water ones ($H_{C+/W} = -390$ kJ.mol^{-1}).

Table 3
Structural parameters of the ion hydration shell. Values obtained in the present work are reported in the first row of the table.
CN: coordination number, d: average distance between ion and water molecules.
$H_{ion/W}$: ions hydration enthalpy. N_W: number of water molecules required to complete the first water coordination layer.

	CN	d (A)	$H_{ion/w}$ (kJ.mol^{-1})	Water cluster geometry
Li^+	**4 (N_w=7)**	**1.99-2.11**	**-590**	
	4-5 [21,39,40]		-580 to -505[46]	
	4[48–50]		-531[42]	
	3.3-5.5[47]		-514[45]	
	3.2-6.5[60]		-529.3[43]	
	5.1[61]			
				Figure 4: *Optimized structure of Li^+, with its tetrahedral coordination geometry.*
				Tetrahedral coordination geometry [21].
Na^+	**5 (N_w=7)**	**2.36-2.53**	**-420**	
	5.2[52]	2.3-2.5[52]	-423.8[46]	
	5.85[39]	2.40 [55]	-416 [42]	
	5-6[55]	2.39[62]	-403[45]	
	4.6[62]		-423.7[43]	
	5.5[63]		-410[41]	
				Figure 5: *Optimized structure of Na^+, with its bipyramidal trigonal coordination geometry.*
				Bipyramidal trigonal coordination geometry [21].
K^+	**6 (N_w=10)**	**2.81-2.92**	**-390**	
	6.1-6.7[52]	2.75-2.80[52]	-370[41]	
	6[51]		-382.2[46]	
			-334 [42]	
			-334[45]	
			-351.8[43]	
				Figure 6: *Optimized structure of K^+, with its octahedral coordination geometry.*
				Octahedral coordination geometry [21].
Mg^{2+}	**6 (N_w=16)**	**1.95-2.12**	**-2150**	
	5-6[55]	2.09[55]	-1949[42]	
	6[53,54,56,59,64]	2.13[59]	-1921[44]	
				Figure 7: *Optimized structure of Mg^{2+}, with its octahedral coordination geometry.*
				Octahedral coordination geometry [19,57].
Ca^{2+}	**8 (N_w=12)**	**2.42-2.52**	**-1650**	
	5-8[59],	2.42-2.58[59]	-1602[42]	
	8[22], 6[64]		-1577[44]	
	8[58]	2.46[58]		
				Figure 8: *Optimized structure of Ca^{2+}, with its square antiprismatic coordination geometry.*
				Square antiprismatic coordination geometry [58,65]
Cl^-	**5 (N_w=12)**	**2.30-2.49**	**-350**	
	≥5-6[55]	2.37[55]	-319.9[46]	
	6[66]	2.24-2.42 [67]	-367[42]	
	6.25[39]		-319.5[43]	
				Figure 9: *Optimized structure of Cl^-, with its coordination geometry.*
SO_4^{2-}	**9 (N_w=10)**	**1.81-1.91**	**-1330**	
	7-8[54]	1.91[55]	-1035[42]	
	10-11[55]			
	9-13[68]			
				Figure 10: *Optimized structure of SO_4^{2-}, with its coordination geometry.*

The coordination number of Cl^- is 5, which is quite close to the 6.25 reported by Ohrn et al. [39] in simulation works. The water arrangement around Cl^- is highly unsymmetrical (Fig. 9), which is consistent with the observations of Ohtaki et al. [57]. Indeed, the hydration energy of Cl^- is low (around -350 kJ.mol^{-1}), which means that a competition exists between forming hydrogen bond with chloride ion and in the water network. A similar observation was reported *in* ab initio QM/MM molecular dynamics simulations of Tongraar et al. [67]. Thus, a competition appears between the hydration of Cl^- and the hydrogen bonds with the neighboring water molecules. The low hydration energy of Cl^- explains why the water around Cl^- forms a loose cluster (distance ion - water molecules between 2.30 and 2.49 Å), with no identifiable geometry.

The SO_4^{2-} ion can be strongly combined with water. According to X-ray diffraction studies on aqueous sulfate solutions [54], 7 to 8 water molecules surround SO_4^{2-}. A coordination number of 9 is found in our study. The SO_4^{2-} coordinated water cluster is very compact (between 1.81 and 1.91 Å) compared to that of Cl^-(2.30–2.49 Å), with 2 to 3 hydrogen bonds per oxygen atom belonging to SO_4^{2-} (Fig. 10). More than, each water molecule belonging to the SO_4^{2-} coordinated water cluster is bound to the other two, which gives a very structured cluster as compared to that of Cl^-. Same remarks are reported in the works of Thaunay et al. [68]. This results are in line with the difference of hydration energy between Cl^- (-350 kJ.mol^{-1}) and SO_4^{2-} (-1330 kJ.mol^{-1}).

In this first part, quantum mechanics calculations have been used to determine the hydration properties of the ions, without counter-ion, in pure water. These calculations enabled to determine the ions solvation enthalpy, the ions coordination number, the ion – water molecules distances and the structure of the water cluster coordinated to the ions. The method developed was tested by comparing the theoretical results obtained with other simulation and experimental works.

3.2. Hydration properties of ions in presence of counter-ions

This study was extended to different salts (LiCl, NaCl, KCl, $MgCl_2$, $CaCl_2$, Na_2SO_4, K_2SO_4 and $MgSO_4$) with water molecules. The hydration energy of the ions is studied, when salts are fully dissociated. That means that distance between cations and anions is larger than the sum of the van der Waals radii of the interacting atom, and that conditions described in II.2 are satisfied.

For example, the evolution of the hydration energy of LiCl, $H_{LiCl/W}$, its derivate, $dH_{LiCl/W}/dN_W$ and the interaction energy Li^+/Cl^-, $H_{Li+/Cl-}$, as a function of the number of water molecules N_W are drawn in Fig. 11.

Fig. 11 shows that between 6 and 9 water molecules, LiCl hydration energy is stable, its derivate becomes positive. However, the number of water molecules in the system is not sufficient to separate the ions. Indeed, the distance between Li^+ and Cl^- (3.59 Å) is smaller than the sum of the van der Waals radii of the interacting atom (3.65 Å), the dissociation of the salt is not complete.

When the 10th water molecule is added, the sharp decrease in energy between Li^+ and Cl^- ($H_{Li+/Cl-}$) shows that the system tends to destabilize. The interaction energy between Li^+ and Cl^- increases and the distance between Li^+ and Cl^- decreases. In the same time, $H_{LiCl/W}$ increases meaning that the interaction between salt and water molecules becomes less strong.

The addition of the 12th water molecule has the effect of restructuring the water network, the distance between Li^+ and Cl^- increases. When the 13th water molecule is added, the dissociation of the salt becomes complete (distance $Li^+/Cl^- = 3.79$ Å). The derivate of LiCl hydration energy becomes positive, and LiCl hydration energy stabilizes. Also, it can be observed that the interaction energy Li^+/Cl^- stabilizes around -400 kJ.mol^{-1}.

When the salts are fully dissociated, the ternary interactions are calculated using Eq. (4). The order of magnitude of the ternary interactions of 10 kJ.mol^{-1} is small compared to other binary interactions, whose values oscillate between -400 and -600 kJ.mol^{-1}. Thus, ternary interactions in each system can be considered as negligible.

3.2.1. Influence of anions on cations hydration properties

In a first step, the anion influence on the cations hydration properties was studied.

3.2.1.1. Influence of Cl^- on the cations properties. The hydration properties of monovalent and divalent cations in the presence of Cl^- are respectively summarized in Tables 4 and 5. The interaction energy between the cation and the anion, $H_{C+/A-}$, the cation coordination number, CN, the distance cation - water $d_{C+/W}$, and the geometry of the water cluster are included in the tables. Results concerning the cations hydration properties in pure water are also indicated in order to analyze the influence of the presence of the anion on the cation hydration properties. N_w corresponds to the water molecules number in the system required for the complete salt dissociation. As previously mentioned, ions are considered dissociated when the distance between cations and anions is larger than the sum of the van der Waals radii of the interacting atom [36,37]. For comparison, properties obtained in other works, within electrolytes, are also indicated in Tables 4 and 5.

The cations coordination numbers, the distance cations - water molecules as well as the water cluster geometry are consistent with those reported either experimentally (Neutron diffraction [48] and sterically exclusion column [70]) or theoretically [71]. For instance, the reported Li^+ coordination number is 4, with a tetragonal structure [48], which correspond to the properties obtained in our work. The consistency between results validates our approach and assumption.

Concerning Na^+, different water cluster geometry is obtained. Octahedral for CN = 6 [72] and tetragonal for CN = 4 [51] arrangements have been obtained in previous investigations, to be compared to a trigonal bipyramid structure obtained for CN = 5 in our work. Those differences arise from the different coordination numbers values obtained, which necessarily lead to different water cluster geometries.

Considering the cations properties in presence of Cl^-, interaction energies between the cation and Cl^-, $H_{C+/A-}$, reported in Table 4, decrease when the size of the cation is increasing. This result is line with the HSAB (Hard and Soft Acids and Bases) properties [76].

Hard acids and bases are small, compact and non-polarizable. The large differences in electronegativity between hard acids and hard bases lead to strong ionic interactions. Indeed, Li^+ is harder acid than Na^+ and K^+. As a result, since Cl^- is relatively hard base, the Li^+/Cl^- interaction enthalpy is higher than the Na^+/Cl^- and K^+/Cl^- one. Comparing the ion hydration energy, $H_{C+/W}$ in presence of Cl^- and in pure water, $H_{C+/W}$, the presence of Cl^- does not impact the monovalent cation hydration energy (Table 4). Different results are obtained for

Notes to Table 3:
[21,22,39–41,52,55,59,64,67,68]: Molecular modeling.
[42–44]: Model for the thermodynamics of hydration.
[45]: Gaz phase experiment.
[46]: Cluster ion solvation data.
[48,51,53,54,62,63,66]: X-ray diffraction.
[49,50,56]: Raman spectroscopy.
[47,60]: Neutron diffraction and isotopic substitution.
[61]: Field evaporation of ions from solution
[58,65]: Large-angle X-ray scattering (LAXS) and X-ray absorption fine structure spectroscopy (EXFAS).

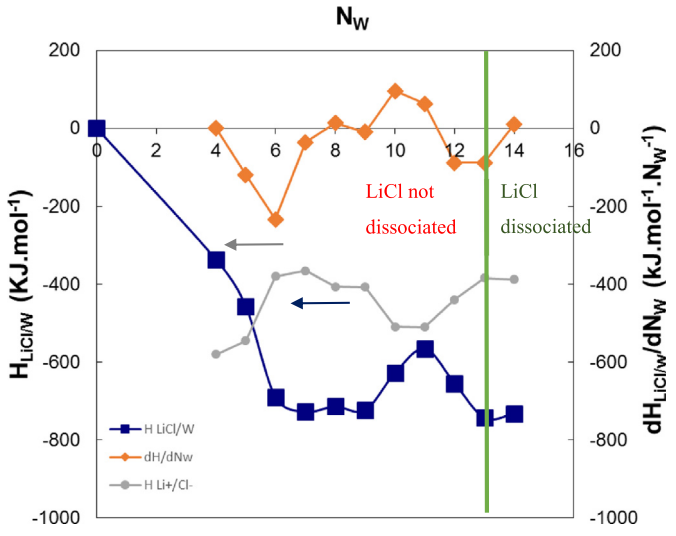


Fig. 11. Evolution of the hydration energy of LiCl, $H_{LiCl/W}$, its derivate, $dH_{LiCl/W}/dN_W$ and the interaction energy Li^+/Cl^-, $H_{Li+/Cl-}$, as a function of the number of water molecules N_W at 298.15 K.

Table 5
Hydration properties of divalent cations, with Cl^- and in pure water, with:
- N_W: number of water molecules required for the complete dissociation of the salt.
- $H_{C+/A-}$: interaction enthalpy between cation and anion.
- $H_{C+/W}$: cation hydration enthalpy.
- CN: ion coordination number.
- $d_{C+/W}$: distance between the cation and the coordinated water molecules.
- Geometry: geometry of the water cluster molecules coordinated to the cation.
Values obtained in the present work are reported in the first row of the table.

		$MgCl_2$ ($N_W = 20$)	$CaCl_2$ ($N_W = 32$)
$H_{C+/W}$ (kJ.mol^{-1})	With Cl^-	−1840	−1750
	In water	−2150	−1650
CN	With Cl^-	6	8
		6 [73]	8 [74]
			7.7 [75]
	In water	6	8
$d_{C+/W}$ (Å)	With Cl^-	2.11–2.12	2.52–2.53
		210–212 [73]	2.46 [58]
	In water	1.95–2.12	2.42–2.52
Geometry	With Cl^-	Octahedron	Square antiprismatic
		Octahedron [73]	
	In water	Octahedron	Square antiprismatic

[58,73,74]: X-ray Diffraction and EXAFS Measurements.
[75]: Molecular modeling

divalent cations. Indeed, results in Table 5 show that the hydration energy of Mg^{2+} is lower in the presence of Cl^- (−1840 kJ.mol^{-1}) than in water (−2150 kJ.mol^{-1}). On the other hand, the hydration energy of Ca^{2+} is lower in water (−1650 kJ.mol^{-1}) than in the presence of Cl^- (−1750 kJ.mol^{-1}). These differences in behavior can be related to the increase of the number of water molecules required for complete dissociation of salts. Indeed, the complete dissociation of $MgCl_2$ requires the presence of 20 water molecules while that of $CaCl_2$ requires 32. The number of water molecules around Mg^{2+} therefore increases from 16 in pure water to 20 in the presence of Cl^- compared to that of Ca^{2+} which increases from 12 in pure water to 32 molecules in the presence of Cl^-. Moreover, unlike monovalent, divalent cations interact with water molecules located beyond the first hydration layer. Therefore, due to a larger number of water molecules in the system, the hydration energy of Ca^{2+}, in the presence of Cl^-, is higher than in water.

Results concerning cations coordination number are in agreement with experimental studies. For instance, the most commonly coordination numbers reported for X-Ray diffraction, neutron diffraction and EXAFS experiments for Ca^{2+} are 6, 7 and 8 [71].

For a given cation valence, the cations coordination number, CN, and the distance cation - water molecules in presence of Cl^-, $d_{C+/W}$, can be ranked as follow: $Li^+ < Na^+ < K^+$ and $Mg^{2+} < Ca^{2+}$. Interestingly enough, these results match the one found in pure water. In the same way, the water cluster geometry in presence of Cl^- remains the same as in pure water. For instance, the optimized water structure of Li^+ in presence of Cl^-, a tetrahedral coordination structure, is, therefore,

Table 4
Hydration properties of monovalent cations, with Cl^- and in pure water, with:
- N_W: number of water molecules required for the complete dissociation of the salt.
- $H_{C+/A-}$: interaction enthalpy between cation and anion.
- $H_{C+/W}$: cation hydration enthalpy.
- CN: ion coordination number.
- $d_{C+/W}$: distance between the cation and the coordinated water molecules.
- Geometry: geometry of the water cluster molecules coordinated to the cation.
Values obtained in the present work are reported in the first row of the table.

		LiCl ($N_W = 13$)	NaCl (Nw = 10)	KCl (Nw = 25)
$H_{C+/A-}$ (kJ/mol)		−390	−300	−300
$H_{C+/W}$ (kJ/mol)	With Cl^-	−580	−480	−410
	In water	−590	−420	−390
CN	With Cl^-	4	5	6
		4 [48]	4–6 [51,72]	6 [51]
		6 [70]	*6* [70]	
	In water	4	5	6
$d_{C+/W}$ (Å)	With Cl^-	2.00	2.38–2.46	2.88
		1.95–2.25 [48]	2.41–2.50 [51]	2.80 [51]
	In water	1.99–2.11	2.36–2.53	2.81–2,92
Geometry	With Cl^-	Tetrahedron	Trigonal bipyramid (CN = 5)	Octahedron
		Tetrahedron [21]	Octahedron (CN = 6) [72]	Octahedron [51]
			Tetragon.(CN = 4) [51]	
	In water	Tetrahedron	Trigonal bipyramid (CN = 5)	Octahedron
			Octahedron (CN = 6)	

[70]: Size exclusion chromatography.
[21]: Molecular modeling.
[48,51]: X-ray Diffraction and EXAFS Measurements.
[72]: Diffractometric studies

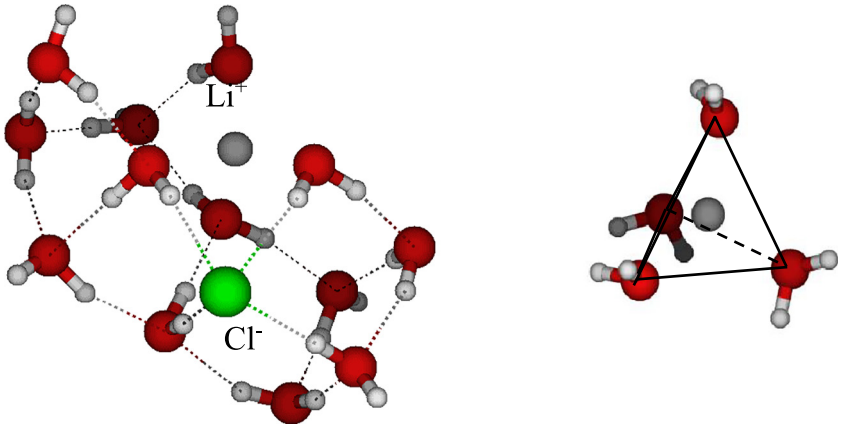


Fig. 12. On the left: optimized structure of hydrated lithium chloride. On the right: optimized structure of Li^+ (in grey) with water molecules in presence of Cl^- - tetrahedral coordination structure of the water.

identical than the one in water (Figs. 12). The coordination water structures of others cations in systems are presented ESI.

To synthesize, results show that the water molecules coordinated with cations, characterized by $H_{C+/W}$, CN, $d_{C+/W}$, and the water cluster geometry, are not affected by the presence of Cl^- in solution.

3.2.1.2. Influence of SO_4^{2-} on the cations hydration properties. The hydration properties of Mg^{2+} in the presence of SO_4^{2-} are reported in Table 6. Properties found in the literature are also indicated in Table 6 for comparison.

The studies from ab initio methods and molecular methods [77,78] showed that Mg^{2+} is hexa-coordinate in $MgSO_4$ aqueous solution, as well as our results. Alike in the case of Cl^-, the hydration sphere of Mg^{2+} is only marginally affected by the presence of SO_4^{2-}. Indeed, a coordination number of 6 is found with or without SO_4^{2-}. Similarly, the distance between the ion and the coordinated water molecules does not change and the geometry of the water cluster remains octahedral. Therefore, the hydration properties of the first hydration sphere of Mg^{2+} are not influenced by the presence of SO_4^{2-}.

To conclude, results show that the cations hydration properties (Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}) do not depend on the presence of the counterion, Cl^- or SO_4^{2-}. The structural parameters of Mg^{2+} hydration are independent of the chemical nature of the anions. In the same trend, a review published by Smirnov et al. showed that structural parameters of Mg^{2+} hydration are independent of the chemical nature of the anions [79]. Results are also in line with the findings of a combined Molecular Dynamics and EXAFS investigation on the influence of triflate, nitrate and bis(trifluoromethylsulfonyl)imide counterions on the hydration structure of Lanthanide ions [80]. In this study, the presence of counterions in the cation first or second shell was found to change neither the first shell distance nor the symmetry of the hydration complex formed in solution.

Table 6
Hydration properties of Mg^{2+}, with SO_4^{2-} and in pure water, with:
- N_W: number of water molecules required for the complete dissociation of the salt.
- $H_{C+/W}$: cation hydration enthalpy.
- CN: ion coordination number.
- $d_{C+/W}$: distance between the cation and the coordinated water molecules.
- Geometry: geometry of the water cluster molecules coordinated to the cation.
Values obtained in the present work are reported in the first row of the table.

		$MgSO_4$ ($N_W = 25$)
$H_{C+/W}$ ($kJ.mol^{-1}$)	With SO_4^{2-}	−1970
	In water	−2260
CN	With SO_4^{2-}	6 6 [54,77,78]
	In water	6
$d_{C+/W}$ (Å)	With SO_4^{2-}	2.11
	In water	2.10
Geometry	With SO_4^{2-}	*Octahedron* *Octahedron* [79]
	In water	Octahedron

[54]: X-ray diffraction and EXAFS measurements.
[77,78]: Molecular modeling.

3.2.2. Influence of the cation on anion hydration properties

In a second step, the cation influence on the anion hydration properties was studied.

3.2.2.1. Impact of the cation on Cl^- hydration properties. The hydration properties of Cl^- in the presence of monovalent and divalent cations are reported in Table 7.

When considering the Cl^- hydration energy, $H_{A-/W}$, in presence of the cation, results in Table 7 show that $H_{A-/W}$ decrease in presence of the cation. For example, the hydration energy of Cl^-, which is $-350\ kJ.mol^{-1}$ in pure water, decreases to $-200\ kJ.mol^{-1}$ in the presence of a monovalent cation such as Li^+. This hydration energy drops to $-150\ kJ.mol^{-1}$ in the presence of Mg^{2+}. Therefore, the Cl^- hydration energy decreases when the cation hydration increases. Indeed, Mg^{2+}, with a hydration energy of $-2260\ kJ.mol^{-1}$, strongly attracts water molecules, compared to K^+, whose hydration energy is $-390\ kJ.mol^{-1}$. As a result, the hydration energy of Cl^-, in the presence of Mg^{2+}, decreases more than in the presence of K^+. The Cl^- hydration energy, $H_{A-/W}$, in the presence of cations, follows the sequence (Table 7): $MgCl_2 < CaCl_2 < LiCl < NaCl < KCl$. This means that the Cl^- ion is more bound to water molecules in the presence of K^+ than in the presence of Mg^{2+}. X-ray scattering measurements also show that Mg^{2+} is strongly hydrated and that it attracts more water molecules than Cl^-, thus making hydration of chlorine ions weaker than in solution containing Cl^- and water molecules [82]. Results of computer simulations suggest that the hydration structure around Cl^- is not well defined and that between 1 and 6 water molecules surround Cl^- ions in presence of Mg^{2+} (Table 7) [81].

Interestingly, the decrease of the Cl^- hydration energy is concomitant with a decrease of its coordination number, CN, (5 in pure water and between 3 and 5 in the presence of cations).

Therefore, Cl^- is dehydrated in presence of the cation. These results are in line with previous theoretical and experimental study on mixtures of water and Hexylammonium Chloride [83] where it was found that the Chloride hydration number decreased due to the presence of the Hexylammonium cation. Cl^- was "dehydrated" as in the present case. Very interestingly, it was also reported that the Chloride ion seemed to prefer a heptacoordinated first shell configuration, independently on the nature of the first shell ligands (either water molecules or Hexylammonium cation).

Table 7
Hydration properties of Cl^- in the presence of monovalent and divalent cations, and in pure water, with:.
- N_W: number of water molecules required for the complete dissociation of the salt.
- $H_{A-/W}$: anion hydration enthalpy.
- CN: ion coordination number.
- $d_{A-/W}$: distance between the anion and the coordinated water molecules.

		LiCl ($N_W = 25$)	NaCl ($N_W = 25$)	KCl ($N_W = 25$)	$MgCl_2$ ($N_W = 25$)		$CaCl_2$ ($N_W = 25$)	
					Cl^- [1]	Cl^- [2]	Cl^- [1]	Cl^- [2]
$H_{A-/W}$ (kJ.mol^{-1})	With cation	−210	−280	−300	−150	−180	−260	−200
	In water	−350						
CN	With cation	4 3–9 [51]	4	5	4 1–6 [81]	4 1–6 [81]	4	3
	In water	5						
$d_{A-/W}$ (Å)	With cation	2.22	2.21	2.32	2.18	2.21	2.15	2.08
	In water	2.30–2.49						

Values obtained in the present work are reported in the first row of the table.
[51]: X-ray Diffraction and EXAFS Measurements.
[81]: Molecular modeling.

Quite unexpectedly, this dehydration renders the first coordination shell of the anion more compact. Indeed, the distances anions/water, $d_{A-/W}$ (in between 2.30 and 2.49 Å in pure water) decrease to a range between 2.08 and 2.32 Å in the presence of the cations. The water molecules coordinated to Cl^- are even closer in the presence of divalent cations ($d_{A-/W}$ between 2.08 and 2.21 Å), than in the presence of monovalent ones ($d_{A-/W}$ between 2.21 and 2.32 Å). However, the gain in compactness does not influence the overall water cluster geometry that remains very asymmetrical. Water molecules belonging to its cluster are located on the same side as the cation. Indeed, the cations attract more water molecules than Cl^-, given their higher hydration energy. Thus the first water molecule in the system is oriented towards the cation. Then, the water molecules establish hydrogen bonds with the water molecules already present in the system and orient themselves under the influence of the forces exerted by the water molecules and those exerted by the cation and the Cl^- anion. This competition results in asymmetric hydration of Cl^-.

Quantities presented in Table 7 ($H_{A-/W}$, CN, $d_{A-/W}$) show that the presence of cations influences the hydration of Cl^- and causes a decrease in its hydration.

3.2.2.2. Impact of the cation on SO_4^{2-} hydration properties. The hydration properties of SO_4^{2-} in the presence of Mg^{2+} are reported in Table 8.

Results in Table 8 indicate that the presence of Mg^{2+} induces a decrease in the SO_4^{2-}hydration energy, $H_{A-/W}$, whose hydration energy changes from −1330 kJ.mol^{-1} in water to −990 kJ.mol^{-1} in the presence of Mg^{2+}. Mg^{2+} has a hydration energy twice as high as that of SO_4^{2-} (−2260 kJ.mol^{-1} versus −1300 kJ.mol^{-1}). Water molecules are therefore more attracted by Mg^{2+} than SO_4^{2-}, which induces a decrease in the hydration energy of SO_4^{2-}. SO_4^{2-} coordination number, CN, slightly increases in the presence of Mg^{2+} while the distance SO_4^{2-}-water molecules is not influenced by the presence of Mg^{2+}. The latter makes sense since the water cluster around sulfate in pure water solution is already more compact than the one of Cl^-.

The anions hydration properties of Cl^- and SO_4^{2-} are influenced by the cation hydration characteristics.

Table 8
Hydration properties of SO_4^{2-} in the presence of Mg^{2+} and in pure water, with:
- N_W: number of water molecules required for the complete dissociation of the salt.
- $H_{A-/W}$: anion hydration enthalpy.
- CN: ion coordination number.
- $d_{A-/W}$: distance between the anion and the coordinated water molecules.
Values obtained in the present work are reported in the first row of the table.

		$MgSO_4$ (Nw = 25)
$H_{A-/W}$ (kJ.mol^{-1})	With Mg^{2+}	−990
	In water	−1330
CN	With Mg^{2+}	11 9, 11, 12 [68]
	In water	9
d (Å)	With Mg^{2+}	1.81–1.85
	In water	1.81–1.91

[68]: Infrared photodissociation

4. Conclusion

In order to describe the hydration properties of ions in water, a methodology using a quantum mechanics method (DFT) is described in this study. This approach, based on the decomposition of the system energy has been carried out in two stages.

The fundamental approach proposed consists, on the one hand, in characterizing the hydration properties of Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, SO_4^{2-} in pure water, without counter-ion. On the other hand, the ions first hydration layers were systematically characterized in presence of counter-ion, and water molecules in different systems (LiCl, NaCl, KCl, $MgCl_2$, $CaCl_2$ and $MgSO_4$).

In the first part, quantum mechanics calculations were used to determine the hydration properties of the ion, without counter-ion, in pure water. The hydration energy of the ions, their coordination number, and the structure of the water cluster coordinated with the ions were determined. The approach used to calculate ions properties was validated by comparing hydration properties provided by experimental and simulation works. As expected, it has been shown that the interaction energy between divalent ions and water is stronger than that of monovalent ions.

In the second part, the hydration characteristics of species in systems containing ion, counter-ion and water molecules were investigated. A methodology, based on the decomposition of the total energy of the ion/counter-ion/water system has made it possible to evaluate the interactions between species in complex systems. The approach was validated by comparing data from experimental and simulation studies from literature.

It has been shown that the presence of an anion (Cl^- or SO_4^{2-}) does not lead to structural and energetic changes in the cation first hydration layer (Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}). The hydration characteristics of the studied cations are not influence by the anion. Conversely, the anion first hydration layer is influenced by the cation of the system.

Declaration of Competing Interest

The authors declare no competing financial interest.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2019.111394.

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Supporting information for:

Investigation of ions hydration using Molecular Modeling

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Optimized hydrated structure of ions in electrolyte.

Optimized hydrated structure of Na^+ in NaCl.

In the NaCl, Na^+ has 5 directly interacting water molecules (Figure ESI-1). When 5 water molecules coordinate Na^+, the structure of the hydration cluster is trigonal bipyramidal (Figure S_1).

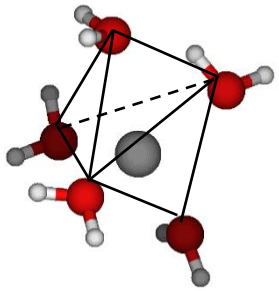

Figure S_1 : *Optimized structure of Na^+ (in grey) in the electrolyte containing Cl^-. NaCl (H_2O). Trigonal bipyramidal structure of the water.*

Optimized hydrated structure of K^+ in KCl.

K^+ in has 5 coordinated water molecules. The structure of the water cluster is of octahedral for a coordination number of 6 (Figure S_2).

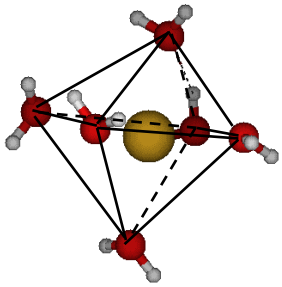

Figure S_2: *Optimized structure of K+ (yellow) in the electrolyte containing Cl^-. KCl (H_2O). Coordinated octahedral structure of the water.*

Optimized hydrated structure of Mg^{2+} in $MgCl_2$ and $MgSO_4$.

Mg^{2+} in the presence of Cl^- has 6 coordinated water molecules, which gives the water cluster an octahedral structure . In $MgSO_4$, Mg^{2+} keeps this same geometry, with a CN of 6 (Figure S_3).

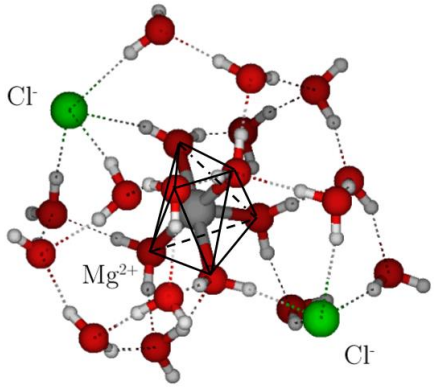

Figure S_3 : *Optimized structure of Mg^{2+} (in grey) in the electrolyte containing $2Cl^-$: $MgCl_2$ (H_2O). Coordinated octahedral structure of the water.*

Optimized hydrated structure of Ca^{2+} in $CaCl_2$

The geometry of the Ca^{2+} coordinated water network, composed of 8 water molecules and in the presence of Cl^-, is square antiprismatic (Figure S_4).

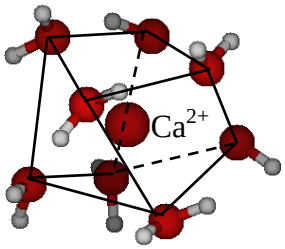

Figure S_4 : *Optimized structure of Ca^{2+} in the electrolyte containing $2Cl^-$: $CaCl_2$ (H_2O). Coordinated square antiprismatic water structure.*

Optimized hydrated structure of SO_4^{2-} in $MgSO_4$.

With regard to SO_4^{2-}, in $MgSO_4$, a coordination number of 11 is obtained. The water network around SO_4^{2-} remains highly structured around the oxygen atoms belonging to the anion (Figure S_5).

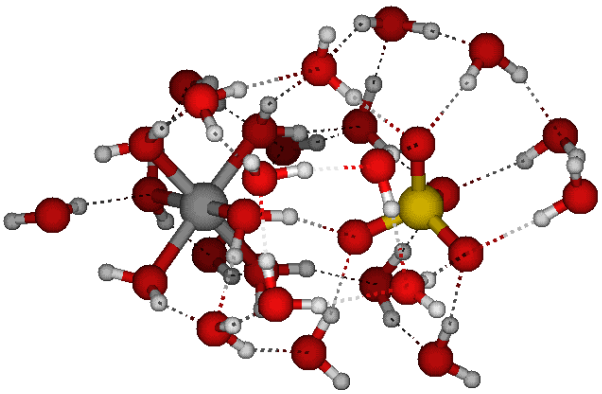

***Figure S*$_5$**: Optimized structure of SO_4^{2-} in the electrolyte containing Mg^{2+}. $MgSO_4$ (H_2O).

Electronic energies, enthalpies and cartesian coordinates of the stationary points on the potential energy surfaces.

$Li^+ (H_2O)_n$

$Li^+ (H_2O)$

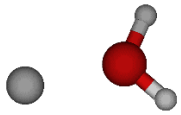

Figure S_6 : Li^+ optimized structure with 1 water molecule.

E = -83.706570

H = -83.705626

Li	-0.111316	0.000000	-0.109711
O	0.093477	0.000000	1.728684
H	0.925639	0.000000	2.219358
H	-0.609240	0.000000	2.391623

$Li^+ (H_2O)_2$

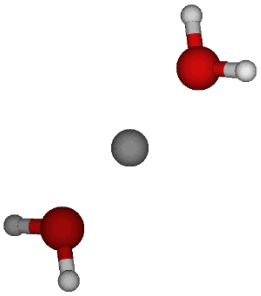

Figure S_7 : Li^+ optimized structure with 2 water molecules.

E = -152.844745

H = -152.843800

O	0.264866	-0.000038	2.035815
Li	-0.974695	0.000096	0.568741
H	1.227958	0.000043	1.972358
H	0.062564	-0.000087	2.979450

O	-2.219997	0.000230	-0.888932
H	-2.016761	-0.000009	-1.832399
H	-3.183108	-0.000234	-0.825908

$Li^+ (H_2O)_3$

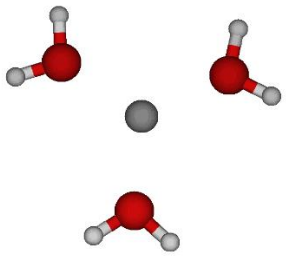

Figure S_8 : Li^+ optimized structure with 3 water molecules.

E = -229.251831

H = -229.250887

O	-0.015661	0.000316	1.767236
Li	-0.797324	0.000013	-0.022581
O	-2.737018	-0.000043	-0.251573
H	0.921694	0.003662	1.991296
H	-0.484930	-0.003957	2.609044
H	-3.222397	0.000064	-1.084201
H	-3.407319	0.000842	0.440933
O	0.369696	-0.000051	-1.588111
H	1.333484	-0.000302	-1.595281
H	0.102808	-0.000086	-2.514286

$Li^+ (H_2O)_4$

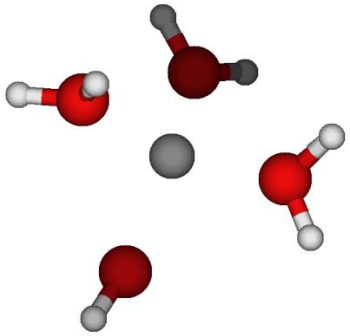

Figure S_9 : Li^+ optimized structure with 4 water molecules.

E = -305.646717

H = -305.645773

O	-0.136238	0.251761	1.702928
Li	-0.999037	-0.423053	0.037620
O	0.214014	-0.077729	-1.507242
O	-2.729947	0.505090	-0.303377
H	-0.057550	1.161152	2.009550
H	0.118122	-0.304697	2.446731
H	-2.944744	0.974517	-1.116444
H	-3.417021	0.738008	0.329778
H	1.043779	0.408212	-1.452921
H	0.203796	-0.493199	-2.375882
O	-1.332949	-2.376930	0.256510
H	-0.699965	-3.098257	0.177410
H	-2.204750	-2.786135	0.268660

$Li^+ (H_2O)_5$

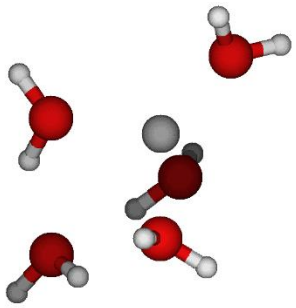

Figure S_{10} : Li^+ optimized structure with 5 water molecules.

E = -382.034409

H = -382.033465

O	0.818674	-0.353806	2.164514
Li	-0.579747	-0.331782	0.769583
O	-2.770497	-0.297458	-1.415445
O	-1.535313	-2.005701	0.340495
O	-0.239573	0.638633	-0.918007
H	1.576102	0.237735	2.228437
H	0.956786	-1.039675	2.826480
H	-3.453102	-0.286575	-2.096229
H	-3.098431	0.221642	-0.663555
H	0.522887	0.651599	-1.504413
H	-1.021674	0.430446	-1.462768
H	-1.216760	-2.899761	0.183774
H	-2.097410	-1.760251	-0.418302
O	-2.329587	0.743057	1.203984
H	-2.222827	1.693479	1.337045
H	-2.851702	0.429746	1.953232

$Li^+ (H_2O)_6$

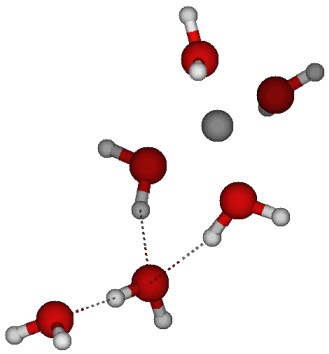

Figure S_{11} : Li^+ optimized structure with 6 water molecules.

E = -458.426216

H = -458.425272

O	0.818674	-0.353806	2.164514
Li	-0.579747	-0.331782	0.769583
O	-1.535313	-2.005701	0.340495
O	-0.239573	0.638633	-0.918007
O	-2.329587	0.743057	1.203984
O	-2.770497	-0.297458	-1.415445
H	1.576102	0.237735	2.228437
H	0.956786	-1.039675	2.826480
H	-3.453102	-0.286575	-2.096229
H	-3.098431	0.221642	-0.663555
H	0.522887	0.651599	-1.504413
H	-1.021674	0.430446	-1.462768
H	-1.216760	-2.899761	0.183774
H	-2.097410	-1.760251	-0.418302
H	-2.222827	1.693479	1.337045
H	-2.851702	0.429746	1.953232
O	-0.328571	-1.170157	-0.716679
H	0.219259	-0.791961	-1.394432
H	-1.033652	-1.664124	-1.118371

$Li^+ (H_2O)_7$

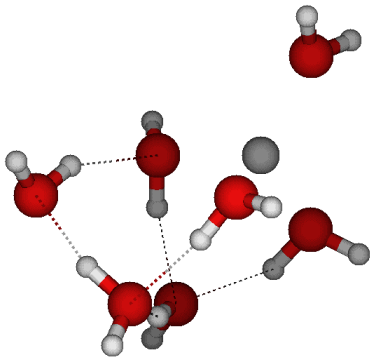

Figure S_{12} : Li^+ optimized structure with 7 water molecules.

E = -534.817476

H = -534.816532

O	1.267867	-1.730082	2.266237
Li	0.105597	-1.119374	0.781848
O	-0.727542	0.777359	-1.815988
O	1.035367	-1.135429	-0.972838
O	-1.697216	-1.908177	0.716444
O	-3.060269	-0.166446	-0.885643
O	-2.983125	1.569231	1.042557
H	2.217084	-1.881884	2.211940
H	0.992714	-2.032065	3.137948
H	-3.894755	-0.287194	-1.352311
H	-3.207707	0.514214	-0.162876
H	-0.743801	1.459815	-2.495749
H	-1.652272	0.446208	-1.694956
H	-1.899103	-2.846332	0.653436
H	-2.315901	-1.439258	0.114612
H	-3.466597	1.455071	1.867534
H	-2.036419	1.456038	1.250643
H	1.321227	-1.884808	-1.503688
H	0.548122	-0.530396	-1.565564
O	-0.262386	0.929407	0.815696

H	-0.326617	1.120988	-0.152082
H	0.435036	1.494700	1.168060

$Li^+ (H_2O)_8$

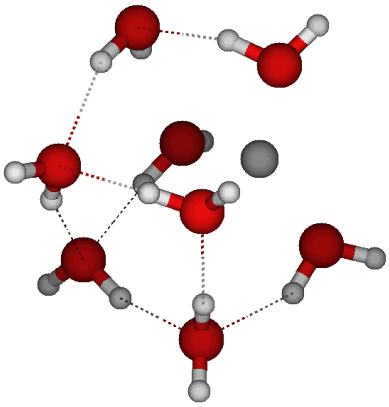

Figure S_{13} : Li^+ optimized structure with 8 water molecules.

E = -611.204611

H = -611.203667

O	1.500144	-1.216588	1.567900
Li	-0.428585	-0.979776	1.606160
O	-1.365364	-2.094219	0.169051
O	1.203842	-1.648857	-1.020402
O	-0.331697	1.005299	0.911500
O	-0.376644	0.698804	-1.723824
O	-2.890308	-0.153512	-0.984986
O	-2.943566	1.174151	1.387008
H	1.626137	-1.390287	0.596943
H	2.127166	-1.766497	2.046266
H	-3.703922	-0.279124	-1.486461
H	-3.112418	0.378793	-0.183328
H	-0.244658	1.361206	-2.411353
H	-1.322599	0.440140	-1.739082
H	-1.814468	-2.890255	0.475493
H	-2.034933	-1.556581	-0.310639

H	-3.444380	1.972049	1.592094
H	-1.994588	1.425363	1.307635
H	0.388824	-2.160357	-0.898874
H	0.900721	-0.847125	-1.476662
H	-0.208723	1.036551	-0.072044
H	0.478567	1.347343	1.309410
O	-1.817035	-0.806213	2.992647
H	-1.827033	-0.855346	3.952799
H	-2.467139	-0.133826	2.719425

$Li^+ (H_2O)_9$

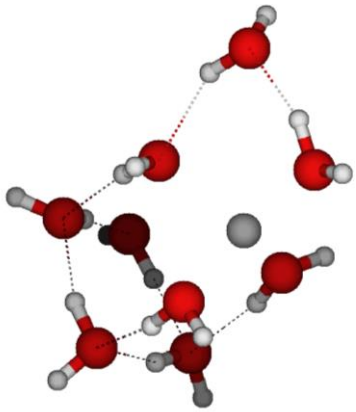

Figure S_{14} : Li^+ optimized structure with 9 water molecules.

E = -687.593539

H = -687.592595

O	0.675643	-3.177079	1.664390
Li	-0.567893	-1.693651	1.464221
O	-1.648918	-0.869320	2.935401
O	-1.713868	-1.985469	-0.094443
O	-0.622210	2.116917	0.442156
O	2.879162	-1.833719	1.106277
O	-1.416401	1.477811	-1.934439
O	-2.879376	1.247528	1.592296
O	-3.452683	0.047319	-0.781116
H	1.594448	-2.856308	1.476838

H	0.742179	-3.899364	2.294255
H	-4.370067	-0.100514	-1.035711
H	-3.455061	0.494321	0.097331
H	-1.605858	2.090416	-2.652054
H	-2.238277	0.977605	-1.751387
H	-1.527979	-2.656738	-0.756770
H	-2.391939	-1.382350	-0.456904
H	-3.428748	1.903219	2.036893
H	-2.067652	1.717370	1.268681
H	3.344410	-1.969438	0.274406
H	2.362511	-1.014915	1.006961
H	-0.856448	1.967902	-0.526668
H	-0.228905	2.994155	0.511697
H	-2.201417	-1.385655	3.530676
H	-2.201922	-0.133239	2.604148
O	0.730664	-0.063196	1.406722
H	0.812529	0.145414	2.345997
H	0.368485	0.753296	0.992665

$Li^+ (H_2O)_{10}$

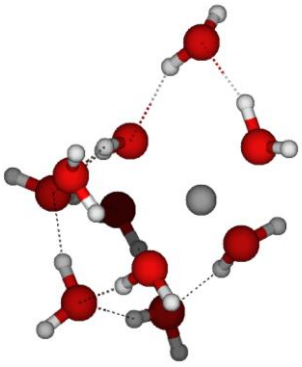

Figure S_{15} : Li^+ optimized structure with 10 water molecules.

E = -763.981303

H = -763.980359

O	0.543817	-3.212290	1.621355
Li	-0.677924	-1.727979	1.379449
O	-2.004733	-1.051750	2.815261
O	0.583020	-0.134389	1.441446
O	-1.813697	-2.039255	-0.195171
O	2.750367	-1.819962	1.359076
O	-3.435565	0.054489	-0.991793
O	-2.960293	1.141191	1.459551
O	-0.723529	2.098343	0.413468
O	-1.375267	1.552219	-2.038891
H	1.476247	-2.877986	1.541269
H	0.565202	-4.066769	2.058232
H	-4.339847	-0.092242	-1.290429
H	-3.480843	0.479661	-0.104326
H	-1.545196	2.185550	-2.743218
H	-2.195908	1.036735	-1.905540
H	-1.499387	-2.622405	-0.892420
H	-2.419533	-1.390736	-0.606175
H	-3.511083	1.791652	1.910554
H	-2.128758	1.613432	1.173512
H	3.289752	-1.896595	0.565433
H	2.191134	-1.025668	1.242941
H	-0.895308	2.005591	-0.571455
H	-0.346800	2.971739	0.567289
H	-2.703207	-1.647997	3.107385
H	-2.448945	-0.264626	2.422623
H	0.572958	0.094762	2.407292
H	0.297030	0.680457	0.982035
O	0.129302	0.274031	4.029607
H	-0.671528	-0.277254	3.994111
H	0.704946	-0.115078	4.696697

$Li^+ (H_2O)_{11}$

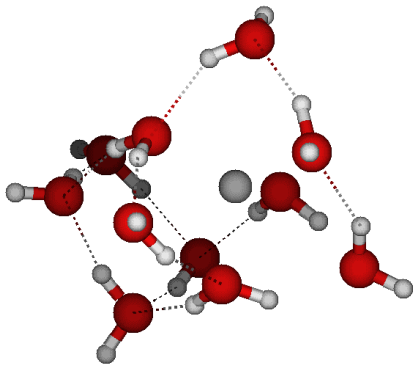

Figure S_{16} : Li^+ optimized structure with 11 water molecules.

E = -840.366244

H = -840.365300

O	0.543817	-3.212290	1.621355
Li	-0.677924	-1.727979	1.379449
O	-1.813697	-2.039255	-0.195171
O	0.583020	-0.134389	1.441446
O	-2.004733	-1.051750	2.815261
O	2.750367	-1.819962	1.359076
O	0.129302	0.274031	4.029607
O	-2.960293	1.141191	1.459551
O	-0.723529	2.098343	0.413468
O	-1.375267	1.552220	-2.038891
O	-3.435565	0.054489	-0.991793
H	1.476247	-2.877986	1.541269
H	0.565202	-4.066769	2.058232
H	-4.339847	-0.092242	-1.290429
H	-3.480843	0.479661	-0.104326
H	-1.545196	2.185551	-2.743218
H	-2.195908	1.036736	-1.905540
H	-1.499387	-2.622405	-0.892420
H	-2.419533	-1.390736	-0.606175
H	-3.511083	1.791652	1.910554
H	-2.128758	1.613432	1.173512

H	3.289752	-1.896595	0.565433
H	2.191134	-1.025668	1.242941
H	-0.895308	2.005591	-0.571455
H	-0.346800	2.971739	0.567290
H	-2.703207	-1.647997	3.107385
H	-2.448945	-0.264626	2.422623
H	0.572958	0.094762	2.407292
H	0.297030	0.680457	0.982035
H	-0.671528	-0.277254	3.994111
H	0.704946	-0.115078	4.696697
O	-1.747677	-3.079940	1.326852
H	-2.631160	-3.295125	1.601901
H	-1.124693	-3.472344	1.927194

$Na^+ (H_2O)$

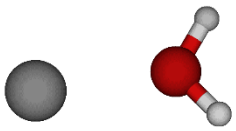

Figure S_{17} : Na^+ optimized structure with 1 water molecule.

E = -76.408209

H = -76.407265

Na	-0.107909	0.000000	-0.183683
O	0.098617	0.000000	2.030680
H	0.914407	0.000000	2.546154
H	-0.606556	0.000000	2.689404

$Na^+ (H_2O)_2$

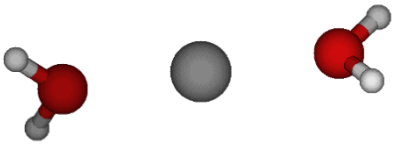

Figure S_{18} : Na^+ optimized structure with 2 water molecules.

E = -152.813067

H = -152.812123

O	0.029916	-0.257099	2.441534
Na	0.427524	0.807546	0.510660
H	0.620120	-0.842347	2.930850
H	-0.777446	-0.226394	2.968434
O	0.830130	1.883065	-1.415490
H	0.708693	1.551577	-2.312960
H	1.165296	2.780350	-1.527864

$Na^+ (H_2O)_3$

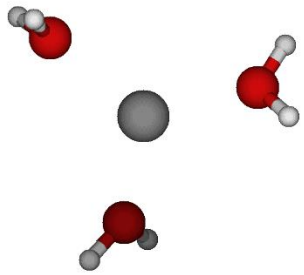

Figure S_{19} : Na^+ optimized structure with 3 water molecules.

E = -229.212399

H = -229.211455

O	-0.165035	-0.754009	1.920779
Na	0.577092	1.216110	1.076036
O	0.593473	1.552682	-1.166871
H	0.308273	-1.358884	2.503103
H	-1.022868	-1.168666	1.775210
H	1.028687	1.014541	-1.837691
H	0.167822	2.265209	-1.656898
O	1.303266	2.846840	2.475611
H	0.818172	3.256988	3.200511
H	2.164236	3.280124	2.475511

$Na^+ (H_2O)_4$

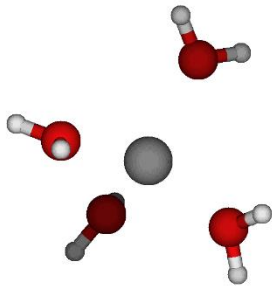

Figure S_{20} : Na^+ optimized structure with 4 water molecules.

E = -305.604745

H = -305.603801

O	-0.382750	-0.545501	1.692928
Na	0.934957	1.048677	0.673539
O	-0.124864	1.887823	-1.193874
O	1.334490	2.782080	2.141326
H	-0.119166	-1.206129	2.342386
H	-1.313722	-0.721761	1.519531
H	0.109006	1.715182	-2.112205
H	-0.857234	2.512057	-1.234491
H	1.158025	2.786275	3.088240
H	1.662323	3.665789	1.943151
O	2.931565	0.066716	0.065436
H	3.815668	0.412433	0.228777
H	3.070467	-0.787504	-0.357308

$Na^+ (H_2O)_5$

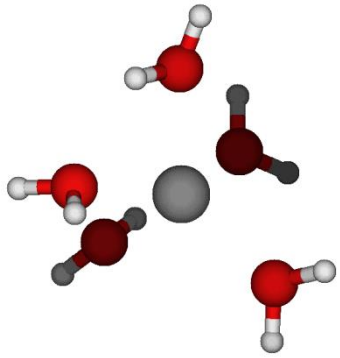

Figure S_{21} : Na^+ optimized structure with 5 water molecules.

E = -381.989449

H = -381.988505

O	-0.351339	-0.663960	1.733218
Na	1.151766	0.907002	0.938066
O	0.561394	1.955909	-1.012212
O	0.873537	2.871389	2.448242
O	2.263717	-0.203846	-1.005877
H	-0.162566	-1.422804	2.295375

H	-1.299728	-0.698530	1.569273
H	1.089679	1.402406	-1.604373
H	0.053592	2.559131	-1.561711
H	0.305805	2.905974	3.226576
H	0.836033	3.757232	2.069393
H	3.219546	-0.128191	-1.107234
H	2.040154	-1.070837	-1.363185
O	3.049468	1.204140	2.189869
H	3.905394	0.956748	2.550341
H	2.749043	1.986015	2.673887

$Na^+ (H_2O)_6$

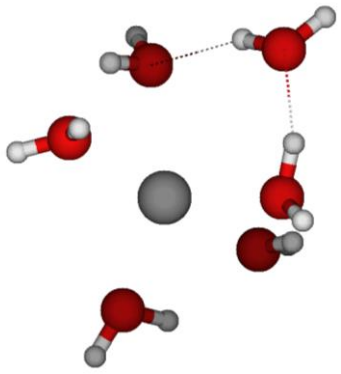

Figure S_{22} : Na^+ optimized structure with 6 water molecules.

E = -458.376198

H = -458.375254

O	0.040906	-0.630113	1.083937
Na	1.190545	1.375132	0.660449
O	0.898207	2.252238	-1.402381
O	2.780869	1.329131	2.469564
O	0.642517	3.049338	2.406349
O	1.793090	-0.310461	-0.970703
H	0.452902	-0.934059	1.934270
H	-0.884432	-0.893263	1.112740
H	1.161815	1.442283	-1.864777
H	0.501454	2.838280	-2.052377

H	-0.088937	2.932059	3.025007
H	0.662309	3.995787	2.219237
H	2.465385	-0.901434	-1.322985
H	1.144376	-0.862203	-0.497320
H	3.730776	1.476477	2.537973
H	2.342807	2.097170	2.873955
O	1.360552	-0.947698	3.345966
H	2.052899	-0.272087	3.235486
H	1.789612	-1.742576	3.678421

$Na^+ (H_2O)_7$

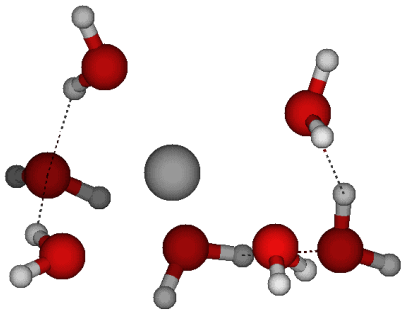

Figure S_{23} : Na^+ optimized structure with 7 water molecules.

E = -534.765590

H = -534.764646

O	0.228849	-0.349015	0.911301
Na	1.930438	1.373728	0.855610
O	0.606690	1.608760	-1.094897
O	2.781638	0.922782	3.204514
O	1.439062	-1.020550	-1.424965
O	0.852185	2.654214	2.627368
O	0.197976	0.136408	3.591189
H	0.027802	-0.466488	1.861107
H	-0.505968	0.150723	0.534183
H	0.821462	0.778885	-1.560887
H	0.437723	2.268180	-1.774660
H	0.291603	1.992844	3.075749

H	0.401021	3.501416	2.702304
H	1.272484	-1.774364	-2.000601
H	0.976574	-1.185853	-0.579831
H	3.650523	0.708886	3.562098
H	2.564968	1.828657	3.475035
H	1.170504	0.122214	3.701306
H	-0.191363	-0.257929	4.379474
O	3.575074	0.261572	-0.272988
H	4.476867	0.303769	-0.601373
H	3.088031	-0.356537	-0.849395

$Na^+ (H_2O)_8$

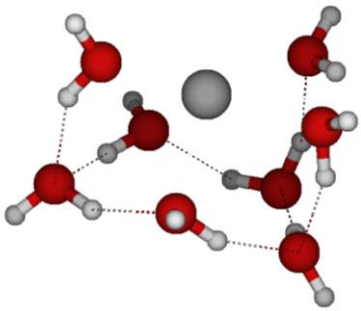

Figure S_{24} : Na^+ optimized structure with 8 water molecules.

E = -611.160863

H = -611.159919

O	-0.002982	0.005891	0.950253
Na	1.660429	1.844663	0.610506
O	3.283857	0.052606	0.348702
O	1.082824	1.684698	-1.591248
O	0.476361	2.733103	2.645725
O	3.118226	0.260307	3.121544
O	1.322293	-1.055994	-1.117717
O	0.575109	0.196453	3.540068
H	0.082636	-0.152988	1.922385

H	-0.926913	0.233010	0.797737
H	1.110950	0.735191	-1.805918
H	1.032124	2.160468	-2.424796
H	0.345384	1.912792	3.175745
H	-0.234987	3.339693	2.875112
H	1.172497	-1.920381	-1.515090
H	0.695409	-0.949691	-0.367496
H	3.306765	-0.091106	2.230610
H	3.361438	1.201304	3.048147
H	1.583718	0.138403	3.484881
H	0.292847	-0.270750	4.333850
H	4.163748	0.117041	-0.037917
H	2.768815	-0.553131	-0.230541
O	3.080720	2.943616	2.247464
H	3.725311	3.647299	2.375854
H	2.252238	3.209537	2.694728

$Na^+ (H_2O)_9$

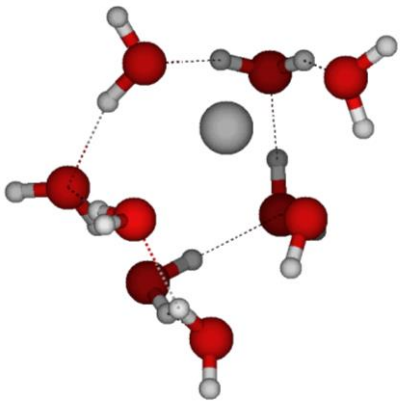

Figure S_{25} : Na^+ optimized structure with 9 water molecules.

E = -687.547731

H = -687.546786

O	-0.620989	-0.405963	0.961132
Na	2.676819	2.224305	0.554858

O	1.067297	1.981661	-1.224820
O	3.581491	2.936636	2.647916
O	3.517707	0.070497	0.283747
O	0.994587	2.736662	2.057098
O	0.593940	0.376104	3.288746
O	3.179969	0.097074	3.097255
O	1.188553	-0.626251	-0.780539
H	-0.261653	-0.317354	1.869660
H	-1.038033	0.460463	0.784886
H	1.057974	0.987974	-1.276279
H	1.086070	2.306709	-2.131819
H	0.756614	1.959750	2.616516
H	0.155074	2.959601	1.617181
H	1.018735	-1.363180	-1.378068
H	0.452373	-0.636749	-0.055000
H	3.409664	-0.177703	2.191423
H	3.529193	1.001626	3.171059
H	1.569620	0.146633	3.318021
H	0.236378	0.254663	4.175043
H	4.324955	-0.305124	-0.083635
H	2.753511	-0.398123	-0.140529
H	4.208597	3.492503	3.123001
H	2.686409	3.253540	2.867168
O	-1.172291	2.273938	0.413482
H	-2.016724	2.653937	0.147342
H	-0.571461	2.302931	-0.357336

$Na^+ (H_2O)_{10}$

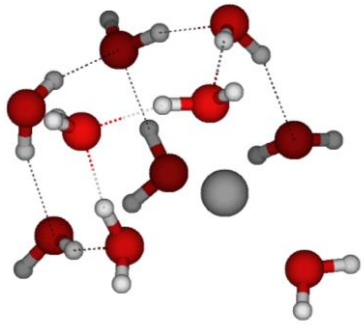

Figure S_{26} : Na^+ optimized structure with 10 water molecules.

E = -763.939139

H = -763.938195

O	-0.713395	-0.451660	1.174553
O	0.945889	-0.810328	-0.693857
O	0.807884	1.736495	-1.384391
Na	2.580114	2.284537	0.259286
O	0.941808	2.609423	1.981035
O	3.307689	0.028280	0.213019
O	3.497321	3.007984	2.461216
O	0.718542	0.308351	3.379573
O	3.290298	0.214402	3.029511
O	-1.243700	2.209618	0.384311
H	-0.262151	-0.334380	2.039241
H	-1.123812	0.413062	0.981389
H	0.812742	0.743117	-1.325080
H	0.756681	1.955623	-2.321046
H	0.763415	1.858680	2.595084
H	0.073934	2.809438	1.584179
H	0.744935	-1.605795	-1.199130
H	0.264652	-0.752700	0.079387
H	3.419927	-0.060229	2.102761
H	3.546801	1.154905	3.031128
H	1.711563	0.151635	3.332917

H	0.442685	0.169310	4.291770
H	4.088937	-0.361357	-0.193705
H	2.525668	-0.476590	-0.125555
H	4.023883	3.629344	2.974578
H	2.555888	3.228563	2.608838
H	-2.077173	2.608380	0.112635
H	-0.667145	2.148476	-0.407343
O	3.823810	3.808901	-0.956882
H	3.728665	4.166166	-1.845586
H	4.593389	4.254095	-0.586680

$Na^+ (H_2O)_{11}$

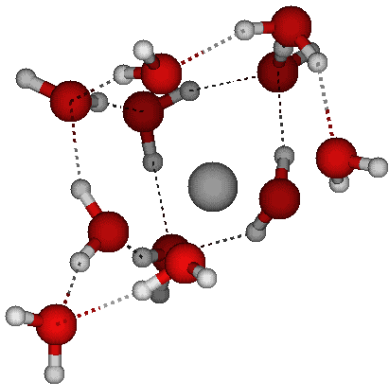

Figure S_{27} : Na^+ optimized structure with 11 water molecules.

E = -840.327442

H = -840.326498

O	-0.741788	-0.163158	0.637903
O	1.318745	-0.558187	-0.791125
O	1.695511	2.093765	-0.854969
Na	2.959853	1.955694	1.235880
O	3.439116	3.704385	-2.446038
O	3.356955	-0.364635	0.909016
O	0.960304	2.350940	2.530043
O	3.331067	2.153353	3.646338
O	0.039976	-0.084977	3.268548

O	2.565959	-0.605128	3.601147
O	-0.662042	2.639153	0.343269
H	-0.553647	-0.283442	1.593902
H	-0.944723	0.787221	0.537451
H	1.581739	1.146361	-1.104167
H	2.161479	2.552735	-1.574286
H	0.508490	1.556799	2.897991
H	0.292853	2.766737	1.953548
H	1.155305	-1.234685	-1.456967
H	0.465940	-0.478906	-0.223770
H	2.912675	-0.754178	2.701437
H	2.946700	0.254528	3.857466
H	0.973449	-0.408849	3.456997
H	-0.512780	-0.336360	4.015837
H	4.165990	-0.816262	0.647247
H	2.656148	-0.629246	0.258789
H	3.823742	2.613491	4.333304
H	2.431524	2.536253	3.617777
H	-1.323001	3.209697	-0.061905
H	0.115270	2.595851	-0.259799
H	3.112621	4.565678	-2.733219
H	3.956156	3.363923	-3.185942
O	4.427649	3.382313	0.202313
H	5.225963	3.851143	0.460902
H	4.245199	3.625365	-0.721121

$Na^+ (H_2O)_{12}$

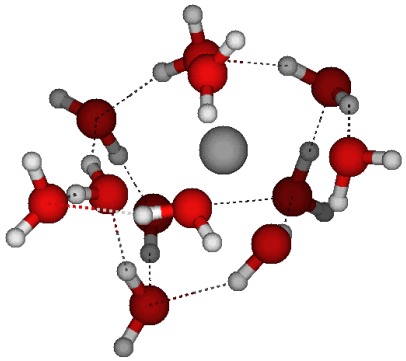

Figure S_{28} : Na^+ optimized structure with 12 water molecules.

E = -916.709122

H = -916.708178

O	-0.964290	0.054262	0.723736
O	0.944283	-0.667761	-0.792290
O	3.006080	-0.773544	0.898599
Na	3.201359	1.620595	1.117559
O	4.135875	3.880922	0.162605
O	1.241410	2.299199	2.488114
O	3.552919	1.780554	3.576299
O	1.796660	1.861625	-0.889989
O	-0.403875	2.792611	0.363713
O	-0.025612	0.056139	3.308428
O	2.388630	-0.840839	3.612880
O	3.413526	3.510436	-2.551338
H	-0.734036	-0.084996	1.667843
H	-1.001944	1.024451	0.616435
H	1.521116	0.942086	-1.120304
H	2.224689	2.271901	-1.659058
H	0.686227	1.579906	2.870261
H	0.629521	2.805639	1.923575
H	0.658255	-1.323925	-1.436412
H	0.137562	-0.451962	-0.196271

H	2.653869	-1.055991	2.697432
H	2.895859	-0.032941	3.814974
H	0.853402	-0.403697	3.489252
H	-0.582660	-0.067541	4.083973
H	3.768929	-1.247648	0.551853
H	2.263282	-0.931601	0.264105
H	4.062285	2.170180	4.293632
H	2.706008	2.269047	3.509387
H	-0.969668	3.445074	-0.060969
H	0.345031	2.591599	-0.245786
H	3.056152	4.163947	-3.164413
H	4.157231	3.101907	-3.011083
H	4.244464	4.776189	0.498612
H	3.875590	3.960778	-0.773416
O	5.437045	1.533578	0.320516
H	6.278408	1.292966	0.719320
H	5.420036	2.504727	0.265497

$Na^+ (H_2O)_{13}$

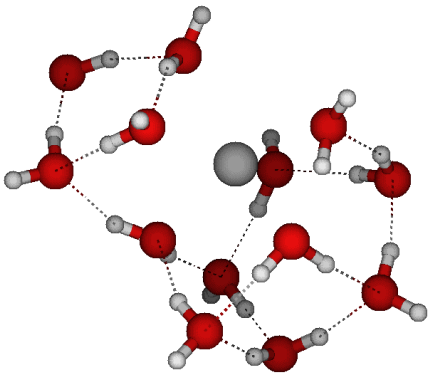

Figure S_{29} : Na^+ optimized structure with 13 water molecules.

E = -993.105967

H = -993.102023

O	-1.206768	0.164724	0.972778
O	0.596494	-0.738747	-0.578048

O	2.729125	-0.857389	0.994766
Na	2.979845	1.523915	1.157870
O	5.431839	1.406495	0.241138
O	1.561904	1.762554	-0.786388
O	1.157136	2.332993	2.607910
O	3.505957	1.731993	3.569939
O	4.016657	3.628757	0.181026
O	-0.512708	2.853040	0.518756
O	-0.201825	0.190170	3.539208
O	2.186927	-0.817931	3.739175
O	3.345069	3.070904	-2.367001
H	-0.964778	0.043843	1.915706
H	-1.196104	1.131790	0.832674
H	1.231173	0.865915	-1.017218
H	2.023967	2.156874	-1.554012
H	0.575001	1.664184	3.037724
H	0.557134	2.847005	2.035080
H	0.243390	-1.411709	-1.169414
H	-0.168965	-0.444787	0.037725
H	2.394979	-1.057048	2.815270
H	2.748882	-0.039376	3.905952
H	0.658129	-0.308699	3.692997
H	-0.734846	0.106240	4.336634
H	3.408454	-1.474850	0.705321
H	1.943529	-0.999101	0.403867
H	4.059898	2.108131	4.261157
H	2.675344	2.252743	3.537001
H	-1.048905	3.535450	0.102601
H	0.196924	2.589810	-0.116216
H	3.260276	3.667948	-3.117878
H	4.110973	2.453679	-2.559028
H	4.171823	4.537944	0.455702
H	3.756931	3.646745	-0.772253
H	6.247497	1.266239	0.734413

H	5.231380	2.369479	0.280345
O	5.402822	1.482823	-2.503972
H	5.558738	1.283569	-1.556181
H	5.421268	0.645743	-2.977753

$Na^+ (H_2O)_{14}$

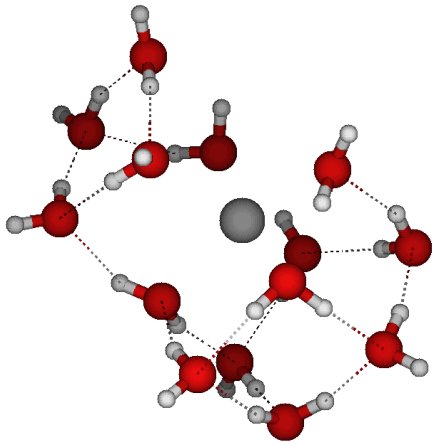

Figure S_{30} : Na^+ optimized structure with 14 water molecules.

E = -1069.489185

H = -1069.488240

O	-1.534817	0.372645	1.172990
O	0.053553	-0.646881	-0.558213
O	2.171026	-1.022638	1.091620
Na	2.711016	1.321388	1.085784
O	1.210747	1.745860	-0.777488
O	1.122208	2.335286	2.669688
O	3.461049	1.436083	3.456110
O	4.008103	3.297907	0.138127
O	6.376650	2.045238	-0.434633
O	-0.641927	3.016866	0.690860
O	3.127316	2.911240	-2.406121
O	5.143445	1.184899	-2.617942
O	-0.332665	0.289497	3.658122
O	1.912232	-0.995988	3.820366
H	-1.217123	0.209742	2.086663

H	-1.444065	1.336434	1.047907
H	0.790889	0.871217	-0.964110
H	1.681214	2.063194	-1.569257
H	0.525950	1.687431	3.115816
H	0.521035	2.898434	2.148143
H	-0.406886	-1.245664	-1.155259
H	-0.631177	-0.313784	0.120298
H	2.030638	-1.283401	2.892176
H	2.556578	-0.271548	3.909892
H	0.475491	-0.302502	3.787213
H	-0.836116	0.271368	4.478649
H	2.984461	-1.210433	0.599581
H	1.417855	-1.132841	0.470394
H	4.107653	1.736804	4.102123
H	2.695385	2.045475	3.497160
H	-1.174074	3.722429	0.309902
H	-0.019872	2.692668	-0.003624
H	3.035419	3.557513	-3.114277
H	3.840039	2.278343	-2.674842
H	3.942737	4.187369	0.502864
H	3.652355	3.343585	-0.781340
H	7.208568	2.503527	-0.277710
H	5.650506	2.622860	-0.108830
H	5.804751	1.550640	-1.978653
H	5.621186	0.835317	-3.377497
O	4.431749	-0.013760	-0.156836
H	5.313431	0.220578	0.165112
H	4.518506	0.105034	-1.118568

$Na^+ (H_2O)_{15}$

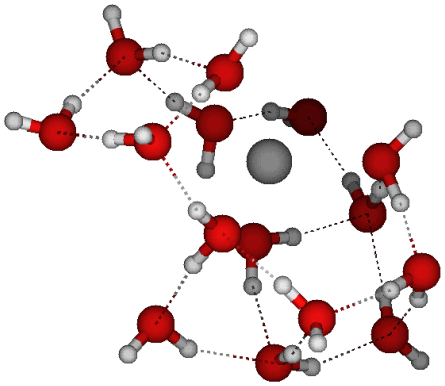

Figure S_{31} : Na^+ optimized structure with 15 water molecules.

E = -1145.872115

H = -1145.871171

O	-1.071925	0.218907	0.740908
O	0.049737	0.455214	-1.759747
O	1.402085	2.487493	-0.649398
Na	2.933408	1.635589	0.999909
O	4.315883	-1.618200	3.198950
O	0.003297	2.557943	3.506582
O	2.524459	2.144913	3.245276
O	4.240607	-0.406224	0.694426
O	4.700964	2.952297	-0.075257
O	-0.739454	2.977481	0.867432
O	-0.747317	-0.157246	3.519303
O	1.920689	-0.546931	3.696170
O	3.322990	3.715227	-2.215672
O	4.165664	1.625903	-3.508000
O	5.706754	0.767389	-1.393177
H	-1.205436	-0.117528	1.647228
H	-1.105792	1.194306	0.823557
H	0.957322	1.758502	-1.157768
H	1.870847	3.046136	-1.300099
H	-0.388921	1.670305	3.632402

H	-0.336837	2.864672	2.643307
H	-0.520238	0.524628	-2.531524
H	-0.507988	0.120228	-1.032996
H	2.746436	-1.093657	3.665964
H	2.235713	0.379337	3.746740
H	0.160218	-0.496816	3.696244
H	-1.318858	-0.532171	4.197953
H	4.479199	-1.285127	2.293444
H	4.508586	-2.560617	3.182344
H	3.023169	2.623551	3.915576
H	1.547903	2.385940	3.389907
H	-1.379520	3.616459	0.537819
H	0.046893	2.996488	0.264935
H	3.338913	4.547629	-2.699257
H	3.624205	2.989718	-2.839695
H	5.261371	3.601736	0.363208
H	4.264103	3.413156	-0.838294
H	6.662610	0.657145	-1.447496
H	5.539838	1.583230	-0.867096
H	4.786999	1.181574	-2.893037
H	4.545960	1.571374	-4.389660
H	4.796918	-0.347335	-0.101674
H	3.359473	-0.740848	0.436973
O	1.634986	-0.325514	1.000398
H	0.687799	-0.237382	0.772016
H	1.655986	-0.552662	1.957132

$Na^+ (H_2O)_{16}$

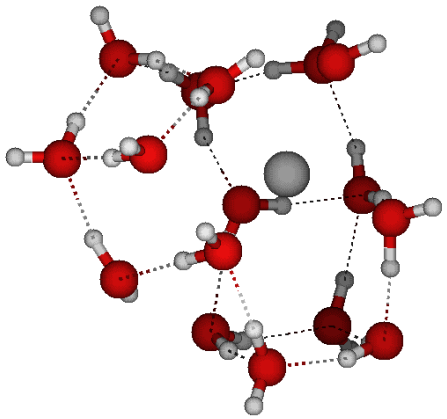

Figure S_{32} : Na^+ optimized structure with 16 water molecules.

E = -1222.265425

H = -1222.264481

O	-0.604666	0.162017	0.397265
O	0.606327	1.297568	-1.959020
O	1.373555	3.182438	-0.310569
Na	2.864457	2.256566	1.282495
O	1.971389	2.507872	3.466598
O	2.008574	0.114314	0.985641
O	4.200288	-1.388813	0.502191
O	4.723711	2.343724	-0.315455
O	-0.582013	2.326960	3.449047
O	3.451158	3.807031	-2.170231
O	3.087866	1.271421	-3.230620
O	-1.063113	2.896708	0.784237
O	2.159919	-0.212366	3.679246
O	4.832482	-0.449914	2.818612
O	-0.564845	-0.477611	3.198797
O	5.045425	0.158460	-1.741498
H	-0.842046	-0.281924	1.230677
H	-0.903123	1.089388	0.504592
H	1.091522	2.440924	-0.926987
H	1.840193	3.795581	-0.902898

H	-0.748118	1.363477	3.452002
H	-0.897553	2.644539	2.579683
H	1.406328	1.011259	-2.437079
H	0.225118	0.534694	-1.500890
H	3.096739	-0.486065	3.597172
H	2.182506	0.762169	3.814324
H	0.363963	-0.626085	3.471544
H	-1.105573	-1.050361	3.753582
H	4.684213	-0.862211	1.901544
H	5.492500	-0.997017	3.258944
H	2.251742	3.095321	4.176261
H	0.953162	2.507258	3.493104
H	-1.806758	3.357634	0.381747
H	-0.239126	3.252120	0.372739
H	3.681232	4.494302	-2.804362
H	3.292294	2.984872	-2.688485
H	5.284412	2.570860	0.447831
H	4.546844	3.109421	-0.900978
H	5.921787	0.028027	-2.120502
H	5.082968	0.980472	-1.182201
H	3.803231	0.740455	-2.799719
H	3.099279	1.051043	-4.168457
H	4.613804	-1.019914	-0.298996
H	3.292750	-1.011709	0.497457
H	1.073096	0.097982	0.662518
H	1.957750	-0.136432	1.936029
O	5.170383	2.178395	2.299550
H	5.596142	2.644843	3.025310
H	5.193459	1.216431	2.537912

$Na^+ (H_2O)_{17}$

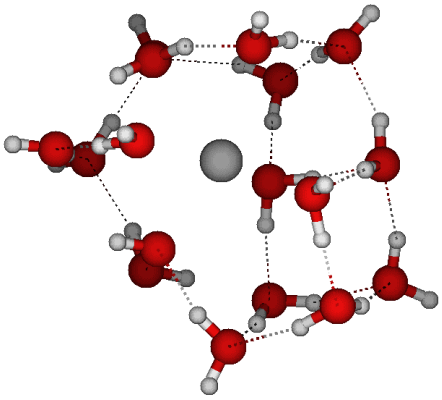

Figure S_{33} : Na^+ optimized structure with 17 water molecules.

E = -1298.650881

H = -1298.649937

O	-0.572190	0.039608	0.357235
O	2.033779	0.370482	0.994717
Na	2.726209	2.609274	1.308174
O	0.983137	3.142030	-0.330951
O	1.766652	2.527530	3.516844
O	5.079234	2.213886	-0.401771
O	5.135087	2.150038	2.271085
O	-0.767426	2.086638	3.476533
O	0.456000	1.217055	-2.001129
O	5.020097	0.047427	-1.800250
O	3.457794	3.932135	-2.109004
O	-1.361287	2.659618	0.846470
O	3.025325	1.342033	-3.044589
O	4.791706	-0.427591	2.914967
O	4.158581	-1.257978	0.570261
O	2.115126	-0.181470	3.657250
O	-0.531275	-0.699949	3.097463
H	-0.753705	-0.471020	1.167487
H	-1.002558	0.908604	0.502754
H	0.792911	2.402549	-0.989403

H	1.273388	3.886848	-0.870866
H	-0.855447	1.113759	3.445140
H	-1.121236	2.402253	2.621133
H	1.327998	0.986006	-2.373149
H	0.133120	0.462762	-1.482854
H	3.061659	-0.430273	3.595953
H	2.098836	0.787111	3.829216
H	0.406244	-0.751259	3.381517
H	-1.013228	-1.347262	3.623352
H	4.656998	-0.812813	1.983628
H	5.423734	-0.996962	3.366961
H	1.971359	3.112234	4.254323
H	0.756081	2.417350	3.529095
H	-2.143273	3.065054	0.457789
H	-0.566754	3.059437	0.412537
H	3.699920	4.471159	-2.869698
H	3.292739	3.028484	-2.466418
H	5.309919	2.314245	0.547481
H	4.885353	3.074934	-0.794734
H	5.831885	-0.176755	-2.268000
H	5.199808	0.869271	-1.261873
H	3.744108	0.761186	-2.681978
H	3.007473	1.195389	-3.997058
H	4.613043	-0.985231	-0.246559
H	3.301557	-0.776120	0.539561
H	1.115285	0.243209	0.651878
H	1.982960	0.077085	1.933722
H	5.732796	2.638052	2.846665
H	5.141327	1.208954	2.585387
O	3.489965	4.715087	0.566409
H	3.700063	5.602045	0.870492
H	3.462801	4.739633	-0.404949

$Na^+ (H_2O)_{18}$

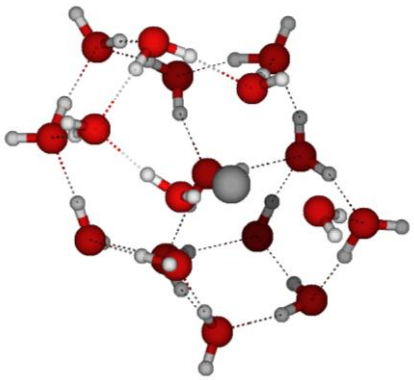

Figure S_{34} : Na^+ optimized structure with 18 water molecules.

E = -1375.047235

H = -1375.046291

O	-0.488367	0.288061	0.311236
O	2.039812	0.849832	1.065236
Na	2.703889	3.100490	1.186708
O	3.129070	4.839757	-0.444542
O	1.239730	2.154965	4.821157
O	0.698696	3.497491	-0.115349
O	-1.050530	1.670121	3.780185
O	0.583961	1.615323	-1.941640
O	4.955160	2.301668	1.708129
O	-1.436759	2.709265	1.221686
O	6.094973	1.985453	-0.808051
O	5.057331	-0.162174	-1.752425
O	4.709592	-0.170921	2.747361
O	3.844130	-1.138340	0.554482
O	3.179825	1.204945	-3.025863
O	2.084462	-0.111181	3.605176
O	-0.405774	-0.907340	2.851228
O	4.416976	3.532137	-2.467977
H	-0.604889	-0.371171	1.021354
H	-1.003317	1.072431	0.599316
H	0.663765	2.840864	-0.872021

H	1.069837	4.317435	-0.470610
H	-1.005438	0.729549	3.518135
H	-1.232462	2.157436	2.951755
H	1.463556	1.332711	-2.252667
H	0.205045	0.877683	-1.434312
H	3.051014	-0.264585	3.541212
H	1.928238	0.666867	4.189007
H	0.529510	-0.858918	3.150899
H	-0.774034	-1.719137	3.215690
H	4.480725	-0.651043	1.875125
H	5.451102	-0.639689	3.145549
H	1.152163	2.241822	5.776614
H	0.300345	2.026988	4.449364
H	-2.270708	3.096601	0.935963
H	-0.708402	3.198072	0.756335
H	4.759863	3.974727	-3.251906
H	3.910872	2.739575	-2.782168
H	5.776446	2.125420	0.109343
H	5.665998	2.674284	-1.349752
H	5.706209	-0.702721	-2.216366
H	5.551339	0.639375	-1.368189
H	3.840097	0.576596	-2.619567
H	3.046595	0.919916	-3.936981
H	4.340921	-0.933094	-0.262414
H	3.092898	-0.503842	0.552724
H	1.128600	0.696802	0.711697
H	1.995851	0.529724	1.997839
H	5.450171	2.871255	2.307753
H	4.932166	1.408977	2.145165
H	3.494829	5.720223	-0.314219
H	3.572614	4.478874	-1.244089
O	2.377150	4.047021	3.257677
H	2.087768	4.928734	3.507513
H	1.983417	3.435692	3.922409

$Na^+ (H_2O)_{19}$

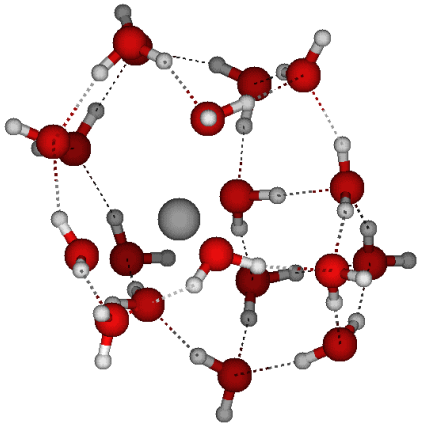

Figure S_{35} : Na^+ optimized structure with 19 water molecules.

E = -1451.420045

H = -1451.419101

O	-0.461022	0.041366	0.312269
O	2.078595	0.677951	0.891788
Na	2.669935	2.928699	0.968519
O	2.666352	4.193106	2.870368
O	2.615017	4.960433	-0.347098
O	0.503135	3.263707	-0.186408
O	4.876267	2.080916	1.690982
O	0.492773	1.401607	-2.045975
O	-1.545059	2.423786	1.190681
O	4.808539	-0.412752	2.623318
O	3.863404	-1.311136	0.425663
O	1.504532	2.366872	4.565099
O	-0.839608	1.659893	3.760165
O	2.262930	-0.027736	3.510494
O	-0.200463	-0.957450	2.940146
O	4.589009	3.489689	-1.712131
O	3.224360	1.434348	-2.870668
O	4.926445	-0.416967	-2.015761

O	6.161820	1.383118	-0.652884
H	-0.511740	-0.581234	1.061684
H	-1.000781	0.812148	0.592760
H	0.481571	2.634208	-0.962243
H	0.902133	4.094876	-0.491578
H	-0.776738	0.703559	3.568011
H	-1.156289	2.058643	2.924641
H	1.423990	1.234555	-2.280883
H	0.186023	0.642429	-1.523624
H	3.213209	-0.263786	3.440184
H	2.165268	0.810824	4.018555
H	0.742823	-0.836551	3.195546
H	-0.508822	-1.753252	3.385882
H	4.557563	-0.852336	1.737336
H	5.557782	-0.893921	2.989096
H	1.468236	2.478680	5.521386
H	0.555072	2.163958	4.269585
H	-2.409708	2.736239	0.905631
H	-0.855257	2.934158	0.685000
H	5.130530	3.932958	-2.374376
H	4.044982	2.823718	-2.202984
H	5.851158	1.441388	0.272892
H	5.778107	2.199223	-1.026073
H	5.495327	-0.933655	-2.597021
H	5.513105	0.220266	-1.491291
H	3.809004	0.656898	-2.650731
H	3.129742	1.446971	-3.829974
H	4.295386	-1.199671	-0.441513
H	3.124789	-0.659561	0.421364
H	1.147965	0.493896	0.605252
H	2.093500	0.439908	1.848906
H	5.305386	2.725893	2.263840
H	4.890605	1.218203	2.177028
H	2.738343	5.759462	0.190269

H	3.393827	4.806941	-0.907137
H	2.329791	5.096884	2.807029
H	2.211383	3.734305	3.605141
O	2.229185	6.885674	1.707878
H	2.798114	7.587125	2.044997
H	1.373300	7.304372	1.559242

$K^+ (H_2O)$

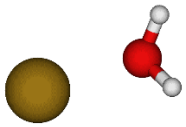

Figure S_{36} : K^+ optimized structure with 1 water molecule.

E = -104.565407

H = -104.564463

K	-0.099939	0.000000	-0.236271
O	0.101647	0.000000	2.398084
H	0.906102	0.000000	2.929567
H	-0.609250	0.000000	3.049574

$K^+ (H_2O)_2$

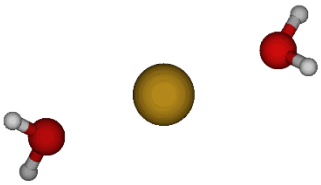

Figure S_{37} : K^+ optimized structure with 2 water molecules.

E = -180.957515

H = -180.956570

O	0.017972	-0.302994	2.871896
K	0.629607	0.666428	0.467144
H	0.596133	-0.757936	3.494736
H	-0.835764	-0.278727	3.318778
O	0.980542	2.166918	-1.706073
H	1.274698	3.083907	-1.748098
H	0.841982	1.922291	-2.628087

$K^+ (H_2O)_3$

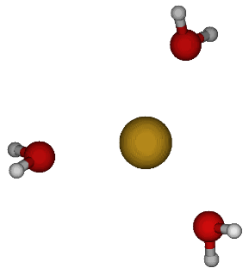

Figure S_{38} : K^+ optimized structure with 3 water molecules.

E = -257.346670

H = -257.345726

O	0.091862	0.049871	2.522424
K	0.911913	0.377853	-0.011047
O	0.472946	2.724434	-1.232437
H	0.624514	-0.175557	3.293129
H	-0.804089	0.128200	2.868327
H	0.772469	3.598500	-0.958916
H	-0.020939	2.886406	-2.043818
O	2.150997	-1.584891	-1.356469
H	1.820626	-2.468283	-1.553917
H	3.028947	-1.566230	-1.753157

$K^+ (H_2O)_4$

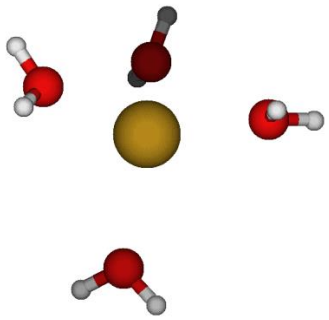

Figure S_{39} : K^+ optimized structure with 4 water molecules.

E = -333.732583

H = -333.731639

O	-0.069197	0.006382	2.143555
K	0.495043	0.354859	-0.483351
O	1.091216	2.938305	-1.040899
O	2.633592	-1.185308	-1.113308
H	-0.078631	-0.816529	2.644109
H	-0.277123	0.684615	2.795169
H	1.953996	3.302472	-1.266313
H	0.496287	3.695093	-1.074443
H	2.724675	-1.776771	-1.868116
H	3.460887	-1.285262	-0.630233
O	-1.649791	-0.341171	-1.984567
H	-2.417169	-0.853190	-1.707424
H	-1.832585	-0.114358	-2.902661

$K^+ (H_2O)_5$

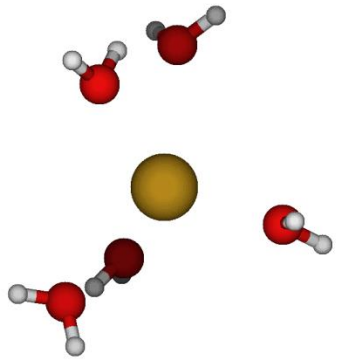

Figure S_{40} : K^+ optimized structure with 5 water molecules.

E = -410.116832

H = -410.115888

O	-0.549768	0.552279	2.159210
K	0.247754	0.627879	-0.426572
O	-1.182639	-0.756502	-2.167386
O	2.349094	2.150864	-0.933630
O	2.983907	-0.545907	-0.660042
H	-0.977442	-0.172939	2.627044

H	-0.463543	1.247758	2.819973
H	2.972428	1.407482	-0.932358
H	2.865604	2.946358	-1.088357
H	3.255419	-1.071960	-1.421271
H	3.534032	-0.860760	0.066558
H	-1.515778	-1.514903	-2.654604
H	-1.712609	0.008418	-2.441514
O	-1.907436	1.927323	-2.029329
H	-1.715401	2.533128	-2.754601
H	-2.775912	2.195101	-1.707209

$K^+ (H_2O)_6$

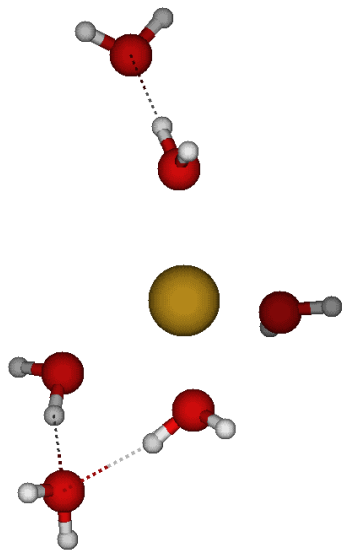

Figure S_{41} : K^+ optimized structure with 6 water molecules.

E = -486.503612

H = -486.502667

O	-1.512073	1.676823	0.996997
K	0.316480	-0.073832	0.093251
O	2.840051	0.722807	0.176581
O	-1.166113	0.286368	-2.119783
O	-3.143933	2.189488	-1.302117
O	4.737809	-0.576514	-1.335083
H	-1.764536	2.121945	1.810735

H	-2.157170	1.960554	0.328313
H	3.547150	0.292851	-0.346490
H	3.268514	1.458491	0.622746
H	5.167459	-0.135735	-2.075522
H	5.429810	-1.088637	-0.903734
H	-1.151569	0.065307	-3.055178
H	-1.894686	0.919568	-2.008582
H	-3.133244	3.073239	-1.688433
H	-4.070137	1.920377	-1.290761
O	-0.045821	-2.584101	1.074974
H	0.111533	-2.897855	1.971607
H	-0.403257	-3.348262	0.610864

$K^+ (H_2O)_7$

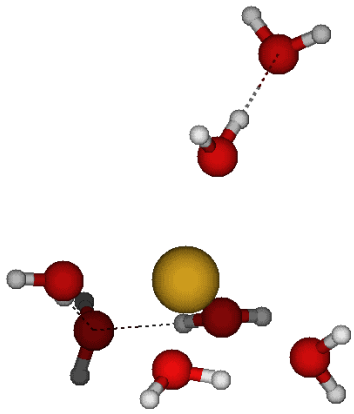

Figure S_{42} : K^+ optimized structure with 7 water molecules.

E = -562.884714

H = -562.883769

O	-1.111647	2.657634	0.276762
K	0.032228	0.231944	0.632616
O	2.700223	0.342335	0.579944
O	-1.404269	-0.122623	-1.641469
O	-0.143150	-2.791686	1.465736
O	4.184627	0.310615	-1.752047
O	-2.829797	2.343856	-1.998645

H	-1.224757	3.457051	0.798324
H	-1.737557	2.730758	-0.461534
H	3.244932	0.328143	-0.232409
H	3.294158	0.643571	1.273253
H	4.577632	1.127690	-2.076044
H	4.854656	-0.367543	-1.887131
H	-1.406343	-0.698540	-2.411048
H	-1.943542	0.646696	-1.889027
H	-2.682179	2.887892	-2.781034
H	-3.784440	2.334741	-1.862100
H	0.639351	-3.315875	1.670003
H	-0.798733	-3.427128	1.157518
O	-0.799229	-0.602917	3.025807
H	-0.696544	-1.545519	2.816866
H	-1.176672	-0.550837	3.907538

$K^+ (H_2O)_8$

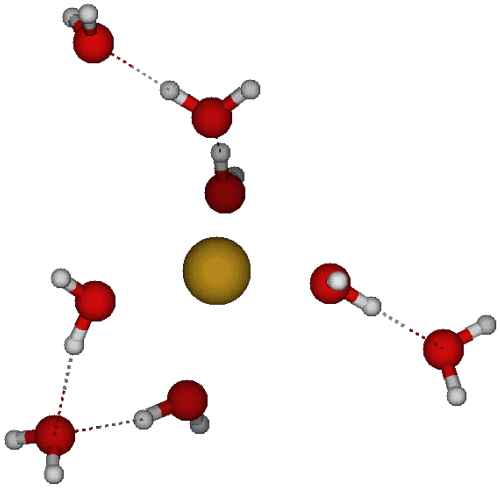

Figure S_{43} : K^+ optimized structure with 8 water molecules.

E = -639.267678

H = -639.266734

O	-0.482720	2.433746	-0.563258
K	0.043369	-0.187904	-0.110156
O	-0.187934	-0.998387	2.431006

O	2.997078	-0.117018	-0.142907
O	-2.451712	-0.248971	-1.197150
O	4.469588	1.980239	-1.117047
O	-1.502483	-3.392468	2.859927
O	-3.072400	2.492353	-1.804934
H	-0.029591	3.280103	-0.520852
H	-1.334242	2.610813	-0.994940
H	3.536515	0.630845	-0.478900
H	3.533584	-0.542258	0.533378
H	5.040620	2.513997	-0.554902
H	4.955698	1.859625	-1.939446
H	-2.934640	-0.910391	-1.700375
H	-2.804497	0.609313	-1.481240
H	-3.168382	2.786360	-2.718137
H	-3.805153	2.891787	-1.321867
H	-1.040828	-4.146402	3.240896
H	-2.391317	-3.420214	3.228364
H	-0.649187	-1.837975	2.627051
H	-0.121597	-0.543767	3.275015
O	1.492611	-1.665864	-1.802426
H	1.790183	-2.360354	-2.394782
H	2.287972	-1.271420	-1.398929

$K^+ (H_2O)_9$

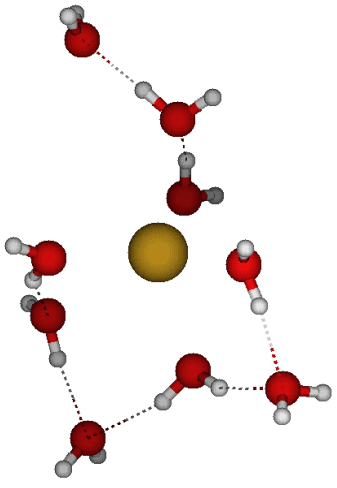

Figure S_{44} : K^+ optimized structure with 9 water molecules.

E = -715.651525

H = -715.650581

O	-0.903066	2.445011	-1.012694
K	0.488720	0.036511	0.154705
O	1.682521	-0.545207	-2.222707
O	0.228973	-1.834646	2.136060
O	-2.114695	-0.730222	-0.099595
O	3.413581	-0.393011	-0.119334
O	5.169763	1.700455	-0.202090
O	-2.512374	-2.700262	1.991880
O	-3.597366	1.561996	-1.155394
H	-0.626465	2.853810	-1.838084
H	-1.846473	2.225141	-1.114294
H	4.057743	0.347465	-0.127819
H	3.899165	-1.157985	0.204271
H	5.679985	2.004627	0.555135
H	5.732918	1.837221	-0.970628
H	-2.483697	-1.302651	0.588058
H	-2.791801	-0.075539	-0.318614
H	-3.966265	1.350143	-2.020791
H	-4.265503	2.095632	-0.709974
H	-2.602457	-3.580491	1.608566
H	-3.104718	-2.685135	2.752015
H	-0.678487	-2.177101	2.192950
H	0.577166	-1.881172	3.030878
H	1.750592	-1.218079	-2.905048
H	2.503738	-0.597950	-1.697412
O	0.365670	2.427291	1.404335
H	0.640309	3.189758	1.919389
H	-0.121923	2.770369	0.634200

$K^+ (H_2O)_{10}$

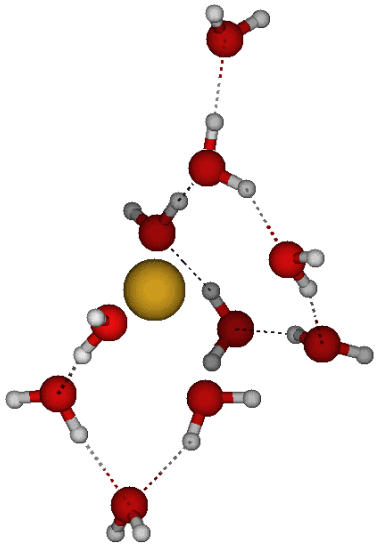

Figure S_{45} : K^+ optimized structure with 10 water molecules.

E = -792.051742

H = -792.050798

O	-1.856640	2.827666	-1.231115
O	-0.311596	3.440278	0.947000
K	0.339313	1.090856	-0.103252
O	1.487307	-0.756583	-1.940110
O	-1.987006	-0.403291	-0.123209
O	2.903379	-0.171261	0.182554
O	5.617133	-0.497179	0.394309
O	0.982153	-0.769285	1.991851
O	-4.214558	1.331123	-0.627611
O	-0.849364	-2.544742	1.210995
H	-1.964744	3.352262	-2.030675
H	-2.713721	2.389967	-1.077208
H	3.870289	-0.286367	0.284654
H	2.460747	-0.570625	0.958007
H	6.188956	0.184006	0.761802
H	6.044774	-1.335464	0.595247
H	-1.972923	-1.085648	0.571107

H	-2.873673	-0.013440	-0.157513
H	-4.809807	1.059445	-1.336466
H	-4.783038	1.677136	0.070647
H	-0.641502	-2.691693	0.235905
H	-1.071356	-3.401245	1.589789
H	0.366579	-1.526269	1.827743
H	1.031318	-0.657559	2.945808
H	1.945268	-0.830714	-2.782890
H	2.183462	-0.689394	-1.233231
H	-0.196963	4.276872	1.404480
H	-0.993157	3.576764	0.265704
O	-0.557766	-2.484278	-1.360592
H	-1.238361	-1.790595	-1.376660
H	0.257932	-2.010634	-1.635121

$K^+ (H_2O)_{11*}$

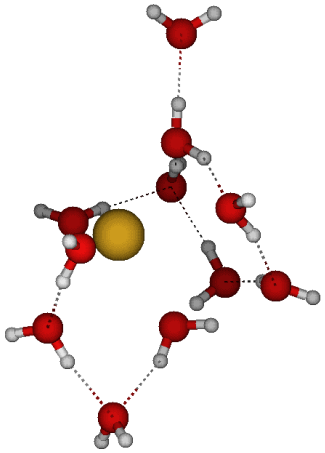

Figure S_{46} : K^+ optimized structure with 11 water molecules.

E = -868.437512

H = -868.436568

O	-2.016625	3.179928	-0.709270
O	-0.241407	3.463765	1.351731
K	0.367756	1.363462	-0.181006
O	-1.847354	-0.300468	-0.307657
O	-0.893291	-2.443897	1.146907

O	-0.498764	-2.527818	-1.400474
O	0.907931	-0.651692	1.945297
O	2.752635	-0.253650	0.049789
O	1.934607	-1.439896	-2.133598
O	5.471057	-0.213882	0.453794
O	-4.195889	1.339466	-0.646426
H	-2.126051	3.806417	-1.431134
H	-2.826128	2.639050	-0.694513
H	3.711974	-0.216486	0.241600
H	2.286667	-0.558825	0.858303
H	5.963689	0.612329	0.487394
H	5.933632	-0.816418	1.044810
H	-1.864818	-0.966723	0.402802
H	-2.737582	0.076477	-0.383475
H	-4.695234	1.182368	-1.456698
H	-4.855045	1.434092	0.051362
H	-0.652700	-2.648019	0.188558
H	-1.190111	-3.263683	1.553823
H	0.282141	-1.399811	1.778322
H	0.994675	-0.569953	2.899479
H	2.589804	-1.984831	-2.581192
H	2.354609	-1.087611	-1.296867
H	-0.166183	4.188146	1.977646
H	-1.021372	3.647105	0.798609
H	-1.060414	-1.739025	-1.487285
H	0.388104	-2.245290	-1.710846
O	1.013185	1.078261	-2.786238
H	1.389353	0.176332	-2.807183
H	1.344347	1.521352	-3.571585

$K^+ (H_2O)_{12}$

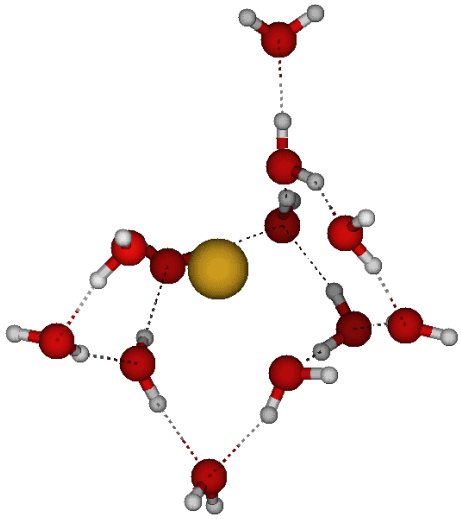

Figure S_{47} : K^+ optimized structure with 12 water molecules.

E = -944.825975

H = -944.825031

O	-1.495070	2.564605	-1.243389
O	-1.018347	4.903445	0.061212
K	0.559026	1.315126	0.386017
O	0.609908	1.396572	-2.543560
O	1.490371	-1.171791	-2.357819
O	2.754189	-0.422659	-0.205484
O	1.323226	-1.041779	1.978452
O	-0.677617	-2.665946	1.303967
O	-0.751494	-2.426485	-1.276289
O	5.489524	-0.327140	-0.247222
O	-1.699209	-0.305663	0.276180
O	-3.938622	1.151537	-0.623844
H	-0.941303	2.149230	-1.931671
H	-2.350796	2.108733	-1.224967
H	3.733288	-0.387770	-0.178957
H	2.436885	-0.840891	0.625031
H	5.971377	0.483254	-0.053381
H	6.060714	-1.046004	0.041488
H	-1.738639	-1.045026	0.906825

H	-2.594723	0.050242	0.151036
H	-4.545766	0.778736	-1.273603
H	-4.476434	1.720716	-0.060735
H	-0.612513	-2.769506	0.306371
H	-0.919244	-3.522124	1.670762
H	0.628469	-1.732299	1.826532
H	1.659520	-1.184001	2.868430
H	2.024452	-1.624493	-3.019029
H	2.078461	-0.983608	-1.568277
H	-0.835010	5.643516	-0.525430
H	-1.266741	4.150875	-0.517389
H	-1.226239	-1.597633	-1.082264
H	0.066719	-2.133561	-1.725426
H	0.878160	0.458190	-2.667027
H	1.139171	1.910252	-3.160934
O	0.991636	3.711835	1.396285
H	1.217977	4.163116	2.213570
H	0.307110	4.276553	0.963205

$K^+ (H_2O)_{13}$

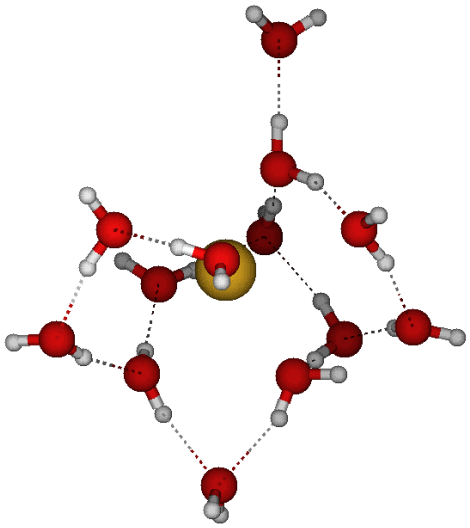

Figure S_{48} : K^+ optimized structure with 13 water molecules.

E = -1021.210956

H = -1021.210012

O	-1.558928	2.575347	-0.951923
O	-0.911082	5.010937	-0.021217
O	1.368850	4.031431	0.895319
K	0.565027	1.281845	0.592063
O	0.473204	1.469254	-2.383070
O	1.514640	-1.032728	-2.370141
O	2.813358	-0.371966	-0.215799
O	1.387428	-1.271570	1.845297
O	-0.633051	-2.857424	1.129834
O	-0.714676	-2.412298	-1.424544
O	5.556620	-0.465044	-0.273825
O	-1.649292	-0.418127	0.291689
O	-3.957481	1.056012	-0.417217
H	-1.020518	2.158813	-1.653924
H	-2.412538	2.116263	-0.912318
H	3.792881	-0.391210	-0.202780
H	2.489217	-0.868444	0.569351
H	6.087879	0.259730	0.071366

H	6.034515	-1.268364	-0.043405
H	-1.653452	-1.199329	0.871866
H	-2.555539	-0.075747	0.225324
H	-4.534075	0.723333	-1.114826
H	-4.536054	1.513910	0.203661
H	-0.576600	-2.885813	0.127012
H	-0.867759	-3.739393	1.434418
H	0.698056	-1.961086	1.679025
H	1.624284	-1.325707	2.775614
H	2.058283	-1.397491	-3.076193
H	2.112877	-0.862012	-1.581242
H	-0.946152	5.695186	-0.696379
H	-1.263057	4.190720	-0.438281
H	-1.185565	-1.601201	-1.157812
H	0.111623	-2.080386	-1.829236
H	0.791427	0.551572	-2.545181
H	0.993288	2.037300	-2.958886
H	2.090076	4.666544	0.929158
H	0.573439	4.521608	0.552698
O	0.598605	2.502178	2.998802
H	0.909366	3.267831	2.473887
H	0.095569	2.864819	3.732591

$K^+ (H_2O)_{14}$

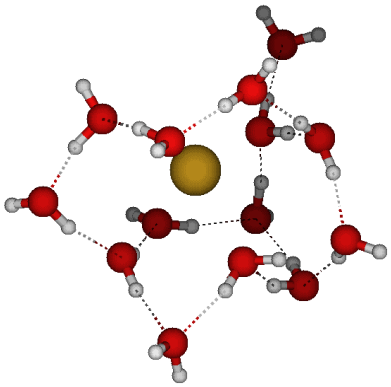

Figure S_{49} : K^+ optimized structure with 14 water molecules.

E = -1097.599949

H = -1097.599005

O	-1.399901	2.565818	-1.012053
O	-0.833599	5.006468	-0.097081
O	1.248233	4.030047	1.146328
O	0.088716	2.562189	3.021519
K	0.770145	1.286682	0.499061
O	0.557962	1.487361	-2.514911
O	1.369969	-1.078054	-2.522152
O	2.755816	-0.466576	-0.442413
O	1.859851	-1.606158	1.717813
O	-0.584174	-2.758275	1.215166
O	-0.822268	-2.332358	-1.353727
O	5.484931	-0.757423	-0.689933
O	-1.479626	-0.302899	0.463653
O	-3.797084	1.064036	-0.414794
H	-0.873647	2.166216	-1.736196
H	-2.249202	2.099638	-0.958451
H	3.732097	-0.519622	-0.509548
H	2.490030	-1.009263	0.356128
H	6.073873	-0.080379	-0.340546
H	5.816731	-1.589469	-0.335474
H	-1.479425	-1.113980	1.007026

H	-2.387470	0.033775	0.399044
H	-4.314549	0.618076	-1.095432
H	-4.433496	1.560732	0.112384
H	-0.580988	-2.823356	0.216846
H	-0.870488	-3.610386	1.558755
H	1.004886	-2.081690	1.658534
H	1.783719	-0.912989	2.403061
H	1.867976	-1.488733	-3.236614
H	2.005299	-0.928846	-1.749265
H	-0.769266	5.663697	-0.796599
H	-1.156930	4.174691	-0.520699
H	-1.184909	-1.487326	-1.031603
H	-0.019246	-2.064944	-1.844155
H	0.795898	0.542286	-2.676739
H	1.017613	1.998534	-3.187222
H	1.951772	4.663734	1.316657
H	0.521623	4.520796	0.663356
H	0.509650	3.293327	2.506696
H	-0.559708	2.953880	3.612965
O	1.942551	0.653312	3.308437
H	2.304911	0.457790	4.177661
H	1.240398	1.328442	3.440892

Mg^{2+} $(H_2O)_n$

Mg^{2+} (H_2O)

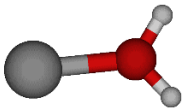

Figure S_{50} : Mg^{2+} optimized structure with 1 water molecule.

E = -275.689796

H = -275.688852

Mg	-0.096933	0.000000	0.172252
O	0.093237	0.000000	2.102208
H	0.928235	0.000000	2.614091
H	-0.625979	0.000000	2.767002

Mg^{2+} $(H_2O)_2$

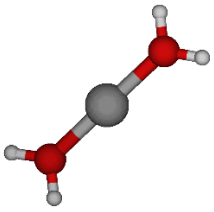

Figure S_{51} : Mg^{2+} optimized structure with 2 water molecules.

E = -352.241551

H = -352.240607

O	0.235421	0.000003	2.372084
Mg	-1.024035	-0.000002	0.870809
H	1.208446	-0.000916	2.323656
H	0.018298	0.000931	3.321844
O	-2.283637	-0.000007	-0.630247
H	-2.066538	0.002410	-1.580021
H	-3.256678	-0.002420	-0.581820

Mg^{2+} $(H_2O)_3$

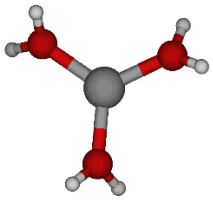

Figure S_{52} : Mg^{2+} optimized structure with 3 water molecules.

E = -428.729600

H = -428.728656

O	-0.005330	0.000782	2.053612
Mg	-0.830643	0.000640	0.247005
O	0.321185	0.007267	-1.371792
O	-2.808112	-0.009567	0.057729
H	0.782651	-0.490848	2.336666
H	-0.307685	0.491798	2.834802
H	0.185589	-0.501133	-2.187809
H	1.134633	0.519367	-1.508981
H	-3.336139	0.490161	-0.585841
H	-3.444342	-0.515047	0.589163

Mg^{2+} $(H_2O)_4$

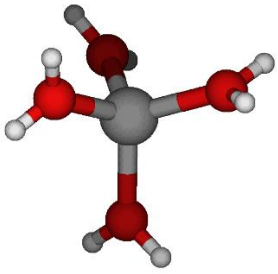

Figure S_{53} : Mg^{2+} optimized structure with 4 water molecules.

E = -505.200068

H = -505.199124

O	0.066778	-0.420516	1.981702
Mg	-0.527978	0.484285	0.278092

O	-2.522778	0.297368	0.030593
O	0.366033	-0.363578	-1.320964
H	0.523849	-1.271096	2.052723
H	-0.029251	-0.090946	2.886869
H	0.148644	-1.210160	-1.737174
H	1.094576	0.010252	-1.837607
H	-3.027536	0.426026	-0.785375
H	-3.166328	0.041190	0.707078
O	-0.020764	2.433821	0.413654
H	0.810664	2.804231	0.743371
H	-0.576140	3.190273	0.175350

Mg^{2+} $(H_2O)_5$

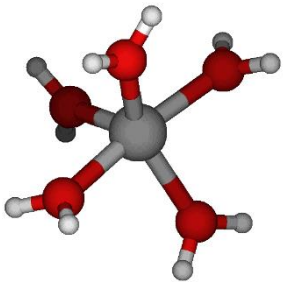

Figure S_{54} : Mg^{2+} optimized structure with 5 water molecules.

E = -581.644672

H = -581.643728

O	0.481386	-0.854822	1.673525
Mg	-0.839745	0.293184	0.610610
O	-0.299248	2.278605	0.686681
O	-2.538293	0.051393	-0.506844
O	0.276741	-0.132515	-1.112492
H	1.291049	-1.259337	1.338094
H	0.425953	-1.076749	2.611293
H	0.369387	-0.969047	-1.585914
H	0.814954	0.510629	-1.591120
H	-2.583462	-0.098292	-1.459350
H	-3.448042	0.089065	-0.186435

H	0.461300	2.653975	1.149706
H	-0.754941	3.018944	0.264817
O	-2.050351	0.372220	2.320342
H	-2.195614	1.164325	2.853143
H	-2.564080	-0.331855	2.736115

Mg^{2+} $(H_2O)_6$

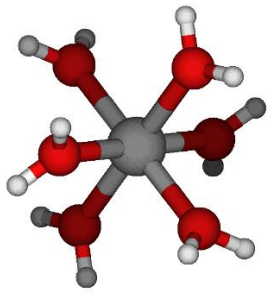

Figure S_{55} : Mg^{2+} optimized structure with 6 water molecules.

E = -658.083768

H = -658.082824

O	0.922975	-0.391707	1.665934
Mg	-0.761991	-0.000468	0.467629
O	-1.984814	-0.041067	2.182044
O	-0.453505	2.065353	0.736424
O	-2.447475	0.394393	-0.731818
O	0.458089	0.039952	-1.246530
H	1.832025	-0.487691	1.360124
H	0.930042	-0.540758	2.618244
H	0.684541	-0.708398	-1.810239
H	0.903257	0.812478	-1.613111
H	-2.453037	0.520694	-1.687364
H	-3.356312	0.503140	-0.429209
H	0.248376	2.467474	1.260656
H	-0.977239	2.785864	0.368226
H	-2.207668	0.705559	2.749454
H	-2.437059	-0.812400	2.542097
O	-1.071892	-2.067293	0.199378

H	-1.777202	-2.474956	-0.315895
H	-0.537028	-2.783487	0.559797

Mg^{2+} $(H_2O)_7$

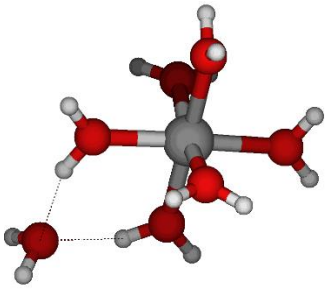

Figure S_{56} : Mg^{2+} optimized structure with 7 water molecules.

E = -734.513070

H = -734.512126

O	1.106837	-0.673579	1.600895
Mg	-0.680451	-0.242042	0.565837
O	-0.825557	-2.309635	0.126919
O	-1.604892	-0.610031	2.441514
O	-0.607459	1.802556	0.959816
O	-2.441446	0.222787	-0.454627
O	0.599885	-0.014108	-1.112143
H	1.997194	-0.619379	1.237538
H	1.185830	-0.837476	2.546735
H	0.736695	-0.668840	-1.805188
H	0.886901	0.832594	-1.469972
H	-3.074457	-0.316209	-0.936641
H	-2.751945	1.152244	-0.489725
H	0.050522	2.305570	1.448546
H	-1.299587	2.418358	0.636954
H	-1.910434	0.076138	3.044105
H	-2.052945	-1.423514	2.696827
H	-1.475458	-2.825909	-0.361634
H	-0.155929	-2.929785	0.436892
O	-2.796452	2.928132	-0.206487

H	-3.523813	3.284282	0.319243
H	-2.717966	3.511392	-0.971945

Mg^{2+} $(H_2O)_8$

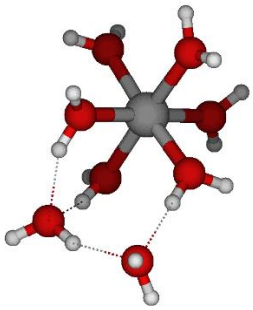

Figure S_{57} : Mg^{2+} optimized structure with 8 water molecules.

E = -810.938972

H = -810.938028

O	1.169981	-0.649274	1.640602
Mg	-0.416626	-0.300401	0.299827
O	1.042523	-0.157893	-1.224855
O	-0.568858	-2.384860	-0.023325
O	-1.706683	-0.458091	1.956925
O	-0.342141	1.771966	0.484833
O	-2.037234	0.009313	-0.985323
O	-2.919651	2.350973	0.040084
H	2.112111	-0.632132	1.442912
H	1.074522	-0.684176	2.598136
H	1.386337	-0.840829	-1.809743
H	1.317059	0.692164	-1.585328
H	-2.100943	-0.158971	-1.929739
H	-2.568817	0.811311	-0.785509
H	0.242528	2.330860	1.003723
H	-1.178512	2.257945	0.308803
H	-2.379163	0.200166	2.230533
H	-2.017254	-1.316216	2.261017
H	-1.278053	-2.831676	-0.497590

H	0.029539	-3.065320	0.302683
H	-3.387982	2.204960	0.886354
H	-3.343842	3.085408	-0.417808
O	-3.726096	1.406685	2.518273
H	-3.626724	1.979129	3.289431
H	-4.615157	1.036320	2.587467

Mg^{2+} $(H_2O)_9$

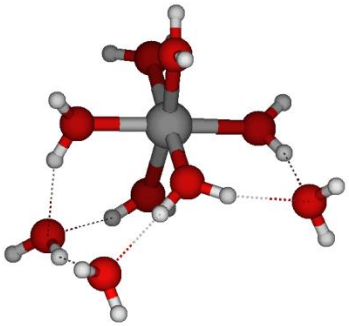

Figure S_{58} : Mg^{2+} optimized structure with 9 water molecules.

E = -887.363901

H = -887.362957

O	1.282881	-0.344659	1.547302
Mg	-0.312424	-0.200300	0.160583
O	-1.902893	0.260938	-1.116025
O	1.196782	0.187767	-1.285419
O	-0.389196	-2.232421	-0.310821
O	-1.607904	-0.618887	1.755867
O	-0.286549	1.865904	0.489449
O	-2.827696	2.530925	0.007257
O	-3.700362	1.267288	2.327636
H	2.221565	-0.376419	1.338706
H	1.179512	-0.569896	2.476729
H	1.571417	-0.318725	-2.012477
H	1.309603	1.119158	-1.505912
H	-2.211932	-0.172570	-1.914730
H	-2.420853	1.077929	-0.962554
H	0.247665	2.324273	1.143367
H	-1.111141	2.376148	0.329404
H	-2.329568	-0.015445	2.013561
H	-1.921120	-1.534245	1.869662
H	0.195900	-2.788648	-0.831287
H	-0.954139	-2.816872	0.238226
H	-3.316814	2.264369	0.810723

H	-3.240061	3.321626	-0.356773
H	-3.601822	1.750219	3.157363
H	-4.602888	0.926192	2.338439
H	-2.892008	-3.766441	1.225767
O	-2.053086	-3.386626	1.512524

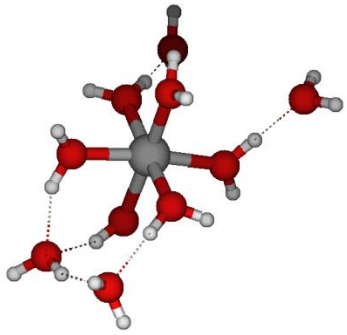

Figure S_{59} : Mg^{2+} optimized structure with 10 water molecules.

E = -963.782903

H = -963.781958

O	1.046521	-0.385676	1.608796
Mg	-0.585304	-0.184304	0.291642
O	-0.520825	1.909331	0.491308
O	-2.314992	0.162512	-0.869912
O	0.740716	-0.000642	-1.282928
O	-0.866816	-2.226933	0.104887
O	-1.796296	-0.313608	2.033998
O	0.816927	-4.190758	0.558398
O	-3.139418	2.498911	0.261661
O	-3.802988	1.542681	2.775305
H	1.961509	-0.545216	1.360434
H	0.964594	-0.536334	2.555036
H	1.158413	-0.647661	-1.909009
H	0.966733	0.882873	-1.585726
H	-2.356228	0.083993	-1.826915
H	-2.825735	0.960258	-0.615540
H	0.083875	2.422884	1.032736

H	-1.366076	2.397783	0.400412
H	-2.455315	0.323882	2.370185
H	-2.128277	-1.196209	2.223910
H	-1.596198	-2.589491	-0.404240
H	-0.222942	-2.966099	0.271732
H	-3.544754	2.333657	1.136110
H	-3.600016	3.238589	-0.148576
H	-3.646851	2.101808	3.546102
H	-4.684698	1.171289	2.901156
H	0.709655	-4.836606	1.262693
H	1.345498	-4.615983	-0.122611
O	1.911498	-1.659115	-2.969182
H	2.868734	-1.710374	-3.046828
H	1.559927	-1.883557	-3.835626

Mg^{2+} $(H_2O)_{11}$

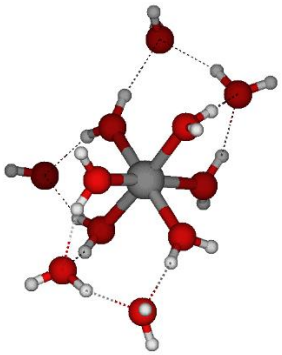

Figure S_{60} : Mg^{2+} optimized structure with 11 water molecules.

E = -1040.209120

H = -1040.208176

O	0.870003	-0.913139	1.411274
Mg	-0.807977	-0.237064	0.360552
O	-2.086676	-0.434209	2.025134
O	-0.433130	1.721005	0.994566
O	-2.390167	0.495514	-0.792129
O	0.339372	-0.198230	-1.392306
O	-1.266464	-2.293423	0.093223
O	1.251416	-3.306700	0.249055
O	2.541715	-1.992498	-1.818061
O	-2.934418	2.706505	0.808433
O	-3.746412	1.528108	3.180624
H	1.175079	-1.827407	1.234804
H	1.021667	-0.707046	2.337148
H	1.135804	-0.720549	-1.588841
H	-0.061386	0.104429	-2.226131
H	-2.242679	0.681099	-1.736811
H	-2.829696	1.269635	-0.392096
H	0.388251	2.215335	0.948586
H	-1.193403	2.338205	0.956441
H	-2.635447	0.206411	2.514365
H	-2.454307	-1.311953	2.160166

H	-1.940659	-2.647026	-0.492640
H	-0.492661	-2.894665	0.083090
H	-3.363584	2.455305	1.650476
H	-3.280193	3.566997	0.550970
H	-3.462037	1.936438	4.006914
H	-4.672211	1.290856	3.310871
H	1.556621	-4.158618	0.577465
H	1.802207	-3.057269	-0.519978
H	3.413135	-1.645882	-1.592490
H	2.640441	-2.392056	-2.690142
O	-1.361567	0.777912	-3.384662
H	-1.193727	1.640759	-3.779713
H	-1.736044	0.237027	-4.088928

Mg^{2+} $(H_2O)_{12}$

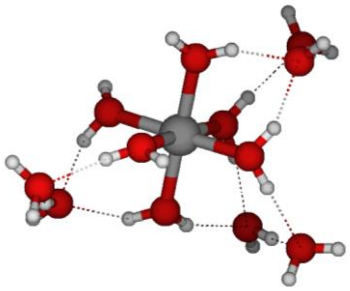

Figure S_{61} : Mg^{2+} optimized structure with 12 water molecules.

E = -1116.627456

H = -1116.626512

O	0.877808	-0.907885	1.502957
Mg	-0.798098	-0.195309	0.474288
O	-1.293996	-2.205255	0.042204
O	-2.001825	-0.403442	2.194464
O	-0.359677	1.752268	1.110326
O	-2.421519	0.546467	-0.605328
O	0.341536	-0.101821	-1.286015

O	1.283232	-3.230804	0.234572
O	-2.797716	2.861369	0.863214
O	2.695362	-1.730817	-1.619082
O	-3.560416	1.702549	3.273567
O	-1.709304	-0.224397	-3.107042
H	1.169891	-1.818818	1.288115
H	0.978396	-0.760609	2.447010
H	1.182964	-0.559420	-1.450161
H	-0.184548	-0.103514	-2.108926
H	-2.354887	0.527286	-1.578870
H	-2.764124	1.409118	-0.306952
H	0.471064	2.196964	0.924720
H	-1.092653	2.397683	1.022746
H	-2.531702	0.280616	2.644224
H	-2.466863	-1.241181	2.272483
H	-1.842801	-2.435512	-0.727933
H	-0.517050	-2.795973	0.046894
H	-3.220316	2.628754	1.713019
H	-3.096039	3.741719	0.614282
H	-3.209197	2.112894	4.072723
H	-4.487876	1.517303	3.461987
H	1.599585	-4.089906	0.531221
H	1.872855	-2.917768	-0.479877
H	3.499448	-1.337666	-1.260160
H	2.927783	-2.027032	-2.506529
H	-1.824358	0.141829	-3.989092
H	-2.110341	-1.114725	-3.089047
O	-2.795336	-2.683437	-2.371663
H	-2.634998	-3.506901	-2.846696
H	-3.749168	-2.647045	-2.235129

Mg^{2+} $(H_2O)_{13}$

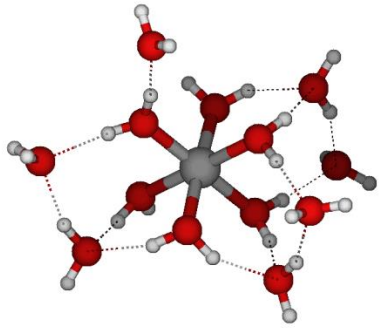

Figure S_{62} : Mg^{2+} optimized structure with 13 water molecules.

E = -1193.040638

H = -1193.039694

O	0.856407	-0.983944	1.454110
Mg	-0.829916	-0.265815	0.439375
O	0.380933	-0.038186	-1.287637
O	-1.257983	-2.240365	-0.166584
O	-1.971774	-0.434202	2.164382
O	-0.400610	1.714427	1.047083
O	-2.430451	0.502681	-0.679756
O	1.337750	-3.230069	0.056976
O	-2.833893	2.835316	0.740530
O	-1.592497	-0.106553	-3.199375
O	2.791960	-1.595748	-1.636704
O	-3.519210	1.802274	3.187816
O	-2.728319	-2.578692	-2.634545
H	1.162965	-1.879903	1.204060
H	0.882594	-0.898402	2.410694
H	1.234998	-0.471978	-1.445258
H	-0.118216	-0.018345	-2.126441
H	-2.311174	0.537784	-1.646608
H	-2.782494	1.355845	-0.362540
H	0.420929	2.137738	0.786060
H	-1.131811	2.355961	0.927589

H	-2.468834	0.292755	2.571878
H	-2.362929	-1.269194	2.504369
H	-1.794599	-2.425285	-0.955778
H	-0.472537	-2.816541	-0.186111
H	-3.236190	2.626504	1.607986
H	-3.138911	3.706914	0.471341
H	-3.151277	2.248478	3.958859
H	-4.430566	1.588504	3.417231
H	1.664544	-4.100379	0.304065
H	1.945311	-2.855531	-0.611324
H	3.567776	-1.205114	-1.218383
H	3.067775	-1.824546	-2.531344
H	-1.680902	0.307373	-4.062969
H	-1.995603	-0.995162	-3.241398
H	-2.589764	-3.380693	-3.150678
H	-3.681335	-2.515368	-2.503682
O	-3.114510	-2.579750	3.310015
H	-3.734163	-3.205909	2.928439
H	-2.879581	-2.922854	4.176114

Mg^{2+} $(H_2O)_{14}$

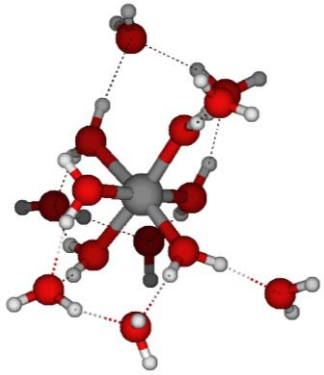

Figure S_{63} : Mg^{2+} optimized structure with 14 water molecules.

E = -1269.453504

H = -1269.452560

O	0.712838	-0.943827	1.476179
Mg	-0.948572	-0.245714	0.472267
O	-2.512286	0.457097	-0.774682
O	0.319201	0.055776	-1.237982
O	-1.295330	-2.218306	-0.175316
O	-2.256422	-0.359510	2.069953
O	-0.552210	1.767542	1.002642
O	-3.475336	-2.465674	3.213506
O	1.244856	-3.239201	0.054659
O	-3.016530	2.823913	0.583447
O	-1.543152	-0.133315	-3.256848
O	-3.869514	1.866476	3.009379
O	2.731042	-1.544519	-1.560063
O	-2.684802	-2.597484	-2.698201
H	1.035853	-1.834377	1.259482
H	1.014188	-0.705815	2.380794
H	1.165012	-0.408368	-1.343433
H	-0.145302	0.033473	-2.095686
H	-2.334235	0.500375	-1.731732
H	-2.897595	1.303248	-0.482041
H	0.222082	2.155889	0.586701

H	-1.307184	2.374299	0.857761
H	-2.739434	0.378744	2.470162
H	-2.650197	-1.186566	2.423264
H	-1.802664	-2.412470	-0.979542
H	-0.499202	-2.784047	-0.167430
H	-3.469402	2.634644	1.430136
H	-3.313276	3.684827	0.274418
H	-3.585368	2.337935	3.800102
H	-4.784550	1.610004	3.168012
H	1.570548	-4.114068	0.283910
H	1.865770	-2.839539	-0.583893
H	3.499908	-1.170856	-1.115315
H	3.019739	-1.738213	-2.458621
H	-1.607750	0.260600	-4.131477
H	-1.926125	-1.030801	-3.294503
H	-2.542009	-3.413949	-3.189536
H	-3.639356	-2.520960	-2.589999
H	-4.062704	-3.092548	2.784822
H	-3.206359	-2.869970	4.042032
O	1.701221	-0.382920	3.903371
H	2.353717	0.298210	4.082899
H	1.445857	-0.747755	4.753695

Mg^{2+} $(H_2O)_{15}$

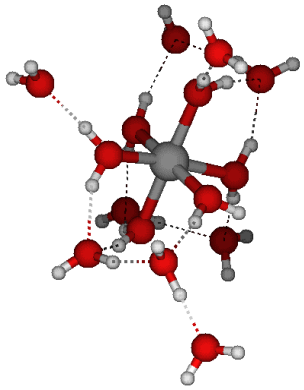

Figure S_{64} : Mg^{2+} optimized structure with 15 water molecules.

E = -1345.871105

H = -1345.870161

O	1.168063	-0.910206	1.133455
Mg	-0.636130	-0.374667	0.277453
O	-0.563037	1.592821	0.883548
O	-2.426756	0.039303	-0.774621
O	0.358656	-0.136742	-1.573242
O	-0.923785	-2.453700	-0.183730
O	-1.796551	-0.851364	1.974555
O	2.017528	-0.530743	3.649200
O	-6.031007	-0.016306	3.859401
O	-3.248705	2.152615	0.734953
O	-1.686509	-0.511837	-3.356125
O	-3.655661	0.867201	3.079578
O	1.707048	-3.244039	-0.228073
O	-2.487452	-3.049690	-2.571656
O	2.895439	-1.473111	-2.001642
H	1.507253	-1.794818	0.915836
H	1.431205	-0.703839	2.057380
H	1.239554	-0.497729	-1.758160
H	-0.189365	-0.212892	-2.376599
H	-2.365392	0.111261	-1.742928
H	-2.901391	0.815723	-0.415249

H	0.168683	2.235123	0.759349
H	-1.409596	2.071963	0.841842
H	-2.461339	-0.287903	2.422972
H	-2.140760	-1.747095	1.926627
H	-1.466066	-2.696322	-0.951728
H	-0.080665	-2.943144	-0.246682
H	-3.549294	1.787595	1.597979
H	-3.771610	2.934256	0.538848
H	-3.311793	1.342416	3.842356
H	-4.544187	0.520483	3.350014
H	2.135965	-4.072147	0.004620
H	2.225035	-2.818626	-0.937489
H	3.616541	-0.989306	-1.584168
H	3.190780	-1.662079	-2.898873
H	-1.882447	-0.167982	-4.231973
H	-1.982827	-1.440973	-3.315920
H	-2.305053	-3.872797	-3.037951
H	-3.426302	-3.073864	-2.356147
H	-6.860252	0.452788	3.736465
H	-6.192255	-0.688288	4.526557
H	2.790786	-0.036531	3.930775
H	1.600621	-0.868511	4.444921
O	1.355079	3.452818	0.557612
H	1.734450	3.978217	1.266067
H	1.551847	3.914313	-0.260805

Mg^{2+} $(H_2O)_{16}$

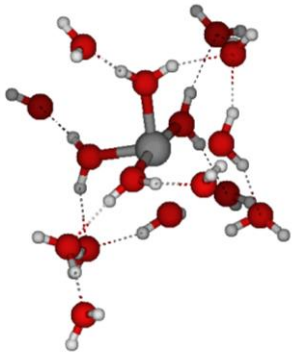

Figure S_{65} : Mg^{2+} optimized structure with 16 water molecules.

E = -1422.281981

H = -1422.281037

O	1.119784	-0.938000	1.272214
Mg	-0.671580	-0.443768	0.383906
O	-1.896909	-0.710697	2.023296
O	-0.601877	1.584021	0.755908
O	-2.465416	-0.057700	-0.827641
O	0.348935	-0.328212	-1.470307
O	-0.890910	-2.600519	-0.046847
O	1.981894	-0.469513	3.761620
O	1.326712	3.426482	0.396958
O	-3.307446	2.084131	0.567525
O	-3.744900	1.151794	3.023290
O	-6.121570	0.271709	3.795490
O	-1.573748	-0.480352	-3.376820
O	1.768090	-3.210718	-0.166318
O	2.932812	-1.511664	-2.006817
O	-2.809954	-2.495366	-1.999803
H	1.521488	-1.788481	1.029546
H	1.395882	-0.711593	2.188143
H	1.264666	-0.595181	-1.642255
H	-0.149159	-0.351007	-2.309756
H	-2.257791	0.188009	-1.748308

H	-2.948030	0.693989	-0.409610
H	0.133005	2.218394	0.611956
H	-1.446891	2.062261	0.702950
H	-2.498293	-0.069797	2.444076
H	-2.223350	-1.621414	2.216365
H	-1.456334	-2.764724	-0.829373
H	-0.003348	-2.983911	-0.209406
H	-3.603540	1.836826	1.477807
H	-3.844557	2.821721	0.266169
H	-3.435866	1.692833	3.756026
H	-4.630046	0.797871	3.294471
H	2.189801	-4.048605	0.044339
H	2.279670	-2.785420	-0.881719
H	3.711700	-1.043388	-1.687103
H	3.124624	-1.748657	-2.920688
H	-1.695115	-0.171404	-4.278714
H	-2.010589	-1.347186	-3.282113
H	-3.494851	-3.153314	-2.154201
H	-3.189595	-1.777142	-1.463232
H	-6.924797	0.797540	3.825717
H	-6.304160	-0.539316	4.276126
H	2.771073	0.014565	4.015480
H	1.539754	-0.723320	4.574771
H	1.717837	3.933865	1.112213
H	1.510368	3.909543	-0.412100
O	-2.566784	-3.258676	2.080596
H	-2.480908	-3.952178	2.738521
H	-1.924583	-3.429759	1.374165

Mg^{2+} $(H_2O)_{17}$

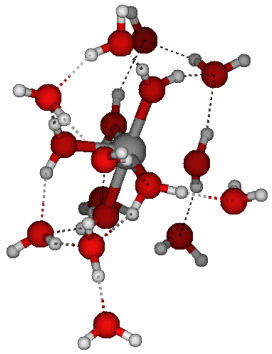

Figure S_{66} : Mg^{2+} optimized structure with 17 water molecules.

E = -1498.701503

H = -1498.700559

O	1.185264	-1.037217	0.983786
Mg	-0.604689	-0.563845	0.133760
O	0.287743	-0.584313	-1.776116
O	-1.730019	-0.728389	1.963750
O	-0.488987	1.482646	0.445867
O	-2.439569	-0.183313	-0.949627
O	-0.859075	-2.731411	-0.164713
O	-2.130772	-3.278745	2.222494
O	2.385812	0.388432	2.801273
O	-3.145263	2.102518	0.233636
O	-3.628339	1.124720	2.622298
O	-6.014030	0.928289	3.778324
O	0.715353	2.539531	2.661026
O	-1.773891	-0.728875	-3.534707
O	-2.901783	-2.723219	-2.011086
O	1.798372	-3.307302	-0.462203
O	2.886058	-1.623974	-2.386109
H	1.613806	-1.876402	0.753564
H	1.709915	-0.550142	1.674114
H	1.216337	-0.758789	-1.993377
H	-0.240402	-0.581853	-2.595003

H	-2.289217	-0.063835	-1.908687
H	-2.877234	0.636120	-0.613158
H	0.045535	1.943896	1.124598
H	-1.322607	1.975819	0.330456
H	-2.573198	-0.235547	2.068645
H	-1.904717	-1.676933	2.217353
H	-1.480331	-2.925053	-0.896441
H	0.023898	-3.093297	-0.395398
H	-3.462964	1.881314	1.147680
H	-3.649257	2.849009	-0.101260
H	-3.011869	1.422015	3.312240
H	-4.521859	1.024071	3.033668
H	2.232329	-4.146425	-0.282984
H	2.268082	-2.878898	-1.204033
H	3.670124	-1.132942	-2.116962
H	3.040631	-1.882723	-3.301249
H	-1.978681	-0.411183	-4.418688
H	-2.184344	-1.603652	-3.412991
H	-3.559230	-3.416306	-2.129695
H	-3.309649	-2.007998	-1.497842
H	-6.583226	1.671883	3.991619
H	-6.461766	0.139372	4.092949
H	2.014134	1.290332	2.809632
H	3.304174	0.433103	3.074109
H	0.039983	2.207912	3.294750
H	0.872069	3.471610	2.837389
H	-1.950951	-3.939636	2.894902
H	-1.627204	-3.498349	1.422278
H	-1.105675	0.317237	3.428684
O	-1.156390	1.120895	3.984088
H	-1.013124	0.850585	4.896414

Mg^{2+} $(H_2O)_{18}$

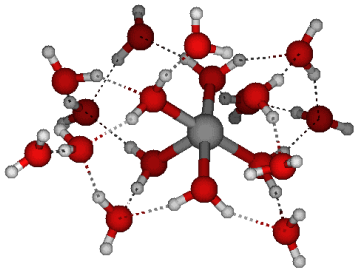

Figure S_{67} : Mg^{2+} optimized structure with 18 water molecules.

E = -1575.114696

H = -1575.113752

O	1.279530	-0.912325	0.881548
Mg	-0.620650	-0.536490	0.095318
O	-2.488199	-0.156996	-0.897406
O	0.186469	-0.584708	-1.836257
O	-1.673419	-0.696637	1.976901
O	-0.460025	1.507371	0.449365
O	-0.868917	-2.708731	-0.123341
O	-2.113483	-3.238284	2.272079
O	1.999004	0.111805	3.155502
O	-3.102893	2.175456	0.255607
O	-3.635986	1.114625	2.598843
O	-6.074985	0.836314	3.620956
O	-1.973677	-0.745229	-3.495518
O	0.679760	2.457963	2.777050
O	-1.251953	1.125688	4.076441
O	1.748989	-3.272395	-0.392470
O	-2.963660	-2.783120	-1.925965
O	2.661092	-1.648892	-2.284031
H	1.619902	-1.807860	0.680820
H	1.571549	-0.630381	1.793961
H	1.069134	-0.906403	-2.113409
H	-0.398102	-0.578117	-2.614974
H	-2.403816	-0.091532	-1.870404

H	-2.897335	0.682402	-0.578776
H	0.034921	1.918977	1.186241
H	-1.287921	2.010743	0.327871
H	-2.520832	-0.205956	2.062250
H	-1.857624	-1.641835	2.235263
H	-1.497136	-2.913481	-0.845858
H	0.010682	-3.093175	-0.344228
H	-3.435512	1.937034	1.159377
H	-3.598220	2.930331	-0.073459
H	-3.063955	1.405377	3.328640
H	-4.546339	0.979586	2.960352
H	2.224392	-4.078814	-0.173466
H	2.183397	-2.860420	-1.179509
H	3.195001	-0.982933	-1.770303
H	3.104348	-1.826752	-3.118379
H	-2.195772	-0.440097	-4.379786
H	-2.340383	-1.637529	-3.368807
H	-3.565416	-3.525154	-2.046049
H	-3.430140	-2.107910	-1.412702
H	-6.672453	1.564675	3.808099
H	-6.509817	0.037618	3.928969
H	1.778719	1.062460	3.119570
H	2.830134	0.003909	3.623574
H	-0.046120	2.192932	3.386467
H	0.906247	3.376454	2.950433
H	-1.950537	-3.906900	2.941131
H	-1.632267	-3.474776	1.463042
H	-1.144184	0.320954	3.532544
H	-1.129160	0.871827	4.996485
H	2.817698	0.105931	0.008104
O	3.586126	0.066714	-0.579640
H	3.924638	0.956688	-0.701832

Mg^{2+} $(H_2O)_{19}$

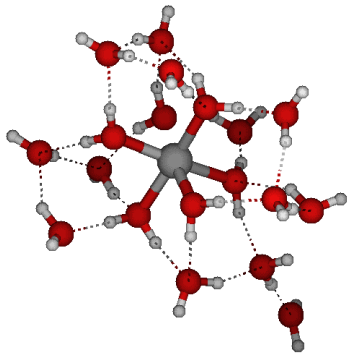

Figure S_{68} : Mg^{2+} optimized structure with 19 water molecules.

E = -1651.526333

H = -1651.525389

O	1.264669	-0.944361	1.029714
Mg	-0.551825	-0.343551	0.172611
O	-0.284464	1.634152	0.778906
O	-2.289943	0.350170	-0.864338
O	0.389393	-0.370578	-1.711823
O	-1.676102	-0.646114	2.006436
O	-0.974922	-2.465776	-0.236709
O	1.891976	-0.257957	3.464065
O	-2.265895	-3.177487	2.080380
O	-2.931020	2.385100	0.765250
O	-3.570414	1.085735	2.948621
O	-6.034421	0.748731	3.881607
O	1.621308	-3.210469	-0.428270
O	2.885979	-1.489022	-2.004864
O	3.798116	-0.051510	-0.051227
O	-1.151570	-0.952829	-3.950331
O	0.823885	2.227493	3.246524
O	-1.176105	0.833434	4.368054
O	-2.886587	-1.984171	-2.117613
H	1.530874	-1.847091	0.757054
H	1.491745	-0.799867	1.989842

H	1.312992	-0.651987	-1.871316
H	-0.086479	-0.524555	-2.551291
H	-2.116453	0.853303	-1.717950
H	-2.766898	1.007657	-0.306534
H	0.213906	1.916983	1.571559
H	-1.113169	2.151861	0.756156
H	-2.495343	-0.133844	2.188748
H	-1.902490	-1.602564	2.169307
H	-1.607521	-2.538346	-0.982750
H	-0.123858	-2.890505	-0.484617
H	-3.291776	2.061434	1.630075
H	-3.405427	3.180718	0.509350
H	-2.999908	1.251172	3.717112
H	-4.491893	0.933385	3.273533
H	2.009244	-4.071367	-0.247553
H	2.171960	-2.763046	-1.116484
H	3.425363	-0.937059	-1.376231
H	3.387419	-1.609979	-2.815964
H	-0.912218	-1.359006	-4.787922
H	-1.860839	-1.487613	-3.539313
H	-3.735712	-2.422883	-2.227860
H	-3.034034	-1.133652	-1.652222
H	-6.613631	1.461072	4.163554
H	-6.511323	-0.070796	4.032410
H	1.779335	0.711358	3.503521
H	2.687393	-0.495707	3.946459
H	0.064886	1.941457	3.803713
H	1.100549	3.103386	3.531618
H	-2.161821	-3.924124	2.674099
H	-1.813942	-3.369872	1.243938
H	-1.092270	0.112666	3.714618
H	-1.030084	0.449163	5.238149
H	2.979745	0.004629	0.462761
H	4.228489	0.806485	-0.041032

H	-1.620606	2.325386	-3.421986
O	-2.031402	1.494482	-3.173404
H	-1.716022	0.802422	-3.781160

Ca^{2+} $(H_2O)_n$

Ca^{2+} (H_2O)

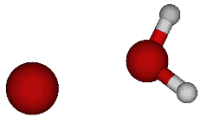

Figure S_{69} : Ca^{2+} optimized structure with 1 water molecule.

E = -112.612598

H = -112.611654

Ca	-0.110102	0.000000	-0.168444
O	0.099127	0.000000	2.038626
H	0.922431	0.000000	2.563995
H	-0.612895	0.000000	2.707177

Ca^{2+} $(H_2O)_2$

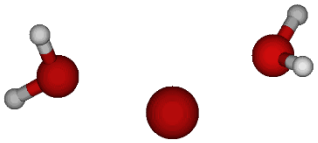

Figure S_{70} : Ca^{2+} optimized structure with 2 water molecules.

E = -189.066054

H = -189.065109

O	0.071916	-0.118496	2.257343
Ca	0.010969	0.065782	0.007284
H	0.827750	-0.374374	2.815807
H	-0.656649	0.025148	2.887664
O	0.793309	1.750540	-1.270898
H	0.847341	1.789615	-2.242717
H	1.150882	2.606493	-0.974372

Ca^{2+} $(H_2O)_3$

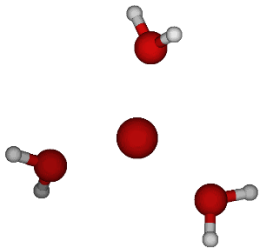

Figure S_{71} : Ca^{2+} optimized structure with 3 water molecules.

E = -265.509450

H = -265.508506

O	0.070970	-0.091605	2.231442
Ca	-0.065735	-0.067463	-0.052560
O	0.854995	1.669168	-1.223354
H	0.815782	0.195859	2.785631
H	-0.602565	-0.392252	2.864267
H	1.324292	1.630874	-2.073551
H	0.863334	2.610569	-0.982101
O	-1.114714	-1.786464	-1.138263
H	-1.695437	-1.733192	-1.915760
H	-1.078841	-2.733943	-0.924871

Ca^{2+} $(H_2O)_4$

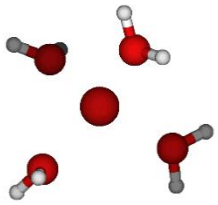

Figure S_{72} : Ca^{2+} optimized structure with 4 water molecules.

E = -341.942811

H = -341.941867

O	0.668360	-0.585933	2.217080
Ca	-0.345441	0.244725	0.309396
O	-1.132530	-1.588136	-0.865283
O	1.154558	1.466606	-0.961431
H	1.526879	-0.329069	2.588486

H	0.337098	-1.276574	2.812155
H	1.584911	1.196629	-1.787804
H	1.479426	2.365165	-0.794472
H	-2.004867	-1.695674	-1.275713
H	-0.670099	-2.422063	-1.042904
O	-2.075513	1.684709	0.850837
H	-2.530549	2.311507	0.266982
H	-2.494400	1.803904	1.717612

Ca^{2+} $(H_2O)_5$

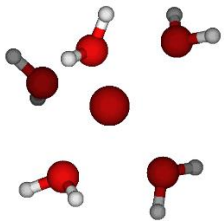

Figure S_{73} : Ca^{2+} optimized structure with 5 water molecules.

E = -418.361494

H = -418.360550

O	1.069265	-1.141286	1.772823
Ca	-0.429588	0.391904	0.759809
O	1.082261	1.510222	-0.632798
O	-1.250927	-1.399195	-0.505573
O	-2.408820	1.569320	0.196021
H	2.018644	-1.213419	1.597477
H	0.883720	-1.819676	2.438168
H	1.324930	1.281552	-1.542160
H	1.599756	2.301693	-0.423310
H	-2.023809	-1.400586	-1.088002
H	-0.888827	-2.295117	-0.558217
H	-2.481351	2.297160	-0.438245
H	-3.306874	1.438915	0.533443
O	-0.418629	1.580721	2.777414
H	0.155972	1.433855	3.542159
H	-0.987933	2.323586	3.023592

Ca^{2+} $(H_2O)_6$

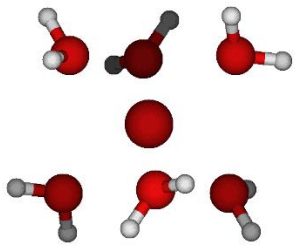

Figure S_{74} : Ca^{2+} optimized structure with 6 water molecules.

E = -494.774601

H = -494.773657

O	1.402221	-0.974673	1.916354
Ca	-0.160194	0.213458	0.560362
O	1.424673	1.971645	0.269438
O	-1.747696	-1.542671	0.851039
O	-1.006707	1.309247	2.502370
O	-1.722141	1.401326	-0.796102
H	2.298115	-0.701232	2.155200
H	1.270968	-1.831727	2.343772
H	2.091489	2.051149	-0.425909
H	1.536907	2.754100	0.825848
H	-2.412965	-1.622357	1.547858
H	-1.862111	-2.324324	0.293946
H	-1.590344	2.257643	-1.224824
H	-2.618524	1.128468	-1.033780
H	-0.708416	1.194912	3.414726
H	-1.720755	1.959579	2.543573
O	0.688521	-0.883766	-1.379606
H	0.391661	-0.769984	-2.292502
H	1.401845	-1.534990	-1.419200

Ca^{2+} $(H_2O)_7$

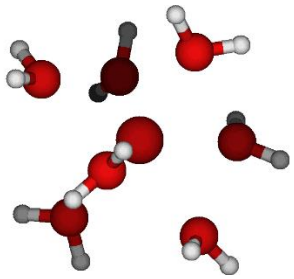

Figure S_{75} : Ca^{2+} optimized structure with 7 water molecules.

E = -571.161906

H = -571.166962

O	1.567735	-0.782605	2.129744
Ca	-0.147251	-0.157993	0.567728
O	1.087722	1.902202	0.324773
O	1.304564	-0.493650	-1.436651
O	-2.163819	-1.082350	1.521855
O	-0.925316	1.294420	2.453566
O	-1.649161	0.785743	-1.054255
H	2.304263	-0.251560	2.457855
H	1.718171	-1.675068	2.466848
H	1.734304	2.107524	-0.361320
H	1.041295	2.681544	0.891666
H	-2.542435	-0.626650	2.283695
H	-2.755057	-1.819220	1.326267
H	-1.562295	1.621207	-1.530319
H	-2.532363	0.456185	-1.264349
H	-0.581686	1.267617	3.355845
H	-1.541791	2.037659	2.432992
H	1.023324	-0.376034	-2.353091
H	2.246654	-0.702066	-1.478832
O	-0.106115	-2.508710	0.014243
H	0.393508	-2.789986	-0.761969
H	-0.482244	-3.310307	0.397386

Ca^{2+} $(H_2O)_8$

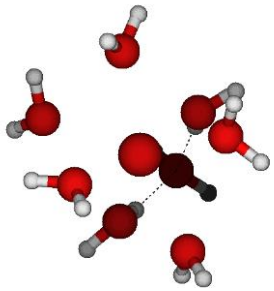

Figure S_{76} : Ca^{2+} optimized structure with 8 water molecules.

E = -647.570531

H = -647.569857

O	1.014267	0.143531	2.009778
Ca	-0.274475	0.236860	0.018054
O	-1.384732	0.095041	-2.110468
O	1.184312	2.054845	-0.610490
O	-1.975597	-0.094830	1.799248
O	-0.727182	-2.136869	-0.195152
O	1.616088	-0.892912	-1.180015
O	-0.591527	-0.487191	4.162292
H	1.855435	0.576757	2.193052
H	0.628963	-0.110015	2.874970
H	1.960627	2.050925	-1.182548
H	1.085490	2.962620	-0.298999
H	-1.665721	-0.275231	2.712577
H	-2.880197	-0.424794	1.744367
H	-1.673671	0.787303	-2.717683
H	-1.786940	-0.723043	-2.427668
H	-0.536163	-1.349171	4.597199
H	-0.690577	0.155650	4.878204
H	1.728729	-0.941019	-2.137798
H	2.461547	-1.168581	-0.803849
H	-0.006819	-2.661564	-0.565815
H	-1.327574	-2.757913	0.233014
O	-1.556282	2.250436	0.402774
H	-1.844308	3.062347	-0.030337

H	-2.159410	2.096372	1.141671

Ca^{2+} $(H_2O)_9$

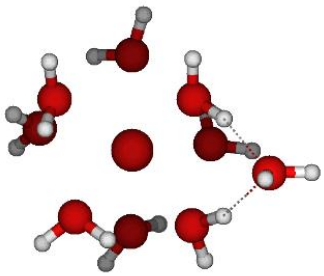

Figure S_{77} : Ca^{2+} optimized structure with 9 water molecules.

E = -723.960264

H = -723.959320

O	1.022596	-0.098044	1.844940
Ca	-0.560186	-0.031821	0.038309
O	-0.522187	0.510575	-2.420405
O	0.812990	2.012053	-0.561191
O	-1.727266	2.155682	0.423427
O	-0.782748	-2.518293	0.142528
O	-1.856875	0.082794	2.178223
O	1.194866	-1.253482	-1.289670
O	-0.173431	-0.127122	4.347140
H	1.982314	-0.023871	1.814422
H	0.774643	-0.143473	2.791171
H	1.740402	2.275990	-0.532067
H	0.310535	2.716861	-0.127284
H	-1.442678	-0.002315	3.063274
H	-2.724019	-0.337019	2.228269
H	-0.069123	1.365256	-2.466751
H	-1.142329	0.472823	-3.158393
H	-0.143340	-0.906849	4.917990
H	-0.064060	0.629677	4.939094
H	1.020404	-0.930877	-2.186904
H	2.121318	-1.520743	-1.259677
H	-0.058274	-2.813232	-0.428252

H	-0.879080	-3.184375	0.833341
H	-2.356325	2.740465	-0.015960
H	-2.095081	1.950460	1.297533
O	-2.766205	-0.825978	-0.622519
H	-2.741812	-1.790278	-0.686518
H	-3.559927	-0.529086	-1.08166

Ca^{2+} $(H_2O)_{10}$

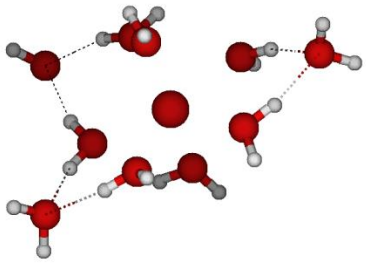

Figure S_{78} : Ca^{2+} optimized structure with 10 water molecules.

E = -800.370142

H = -800.369198

O	1.231045	-0.159156	1.829531
Ca	-0.352422	-0.076059	0.027586
O	-4.290729	0.042772	1.810345
O	-0.760213	-2.435328	-0.123218
O	-1.628746	-0.877982	1.981894
O	-2.598340	0.847909	-0.220127
O	1.763197	-0.103401	-1.121679
O	1.343282	0.587512	-3.780346
O	-0.248310	2.315856	0.098042
O	0.069293	-0.904618	4.220482
H	2.123267	0.200530	1.864447
H	0.984452	-0.398291	2.746471
H	0.389277	3.017720	0.267704
H	-1.122424	2.722047	0.045912
H	-1.223555	-0.926278	2.868431
H	-2.566293	-0.632628	2.099134
H	1.488056	1.496830	-4.073861

H	1.658341	0.030698	-4.504812
H	0.317633	-1.740541	4.636954
H	-0.002933	-0.267224	4.942980
H	1.817538	0.143601	-2.066971
H	2.593381	-0.535208	-0.895130
H	-0.400002	-3.245708	-0.499591
H	-1.220083	-2.668552	0.694998
H	-2.930508	0.895197	-1.123984
H	-3.355781	0.664871	0.371101
H	-5.003206	-0.592938	1.662055
H	-4.659834	0.706858	2.407324
O	-0.955443	-0.093894	-2.358288
H	-1.410818	-0.849488	-2.746903
H	-0.286661	0.186151	-3.015349

$Ca(H_2O)_{11}$

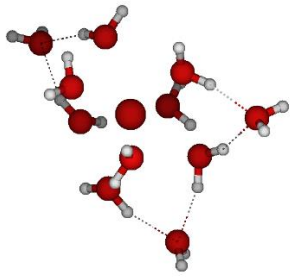

Figure S_{79} : Ca^{2+} optimized structure with 11 water molecules.

E = -876.752275

H = -816.751331

O	1.197283	-0.140257	2.026511
Ca	-0.425822	0.391289	0.335971
O	0.611076	2.476420	-0.298063
O	-0.648070	-2.015994	-0.338587
O	1.732471	0.201683	-1.097691
O	-2.815768	0.921754	0.052614
O	-1.187517	0.174144	-2.032023
O	-1.683040	-1.210899	1.930016
O	-0.019728	-1.397214	4.177998

O	-4.433504	-0.678820	1.654191
O	1.007716	0.335538	-3.798555
H	2.063684	0.246873	2.189526
H	0.908539	-0.552440	2.866933
H	1.436557	2.253885	-0.749773
H	0.503456	3.432880	-0.311316
H	-1.300502	-1.346937	2.817759
H	-2.648248	-1.097767	2.028279
H	1.227216	1.141536	-4.284284
H	1.129385	-0.381778	-4.434520
H	0.298598	-2.263245	4.465510
H	-0.194149	-0.903577	4.989971
H	1.624896	0.161183	-2.070241
H	2.538681	-0.283446	-0.889886
H	-0.038023	-2.735636	-0.533067
H	-1.107090	-2.237199	0.494387
H	-2.998894	0.983630	-0.894138
H	-3.549627	0.430197	0.471018
H	-4.981972	-1.389905	1.297459
H	-4.983232	-0.242136	2.318005
H	-1.336066	-0.782482	-2.032467
H	-0.607877	0.344949	-2.797546
O	-1.261536	1.991004	2.002782
H	-2.099055	2.316502	1.647070
H	-0.851210	2.721424	2.477958

Ca^{2+} $(H_2O)_{12}$

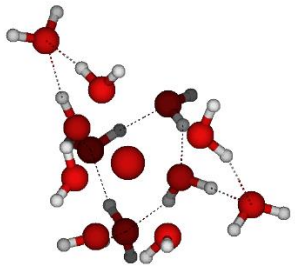

Figure S_{80} : Ca^{2+} optimized structure with 12 water molecules.

E = -953.151672

H = -953.150728

O	1.559935	-0.102841	1.874752
Ca	-0.161185	0.791625	0.495404
O	0.322611	3.079655	-0.059059
O	-0.653806	1.779161	2.808106
O	-2.479341	1.633838	0.801425
O	-0.979569	0.023817	-1.553248
O	-1.287247	-3.281598	-0.367384
O	-1.276624	-1.151679	1.525033
O	1.788825	1.001662	-1.038154
O	-0.083163	-0.717227	3.934834
O	-3.842656	-0.648033	0.852028
O	1.076802	-0.011256	-3.482603
H	2.421535	-0.511965	1.745903
H	1.222107	-0.407547	2.744705
H	1.064913	3.027807	-0.677263
H	0.068112	4.006024	0.011492
H	-0.993070	-1.238820	2.460343
H	-2.259868	-1.100989	1.506823
H	1.039220	0.563144	-4.258853
H	1.439179	-0.850234	-3.796322
H	-0.002747	-1.127916	4.804582
H	-0.402233	0.192870	4.056324
H	1.695778	0.662169	-1.955893
H	2.726710	0.955301	-0.820883

H	-1.351435	-4.214446	-0.134125
H	-1.125492	-2.783771	0.453308
H	-2.842628	2.322718	0.232299
H	-3.150047	0.904232	0.820067
H	-3.787171	-1.076944	-0.042210
H	-4.705735	-0.845457	1.234764
H	-1.771845	-0.551496	-1.657968
H	-0.432809	-0.078396	-2.352632
H	-1.551780	2.054259	2.552034
H	-0.208220	2.563419	3.153062
O	-3.066810	-1.723714	-1.434821
H	-3.597747	-2.033878	-2.178164
H	-2.488896	-2.479677	-1.121276

Ca^{2+} $(H_2O)_{13}$

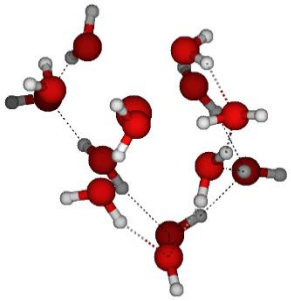

Figure S_{81} : Ca^{2+} optimized structure with 13 water molecules.

E = -1029.541242

H = -1029.540298

O	1.615711	-0.021352	2.107070
Ca	-0.009562	0.504883	0.436544
O	-1.062718	0.162647	-1.687907
O	0.412064	2.853108	-0.025447
O	-1.389368	-1.201487	1.687468
O	-2.312225	1.555491	0.671578
O	1.909849	1.075673	-1.282975
O	-0.674117	1.781263	2.754331
O	-3.865044	-0.622916	0.765226
O	-2.912062	-1.898419	-1.422886
O	-1.136264	-3.327168	0.056967
O	-0.288286	-0.543227	4.043207
O	0.780793	0.768302	-3.782393
H	2.118951	-0.807934	1.862664
H	1.214632	-0.220344	2.976548
H	1.185809	2.747391	-0.603285
H	0.423414	3.750174	0.323292
H	-1.116852	-1.154615	2.636004
H	-2.358154	-1.042244	1.629950
H	0.586580	1.581959	-4.266617
H	1.099951	0.146841	-4.449818
H	-0.328912	-0.828646	4.963841
H	-0.576952	0.388838	3.990965

H	1.697579	0.976042	-2.235685
H	2.868612	1.023975	-1.193189
H	-1.148771	-4.260743	0.302161
H	-1.280760	-2.792716	0.870698
H	-2.494593	2.198147	-0.024208
H	-3.056038	0.907796	0.666564
H	-3.759169	-1.119139	-0.080766
H	-4.771849	-0.735638	1.074083
H	-1.743675	-0.533856	-1.789913
H	-0.596605	0.259954	-2.536188
H	-1.508396	2.022967	2.309194
H	-0.264203	2.599055	3.059873
H	-3.430156	-2.308353	-2.126482
H	-2.347360	-2.600754	-1.022318
O	1.025324	-1.672421	-0.147946
H	0.403177	-2.430674	-0.175391
H	1.626415	-1.786276	-0.890801

Ca^{2+} $(H_2O)_{14}$

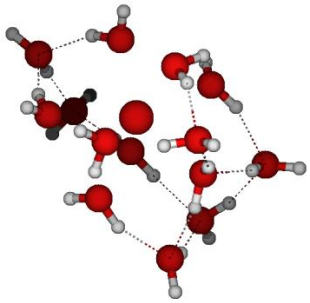

Figure S_{82} : Ca^{2+} optimized structure with 14 water molecules.

E = -1105.937346

H = -1105.936401

O	1.371361	-0.208504	2.693035
Ca	0.078279	0.403796	0.763622
O	-0.660189	-0.027674	-1.487216
O	0.196350	2.740320	-0.071679
O	1.067967	-1.848677	0.465756
O	-1.565367	-1.228595	1.865810

O	-2.220646	1.498524	0.718604
O	2.052202	2.488791	-2.056563
O	-0.814946	1.888227	2.916516
O	-3.848827	-0.615397	0.524053
O	-0.837010	-0.429434	4.326936
O	-1.146960	-3.439671	0.384657
O	-2.585093	-2.032866	-1.410947
O	0.645124	0.972046	-3.883067
H	1.705217	-1.085648	2.458433
H	0.849985	-0.328958	3.509965
H	0.814325	2.832502	-0.830885
H	0.336573	3.522621	0.472768
H	-1.452184	-1.123534	2.840659
H	-2.502621	-1.037976	1.640868
H	0.066394	1.449203	-4.492781
H	1.156004	0.367352	-4.437663
H	-1.057789	-0.621668	5.245852
H	-1.002124	0.519529	4.157137
H	1.652406	2.043524	-2.834064
H	2.663537	3.158505	-2.385877
H	-1.247426	-4.355437	0.671929
H	-1.371108	-2.851123	1.142074
H	-2.165503	2.128779	-0.010229
H	-2.987854	0.902951	0.557727
H	-3.610354	-1.150409	-0.269104
H	-4.794533	-0.714789	0.684106
H	-1.323676	-0.730501	-1.647135
H	-0.263161	0.211914	-2.342076
H	-1.602279	2.055111	2.361009
H	-0.553604	2.725149	3.318168
H	-2.995220	-2.474936	-2.164175
H	-2.120553	-2.725221	-0.880071
H	0.476148	-2.612850	0.313472
H	1.762634	-1.873370	-0.201499

O	2.358612	0.626752	-0.075155
H	2.504525	1.276547	-0.793647
H	3.092744	0.717760	0.543250

Ca^{2+} $(H_2O)_{15}$

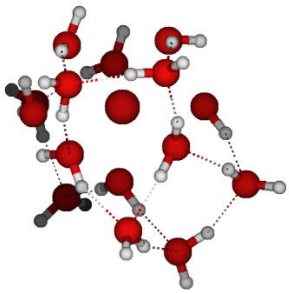

Figure S_{83} : Ca^{2+} optimized structure with 15 water molecules.

E = -1182.334527

H = -1182.333583

O	1.464020	-0.427377	2.688504
Ca	0.392227	0.314988	0.626319
O	-0.587987	-0.165060	-1.512368
O	2.546905	0.594930	-0.432283
O	1.240619	-1.983810	0.330884
O	0.265845	2.623912	-0.418986
O	-1.823145	1.606915	0.939047
O	-1.381943	-1.201066	1.785012
O	-1.409341	2.254093	3.542181
O	-3.602347	-0.386283	0.454473
O	-0.800421	-0.303729	4.265483
O	-1.083402	-3.447438	0.376080
O	-2.571294	-2.072326	-1.403795
O	2.086812	2.383515	-2.450775
O	0.356780	0.938900	-4.044970
H	1.783644	-1.328225	2.551852
H	0.865354	-0.449972	3.461899
H	0.829559	2.788124	-1.201795
H	0.692582	3.066771	0.332391

H	-1.299341	-1.035302	2.753834
H	-2.290551	-0.934086	1.519137
H	-0.271948	1.473129	-4.548342
H	0.717797	0.305118	-4.678853
H	-0.999333	-0.634444	5.149303
H	-1.092441	0.635404	4.222946
H	1.600865	1.935325	-3.174279
H	2.673768	3.035760	-2.851278
H	-1.199202	-4.349805	0.697670
H	-1.271034	-2.825621	1.118923
H	-1.577745	2.251537	0.253230
H	-2.592248	1.086979	0.619115
H	-3.438339	-0.977597	-0.316810
H	-4.544673	-0.418986	0.656008
H	-1.270840	-0.851941	-1.658425
H	-0.332431	0.186460	-2.382272
H	-1.828761	2.156484	2.658121
H	-1.865006	2.960016	4.016444
H	-3.022776	-2.522081	-2.127765
H	-2.114656	-2.761027	-0.862109
H	0.567701	-2.689236	0.234880
H	1.876732	-2.104966	-0.382403
H	2.590597	1.228614	-1.181333
H	3.435815	0.515152	-0.070558
O	0.923243	2.292227	2.160691
H	1.723823	2.136501	2.676021
H	0.209240	2.479770	2.808074

Ca^{2+} $(H_2O)_{16}$

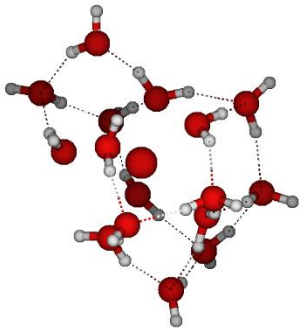

Figure S_{84} : Ca^{2+} optimized structure with 16 water molecules.

E = -1258.726702

H = -1258.725758

O	1.286022	-0.721450	2.039247
Ca	-0.004221	0.581607	0.487895
O	-1.241301	0.094363	-1.462662
O	3.547195	1.442809	-0.943170
O	1.567435	-2.847616	0.308250
O	0.356008	2.706193	-0.514741
O	0.813539	2.175979	2.168371
O	-2.129359	1.826570	1.063173
O	-1.575109	-1.081093	1.622530
O	-1.205229	-3.315430	0.178020
O	-3.081311	-1.918444	-1.313110
O	-0.694028	-0.528577	4.076132
O	-1.390562	2.122364	3.738755
O	-3.920709	-0.219932	0.654389
O	1.860893	2.682689	-2.756775
O	0.765210	0.277846	-3.348274
H	1.527260	-1.609173	1.710891
H	0.891062	-0.814232	2.923093
H	0.819332	2.859255	-1.371741
H	0.815576	3.237109	0.149099
H	-1.378025	-1.022262	2.590803
H	-2.523272	-0.849393	1.490195
H	0.885329	-0.226467	-4.161475

H	1.252951	-0.180972	-2.624372
H	-0.835569	-0.966390	4.923738
H	-0.962801	0.410031	4.181613
H	1.474322	1.902920	-3.217498
H	1.959459	3.390634	-3.404220
H	-1.484033	-4.161849	0.550457
H	-1.353018	-2.627985	0.873906
H	-2.121184	2.584897	0.462391
H	-2.896512	1.267544	0.804180
H	-3.852159	-0.798597	-0.138901
H	-4.834842	-0.252045	0.960481
H	-1.926872	-0.590771	-1.597282
H	-0.745191	0.188191	-2.300785
H	-1.924081	2.168541	2.919561
H	-1.747539	2.768077	4.360885
H	-3.565573	-2.333586	-2.036700
H	-2.489244	-2.597353	-0.917627
H	0.659510	-3.181251	0.143425
H	2.162838	-3.605528	0.273576
H	3.207684	2.015492	-1.659602
H	4.504787	1.398645	-1.036955
H	1.666328	1.985534	2.577035
H	0.182597	2.360712	2.895753
O	1.733284	-0.400390	-0.934904
H	2.571728	0.148422	-0.890155
H	1.908744	-1.316175	-0.629921

Ca^{2+} $(H_2O)_{17}$

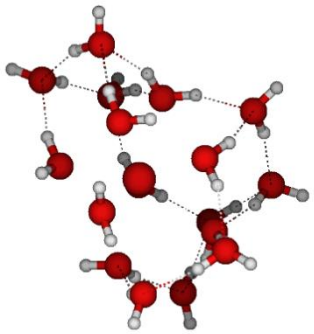

Figure S_{85} : Ca^{2+} optimized structure with 17 water molecules.

E = -1335.116543

H = -1335.115599

O	1.314255	-0.843757	2.089015
Ca	0.166273	0.745490	0.556512
O	-1.212467	0.256356	-1.338880
O	0.431750	2.786744	-0.660103
O	1.670795	-0.582707	-1.074002
O	0.423600	2.423700	2.258780
O	-2.170694	1.773437	1.216553
O	-1.523275	-1.112615	1.581618
O	3.813117	1.068646	-1.297646
O	-0.668595	-0.711797	4.079532
O	-3.913144	-0.262215	0.665844
O	-1.315703	-3.328899	0.140605
O	0.664673	0.309246	-3.398196
O	2.085204	2.516431	-2.827863
O	-1.612784	1.844529	3.934340
O	-3.041652	-1.816159	-1.373887
O	1.396081	-2.938480	0.269788
H	1.402564	-1.732763	1.690942
H	0.864032	-0.933834	2.949571
H	0.979430	2.863559	-1.472527
H	0.706351	3.500116	-0.072121
H	-1.339630	-1.107620	2.552647
H	-2.465534	-0.857707	1.457101

H	0.651917	-0.178053	-4.230149
H	1.100490	-0.252656	-2.715567
H	-0.797926	-1.198928	4.901534
H	-0.995033	0.206246	4.226831
H	1.579277	1.792266	-3.269797
H	2.253443	3.202084	-3.485461
H	-1.654358	-4.145642	0.528729
H	-1.415009	-2.610621	0.822173
H	-2.225877	2.612249	0.740804
H	-2.899646	1.211257	0.872868
H	-3.842372	-0.798995	-0.156063
H	-4.822305	-0.322926	0.980800
H	-1.877999	-0.446726	-1.474020
H	-0.779555	0.394906	-2.202134
H	-2.073516	1.904558	3.070558
H	-2.111706	2.363811	4.575906
H	-3.496460	-2.169566	-2.147227
H	-2.496511	-2.537380	-0.985188
H	0.474700	-3.251524	0.116244
H	1.971980	-3.711624	0.240244
H	3.389459	1.698068	-1.925244
H	4.740765	0.984169	-1.545694
H	1.369684	2.488812	2.447418
H	-0.084091	2.457855	3.090362
H	2.580418	-0.208464	-1.109751
H	1.718740	-1.507303	-0.741156
O	2.572800	1.365386	1.119709
H	2.765640	0.562491	1.626005
H	3.224276	1.408287	0.391549

Ca^{2+} $(H_2O)_{18}$

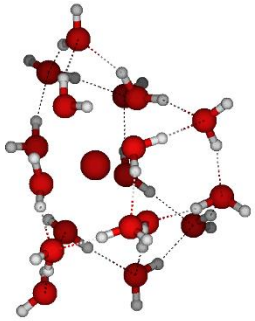

Figure S_{86} : Ca^{2+} optimized structure with 18 water molecules.

E = -1411.510572

H = -1411.509582

O	1.287164	-0.827210	1.972593
Ca	0.160483	0.709940	0.352569
O	0.415333	2.760485	-0.916009
O	-0.985946	0.035297	-1.669061
O	0.262947	2.284867	2.147516
O	2.511338	1.416052	1.043894
O	1.860174	-0.647389	-1.123259
O	-3.261313	2.426495	2.821422
O	1.052689	0.085558	-3.555156
O	2.249270	2.400561	-2.923196
O	-1.242500	1.837040	4.344609
O	-1.552696	-0.923262	1.354536
O	-1.260766	-3.284265	0.135954
O	-0.741532	-0.735310	3.883033
O	-3.822550	-0.206258	0.101549
O	-2.861708	-1.998816	-1.679111
O	3.958688	1.080078	-1.241395
O	1.467139	-2.976561	0.251723
H	1.430451	-1.724110	1.610579
H	0.784685	-0.910868	2.807355
H	1.026356	2.781066	-1.687461
H	0.676361	3.494366	-0.346703
H	-1.433206	-0.906947	2.338738

H	-2.476165	-0.657100	1.135826
H	1.156475	-0.433626	-4.360959
H	1.455128	-0.414574	-2.804951
H	-0.945798	-1.326630	4.616459
H	-0.924931	0.190988	4.194586
H	1.832099	1.629512	-3.380311
H	2.443677	3.066781	-3.593603
H	-1.626184	-4.047374	0.601186
H	-1.398642	-2.489390	0.718185
H	-3.799259	3.215400	2.948429
H	-2.875822	2.480435	1.923984
H	-3.735377	-0.866239	-0.621899
H	-4.747194	-0.174206	0.371932
H	-1.660142	-0.658616	-1.809012
H	-0.475681	0.100589	-2.498170
H	-2.095344	2.104535	3.886280
H	-1.205128	2.285926	5.197025
H	-3.257386	-2.439426	-2.439890
H	-2.354764	-2.668160	-1.166873
H	0.534046	-3.259401	0.112758
H	2.011920	-3.772099	0.268463
H	3.546386	1.668182	-1.913525
H	4.905800	1.047886	-1.417524
H	1.213821	2.408147	2.278510
H	-0.175757	2.274541	3.026357
H	2.764207	-0.264448	-1.085112
H	1.880000	-1.561634	-0.761713
H	2.658225	0.612409	1.567107
H	3.222758	1.455115	0.373598
O	-2.119098	1.917254	0.332981
H	-2.806541	1.296043	0.010524
H	-1.927473	2.530000	-0.390297

Ca^{2+} $(H_2O)_{19}$

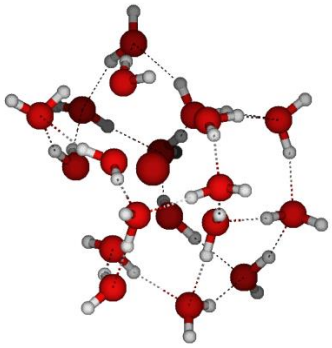

Figure S_{87} : Ca^{2+} optimized structure with 19 water molecules.

E = -1487.902705

H = -1487.901761

O	1.356621	-0.694774	1.949405
Ca	0.098754	0.713729	0.345666
O	0.111274	2.064683	2.296307
O	-1.086057	-0.019070	-1.653292
O	0.244249	2.782125	-0.909309
O	2.517878	1.610998	0.830944
O	-1.522871	-0.990964	1.334028
O	-2.212725	1.863962	0.280211
O	1.778147	-0.679289	-1.152709
O	-0.737346	-0.809418	3.859451
O	-1.607506	1.654144	4.345355
O	-3.545762	2.164303	2.684865
O	0.900454	-0.014327	-3.581030
O	-1.169534	-3.368237	0.185887
O	2.066525	2.332518	-3.009669
O	-3.820907	-0.352858	0.102063
O	-2.833008	-2.175207	-1.638348
O	3.859199	1.034687	-1.437576
O	1.536150	-2.947487	0.321751
H	1.524373	-1.602014	1.628964
H	0.862210	-0.765101	2.788844
H	0.801844	2.771537	-1.713911
H	0.638612	3.461569	-0.320895

H	-1.399089	-0.984305	2.319082
H	-2.452906	-0.741928	1.116343
H	0.989901	-0.550146	-4.377352
H	1.317355	-0.496672	-2.826958
H	-0.880463	-1.448256	4.566870
H	-1.058340	0.069713	4.192239
H	1.642222	1.551685	-3.441564
H	2.234696	2.986678	-3.698607
H	-1.516615	-4.121614	0.679894
H	-1.333880	-2.553162	0.734571
H	-4.151934	2.903893	2.800178
H	-3.091811	2.293656	1.827031
H	-3.749036	-1.039286	-0.596129
H	-4.732458	-0.331176	0.414049
H	-1.710908	-0.762825	-1.762762
H	-0.592323	0.043707	-2.492387
H	-2.439716	1.874444	3.831255
H	-1.645269	2.104820	5.196193
H	-3.204248	-2.636067	-2.399197
H	-2.296047	-2.818003	-1.123736
H	0.614456	-3.274034	0.200443
H	2.116826	-3.717004	0.338919
H	3.396481	1.612612	-2.089979
H	4.794349	1.004943	-1.668360
H	0.484210	2.955669	2.157873
H	-0.443917	2.074044	3.103514
H	2.681864	-0.297435	-1.180924
H	1.827691	-1.577395	-0.751932
H	2.630962	0.955743	1.537147
H	3.195881	1.435768	0.143053
H	-2.846529	1.221620	-0.097969
H	-1.957864	2.476733	-0.425260
O	1.520280	4.072534	1.143306
H	1.924951	4.918067	1.365168

H	2.211001	3.377870	1.152528

Ca^{2+} $(H_2O)_{20}$

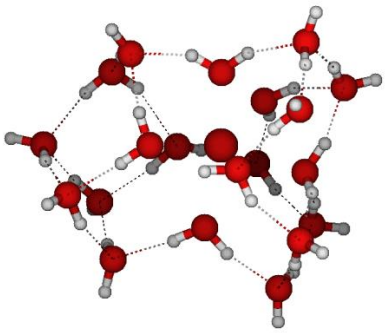

Figure S_{88} : Ca^{2+} optimized structure with 20 water molecules.

E = -1564.292526

H = -1564.291582

O	0.651817	-0.917500	2.567642
Ca	-0.158143	0.426131	0.739742
O	0.071450	2.043812	2.396082
O	0.261899	2.477392	-0.522853
O	-0.774507	-0.406057	-1.426006
O	-2.035576	-1.074046	1.540630
O	-2.291319	1.719914	0.365558
O	3.636551	1.769012	0.667014
O	3.136898	-0.610560	-2.481802
O	-1.620024	-0.734253	4.148841
O	-1.684825	1.891638	4.472597
O	-3.523246	2.522819	2.741014
O	-1.381555	-3.466625	0.550359
O	0.860750	0.101085	-3.663314
O	1.901099	3.614209	1.283804
O	1.518058	2.629047	-3.016518
O	-3.983664	-0.377367	-0.192927
O	3.992869	1.878668	-2.179551
O	-2.698926	-2.365291	-1.564694
O	1.351661	-3.103919	1.099960
H	0.961327	-1.821102	2.375759

H	0.067837	-0.953492	3.347746
H	0.641694	2.572300	-1.419729
H	0.775008	3.098410	0.047324
H	-2.069775	-0.980970	2.528576
H	-2.900345	-0.813103	1.150494
H	0.653433	-0.218964	-4.549088
H	1.718762	-0.310172	-3.389370
H	-1.962705	-1.255130	4.883349
H	-1.687431	0.224489	4.407779
H	1.210528	1.792363	-3.442049
H	1.295345	3.356858	-3.609072
H	-1.780454	-4.222474	0.999307
H	-1.653831	-2.653640	1.054769
H	-4.001383	3.358373	2.728802
H	-3.102746	2.417191	1.864575
H	-3.742105	-1.098653	-0.813796
H	-4.944869	-0.360348	-0.123285
H	-1.435999	-1.098255	-1.627455
H	-0.268413	-0.246298	-2.246341
H	-2.447828	2.224440	3.914267
H	-1.709635	2.346071	5.322039
H	-2.967024	-2.897812	-2.321994
H	-2.276572	-2.966910	-0.907374
H	0.466098	-3.399743	0.800998
H	1.881144	-3.890483	1.270962
H	3.201114	2.342919	-2.538579
H	4.776039	2.290161	-2.563855
H	0.741753	2.751064	2.285053
H	-0.368075	2.116020	3.266164
H	3.634462	0.248312	-2.441023
H	3.767273	-1.301873	-2.715810
H	3.246782	0.882452	0.738477
H	3.894972	1.858681	-0.267246
H	-2.940441	1.174480	-0.121913

H	-1.841453	2.319413	-0.251267
H	2.273392	4.474490	1.503352
H	2.655288	2.972120	1.126215
O	1.997877	-0.582263	0.073466
H	2.352978	-0.663850	-0.836190
H	1.979843	-1.494262	0.430149

$Cl^-(H_2O)n$

$Cl^-(H_2O)$

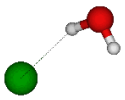

Figure S_{89} : Cl^- optimized structure with 1 water molecule.

E = -91.512984

H = -91.512040

Cl	-0.649291	0.000000	-0.251105
H	0.870475	0.000000	1.437539
O	1.201069	0.000000	2.359619
H	0.369090	0.000000	2.837272

$Cl^-(H_2O)_2$

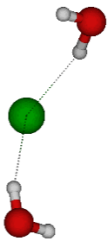

Figure S_{90} : Cl^- optimized structure with 2 water molecules.

E = -167.922326

H = -167.921382

O	1.134140	-0.232321	2.629025
Cl	-0.543779	0.064776	-0.089069
H	0.645299	-0.401915	1.800522
H	1.040523	0.720159	2.696822
H	-2.788489	0.413486	-0.268952
O	-3.734873	0.196878	-0.377483
H	-3.693579	-0.761063	-0.412109

$Cl^-(H_2O)_3$

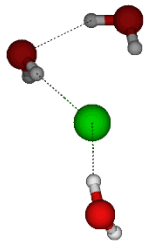

Figure S_{91} : Cl^- optimized structure with 3 water molecules.

E = -244.333935

H = -244.332991

O	1.480863	-0.155569	2.287681
Cl	-1.290082	0.045461	0.286203
O	-4.394216	0.072002	-0.580261
H	0.531347	-0.217095	2.115505
H	1.795546	0.228148	1.455785
H	-3.497752	0.350651	-0.320621
H	-4.293829	-0.882069	-0.584714
H	0.732131	0.648467	-0.393993
O	1.699432	0.571954	-0.539998
H	1.788884	-0.363773	-0.737050

$Cl^-(H_2O)_4$

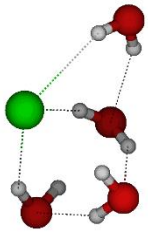

Figure S_{92} : Cl^- optimized structure with 4 water molecules.

E = -320.751327

H = -320.750383

O	1.639905	-0.479970	2.014080
O	0.571905	-0.001875	-0.759808
Cl	-1.393970	1.250096	1.416010
O	-1.926216	-1.350082	-0.587207

H	0.836096	-0.001622	2.253774
H	1.591138	-0.491382	1.049281
H	-1.972803	-0.911607	0.277464
H	-2.169634	-0.623157	-1.188061
H	0.192459	0.582202	-0.074582
H	-0.076932	-0.731137	-0.759551
H	-1.990166	1.529182	-0.926333
O	-1.879807	1.209743	-1.838960
H	-0.933832	0.999069	-1.859409

$Cl^-(H_2O)_5$

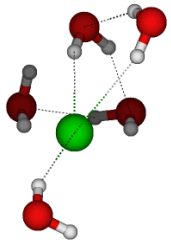

Figure S_{93} : Cl^- optimized structure with 5 water molecules.

E = -397.156483

H = -397.155539

O	1.750113	-0.787471	1.780304
O	0.664576	-0.009019	-0.920125
O	-1.777919	-1.461117	-0.866361
O	-1.838544	1.188771	-1.887568
Cl	-1.326060	0.970243	1.384103
H	0.950609	-0.341007	2.083844
H	1.695839	-0.684157	0.821401
H	-1.862150	-1.132013	0.040908
H	-2.055260	-0.686466	-1.388699
H	0.293041	0.507872	-0.182074
H	0.031921	-0.751262	-0.970952
H	-1.966497	1.452585	-0.961747
H	-0.883795	1.022902	-1.919616
H	-2.089223	2.507079	2.982229
O	-2.599885	2.791839	3.757205

H	-3.005757	1.967087	4.031756

$Cl^-(H_2O)_6$

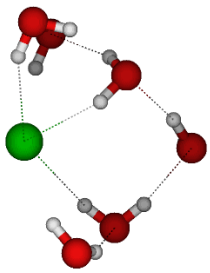

Figure S_{94} : Cl^- optimized structure with 6 water molecules.

E = -473.569217

H = -473.568272

O	-0.809345	0.840891	0.330075
O	0.064513	0.758516	2.937239
O	2.511508	-0.494726	3.431260
O	1.596505	1.249313	5.457232
Cl	2.506460	2.739184	2.674636
O	0.668937	5.460340	1.131151
H	-0.233052	0.177469	-0.055929
H	-0.645613	0.769766	1.296201
H	2.899878	0.261093	2.963060
H	2.374274	-0.124073	4.323152
H	0.603657	1.566314	2.811507
H	0.766122	0.077788	2.999106
H	2.025070	1.945198	4.930379
H	0.747407	1.146933	5.005571
H	0.643756	4.735309	0.483687
H	1.202763	5.081297	1.837158
H	1.621388	2.847707	0.414352
O	0.988393	2.992569	-0.305439
H	0.259589	2.375873	-0.113215

$Cl^-(H_2O)_7$

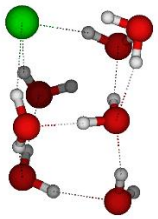

Figure S_{95} : Cl^- optimized structure with 7 water molecules.

E = -549.988961

H = -549.988017

O	-0.388579	0.834386	0.004342
O	0.111526	1.292430	2.644093
O	2.811207	0.547607	3.174965
O	1.001400	0.879883	5.307046
O	1.053548	3.287593	-0.209472
O	0.269984	3.926580	2.341153
Cl	3.124911	3.572009	3.882584
H	0.239518	0.133716	-0.183741
H	-0.365125	0.925595	0.986127
H	3.106719	1.442988	3.449016
H	2.343017	0.250007	3.975051
H	0.076605	2.290661	2.597778
H	1.065440	1.080920	2.622617
H	1.444441	1.734743	5.384262
H	0.395789	1.004840	4.553931
H	0.529893	3.890312	1.391455
H	1.095655	4.088975	2.830686
H	1.937196	2.950261	0.038398
H	0.500365	2.490472	-0.302776
H	3.540585	2.904548	1.634103
O	3.450139	2.307135	0.869937
H	3.305602	1.450076	1.289146

$Cl^-(H_2O)_8$

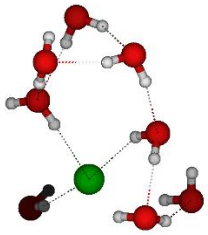

Figure S_{96} : Cl^- optimized structure with 8 water molecules.

E = -626.386999

H = -626.386055

O	-0.300753	-0.111349	0.337968
O	0.247724	0.479200	3.008964
O	-0.105831	-2.920390	-0.003305
O	1.641517	-4.619972	-1.374620
O	2.321975	0.758953	1.103683
O	-0.454604	-5.805991	0.106618
O	2.416830	-1.490791	2.885704
Cl	1.942704	-4.460619	1.995628
H	0.631551	0.156959	0.266413
H	-0.314855	-1.065412	0.140647
H	2.231605	-4.597210	-0.608859
H	0.964921	-5.265648	-1.097047
H	0.381376	-3.146759	0.806330
H	0.496238	-3.254310	-0.698843
H	0.139860	-5.794220	0.871669
H	-0.769539	-4.888660	0.076339
H	1.712682	1.064896	1.798705
H	2.622170	-0.079660	1.487143
H	0.815210	-0.287703	3.178385
H	-0.199517	0.253015	2.167902
H	2.250668	-2.411411	2.591763
H	3.071548	-1.575174	3.581918
O	3.314629	-5.970139	4.541553
H	2.436665	-5.961982	4.928274
H	3.152730	-5.585962	3.666317

$Cl^-(H_2O)_9$

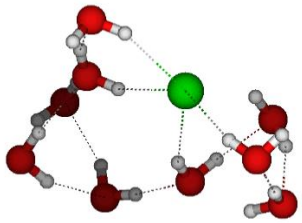

Figure S_{97} : Cl^- optimized structure with 9 water molecules.

E = -702.800899

H = -702.799955

O	-0.157012	-0.183444	0.656678
O	0.433283	0.295893	3.340909
O	2.407748	0.886408	1.382385
O	0.105223	-2.963792	0.116945
O	1.912793	-4.519475	-1.296873
O	-0.584909	-5.655330	-0.864210
O	2.626846	-1.549176	2.833677
Cl	2.042953	-4.741401	2.097628
O	3.653674	-3.517699	4.550907
H	0.750237	0.157089	0.571915
H	-0.117564	-1.123713	0.405101
H	2.341519	-4.718140	-0.453134
H	1.127860	-5.106288	-1.309292
H	0.434755	-3.359736	0.938443
H	0.792707	-3.233125	-0.528522
H	-0.492289	-6.208169	-0.064282
H	-0.763776	-4.762883	-0.530863
H	1.802600	1.098744	2.114070
H	2.803727	0.063743	1.710865
H	1.084407	-0.421118	3.399817
H	-0.032138	0.101601	2.502313
H	2.295708	-2.297275	2.316956
H	3.161522	-1.994278	3.516651
H	2.930269	-3.572642	5.180759

H	3.357339	-4.094029	3.820922
H	0.581132	-6.381848	1.862394
O	0.056137	-7.105005	1.466131
H	0.725891	-7.725624	1.168674

$Cl^-(H_2O)_{10}$

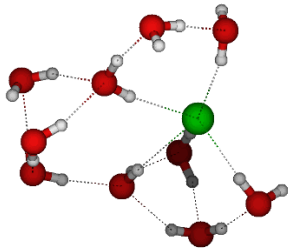

Figure S_{98} : Cl^- optimized structure with 10 water molecules.

E = -779.210060

H = -779.209116

O	0.256947	-0.077160	0.246142
O	0.241826	0.280946	3.029762
O	2.707441	0.453044	1.613305
O	2.194599	-1.867406	3.133037
O	3.219425	-2.990373	5.451540
O	0.160145	-2.881401	-0.260658
O	1.769748	-4.798388	-1.470474
O	-0.920742	-5.424517	-1.187503
O	-0.737125	-6.863557	1.235841
Cl	1.648597	-4.901682	1.932330
H	1.203200	0.076451	0.416843
H	0.183527	-1.011283	-0.016736
H	2.087840	-5.018476	-0.584461
H	0.888859	-5.225850	-1.519162
H	0.389149	-3.245197	0.606962
H	0.843725	-3.280284	-0.838257
H	-0.999450	-5.950046	-0.368833
H	-0.942819	-4.500546	-0.891984
H	2.008121	0.817521	2.181844

H	2.820037	-0.424376	2.018067
H	0.733612	-0.533392	3.223975
H	-0.024398	0.167059	2.095978
H	1.978975	-2.703331	2.691606
H	2.622844	-2.136888	3.971483
H	2.435981	-3.124902	5.989247
H	3.441113	-3.881033	5.098062
H	-0.114292	-6.231338	1.643077
H	-0.176519	-7.608504	1.005642
H	2.971213	-5.377124	3.577611
O	3.674964	-5.405714	4.259604
H	4.487679	-5.374074	3.748969

$Cl^-(H_2O)_{11}$

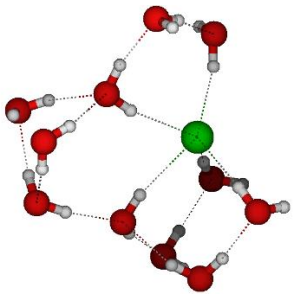

Figure S_{99} : Cl^- optimized structure with 11 water molecules.

E = -855.615745

H = -855.614801

O	0.405792	-0.134309	0.271085
O	-0.063703	0.266800	2.994084
O	2.585530	0.570029	2.000903
O	1.965397	-1.783158	3.448245
O	2.756223	-2.894548	5.863903
O	3.882840	-5.047817	4.607936
O	0.549549	-2.905922	-0.257518
O	1.481623	-4.640102	-2.146712
O	-0.954437	-5.271729	-0.939436
O	-0.672337	-6.551639	1.586178
Cl	1.967859	-4.854220	2.128495

H	1.307048	0.078046	0.568891
H	0.425140	-1.073345	0.011172
H	2.201419	-5.120897	-1.701045
H	0.659039	-5.102601	-1.892827
H	0.956071	-3.314321	0.519707
H	1.019271	-3.317724	-1.019641
H	-0.946242	-5.786343	-0.112778
H	-0.805176	-4.356584	-0.650175
H	1.775412	0.891332	2.432498
H	2.678507	-0.296358	2.431836
H	0.423343	-0.519539	3.286589
H	-0.169999	0.120238	2.032252
H	1.888788	-2.618469	2.965260
H	2.278431	-2.040425	4.339358
H	1.935739	-3.224697	6.236485
H	3.213294	-3.688455	5.508175
H	0.032486	-5.959890	1.908047
H	-0.243450	-7.408175	1.530643
H	3.254030	-5.120462	3.861076
H	4.704759	-4.776132	4.191789
H	3.088622	-5.547783	0.318962
O	3.373508	-5.984755	-0.504887
H	3.107779	-6.898814	-0.383457

$Cl^-(H_2O)_{12}$

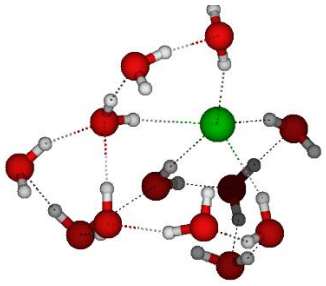

Figure S_{100} : Cl^- optimized structure with 12 water molecules.

E = -932.034709

H = -932.033765

O	-0.057007	-0.816610	0.438194
O	-0.372874	-1.678374	3.016078
O	1.488195	-2.889144	-0.494088
O	1.771334	-4.929202	-2.265365
O	-0.692341	-4.884062	-1.032443
O	2.997705	-6.718191	-0.408675
O	-0.379153	-6.081156	1.435471
O	1.467354	0.760724	2.255600
O	2.458364	-1.640388	3.258718
O	3.456725	-2.597719	5.617391
O	4.501384	-4.886973	4.568460
Cl	2.589507	-4.717335	2.099237
H	0.574541	-0.150008	0.756873
H	0.472701	-1.486720	-0.036101
H	2.294937	-5.574093	-1.757049
H	0.842273	-5.114408	-2.012448
H	1.835898	-3.337463	0.289182
H	1.722913	-3.481744	-1.247226
H	-0.696585	-5.398620	-0.197442
H	-0.367553	-4.014975	-0.760352
H	0.662297	0.619307	2.764893
H	2.036847	0.028530	2.555737
H	0.584030	-1.686537	3.199112
H	-0.425463	-1.457652	2.056457
H	2.630689	-2.416359	2.703287
H	2.848360	-1.867119	4.132642
H	2.699924	-2.888682	6.131224
H	3.896960	-3.425734	5.317991
H	-0.766259	-5.511518	2.133383
H	0.565767	-5.915610	1.559679
H	3.873539	-5.008363	3.826479
H	5.346041	-4.744004	4.134568
H	3.077406	-6.108796	0.345477
H	2.270427	-7.295792	-0.162828

H	-0.735943	-3.388828	3.342998
O	-0.662626	-4.347428	3.560708
H	0.289286	-4.486129	3.616480

$Cl^-(H_2O)_{13}$

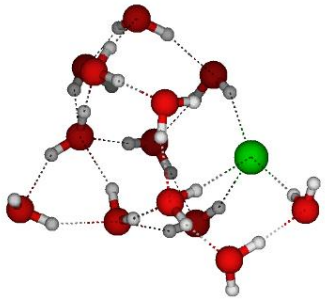

Figure S_{101} : Cl^- optimized structure with 13 water molecules.

E = -1008.453875

H = -1008.452931

O	-0.021522	-2.402198	0.192489
O	0.326201	-2.055904	2.952189
O	-0.306483	-4.765625	3.628858
O	2.280696	-2.358245	-0.931085
O	1.774691	-4.737329	-2.073337
O	-1.027761	-4.224877	-1.834681
O	-0.770652	-5.008516	0.923628
O	2.971684	-2.281470	3.510647
O	4.217038	-2.422382	5.937854
O	4.919306	-5.003759	5.472513
O	-0.636981	0.057082	1.450826
O	1.545851	-6.327908	0.160783
Cl	2.953407	-5.376684	3.076458
H	-0.384664	-1.507624	0.323246
H	0.900611	-2.320905	-0.232561
H	1.837792	-5.368276	-1.322582
H	0.814047	-4.639463	-2.208579
H	3.016081	-2.476725	-0.294846
H	2.217176	-3.206698	-1.441875
H	-1.256740	-4.860077	-1.143243
H	-0.828468	-3.425492	-1.319890
H	-0.407179	-0.520860	2.207122
H	0.148781	0.589902	1.307820
H	1.269527	-1.993805	3.224918

H	0.343318	-2.365691	2.024277
H	2.921629	-3.258253	3.436792
H	3.429327	-2.137933	4.368983
H	3.549717	-2.487044	6.624516
H	4.547878	-3.344347	5.820357
H	-0.794505	-5.076014	1.902126
H	-0.534641	-4.078955	0.755303
H	4.251184	-5.281753	4.808707
H	5.755852	-5.108253	5.012943
H	2.124995	-6.210736	0.925829
H	0.686447	-5.953559	0.448800
H	-0.183545	-3.799017	3.598295
H	0.595951	-5.120966	3.617931
H	4.083504	-3.757271	1.247636
O	4.192014	-2.821569	1.035426
H	3.896438	-2.379868	1.851336

Cl^- $(H_2O)_{14}$

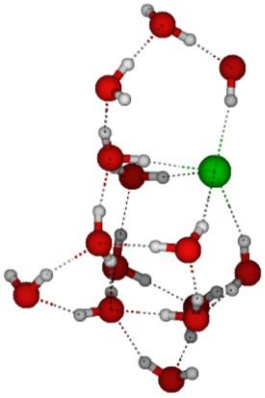

Figure S_{102} : Cl^- optimized structure with 14 water molecules.

E = -1084.861191

H = -1084.860247

O	0.013491	-2.271132	-0.031901
O	2.323851	-2.618092	-1.090199
O	1.427069	-4.889625	-2.214611
O	0.877621	-6.407414	0.014819
O	-1.174698	-4.695072	0.740044

O	-0.612705	-4.555120	3.436387
O	4.063412	-3.305216	0.983524
O	0.451663	-2.011805	2.740566
O	2.963154	-2.609325	3.511679
O	3.579245	-2.665655	6.155397
O	5.571244	-4.481577	6.353042
O	-0.117607	0.239839	1.261966
O	-1.254704	-3.904026	-2.049212
Cl	2.592379	-5.652544	2.866687
H	-0.179705	-1.329019	0.126468
H	0.943700	-2.344559	-0.436930
H	1.357803	-5.517106	-1.461491
H	0.503121	-4.623527	-2.376333
H	3.003220	-2.835303	-0.420019
H	2.130372	-3.457460	-1.582740
H	-1.598204	-4.489523	-1.361973
H	-0.934860	-3.145739	-1.532052
H	0.004997	-0.378678	2.011987
H	0.753371	0.617089	1.117265
H	1.380776	-2.113364	3.058716
H	0.443626	-2.325554	1.815684
H	2.826910	-3.574746	3.421320
H	3.224903	-2.486390	4.453736
H	2.818173	-3.077781	6.570377
H	4.316524	-3.312052	6.266433
H	-1.192173	-4.758340	1.718616
H	-0.787782	-3.818947	0.562253
H	5.396739	-5.233642	5.735976
H	6.392035	-4.086961	6.052361
H	1.480394	-6.374433	0.769581
H	0.100723	-5.878502	0.296153
H	-0.335708	-3.620612	3.392630
H	0.218775	-5.051894	3.423919
H	3.774030	-4.194053	1.235783

H	3.885391	-2.790871	1.787614
H	4.192153	-6.313244	4.158428
O	5.047524	-6.471789	4.613621
H	5.663584	-6.628475	3.894567

$Cl^-(H_2O)_{15}$

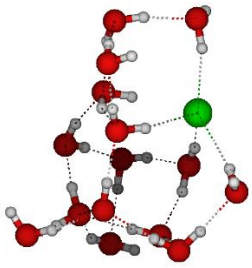

Figure S_{103} : Cl^- optimized structure with 15 water molecules.

E = -1161.275113

H = -1161.274169

O	0.320885	-2.293988	0.154461
O	2.794182	-2.551069	-0.564994
O	2.182286	-4.836199	-1.812291
O	1.362241	-6.393313	0.304523
O	-0.865463	-4.810524	0.546643
O	-1.775119	-4.476051	3.079249
O	4.028591	-3.417891	1.841494
O	-0.019872	-2.198576	2.945653
O	2.396449	-2.854353	3.998301
O	4.485549	-2.459007	5.621053
O	6.071965	-3.600702	3.813760
O	5.645748	-6.308535	4.299708
O	-0.259726	0.127118	1.476760
O	-0.503058	-3.955764	-2.128764
Cl	2.634743	-5.963835	3.468399
H	0.059820	-1.365587	0.296249
H	1.298892	-2.320622	-0.098612
H	2.022634	-5.474544	-1.083002

H	1.285241	-4.614303	-2.127195
H	3.360517	-2.785480	0.191213
H	2.693081	-3.385757	-1.096300
H	-0.927286	-4.533785	-1.476657
H	-0.317171	-3.164732	-1.599394
H	-0.308624	-0.522983	2.207512
H	0.586961	0.563445	1.596487
H	0.811594	-2.321974	3.451137
H	0.202228	-2.455326	2.029256
H	2.347533	-3.829531	4.026046
H	3.068496	-2.604278	4.682092
H	4.497147	-3.060663	6.368414
H	5.165469	-2.820126	4.987927
H	-1.348239	-4.813136	1.407079
H	-0.481062	-3.918328	0.488737
H	6.038684	-4.561235	3.999977
H	5.547195	-3.487821	2.999554
H	1.799526	-6.414935	1.164785
H	0.512585	-5.923498	0.454434
H	-1.275824	-3.652773	3.220531
H	-1.327355	-5.155951	3.618635
H	3.739408	-4.342274	1.867206
H	3.444112	-3.007294	2.515271
H	4.674899	-6.313856	4.179155
H	5.969888	-6.884948	3.603787
H	0.535349	-6.433696	4.140063
O	-0.331888	-6.360043	4.578009
H	-0.117168	-6.030524	5.453319

$Cl^-(H_2O)_{16}$

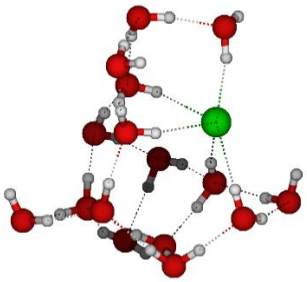

Figure S_{104} : Cl^- optimized structure with 16 water molecules.

E = -1237.691125

H = -1237.690181

O	0.334936	-2.425108	0.194309
O	2.761914	-2.954295	-0.553517
O	1.960588	-5.386561	-1.421000
O	1.096787	-6.473885	1.056598
O	-0.937726	-4.760950	0.938062
O	-1.658179	-4.264958	3.450247
O	-0.186001	-6.237485	4.672536
O	0.138048	-2.014718	3.012561
O	2.623935	-2.531893	3.979623
O	4.713368	-1.822069	5.478059
O	6.317545	-3.109769	3.783584
O	-0.082982	0.120989	1.285563
O	4.220780	-3.297971	1.857444
O	5.967330	-5.752939	4.573004
O	-0.626953	-4.339949	-1.831157
Cl	2.945099	-5.700567	3.664691
H	0.141319	-1.471792	0.270902
H	1.297985	-2.545705	-0.076605
H	1.767659	-5.919128	-0.626659
H	1.077814	-5.121821	-1.747832
H	3.389934	-3.047649	0.184809
H	2.612797	-3.861157	-0.921245
H	-1.073495	-4.774988	-1.088774
H	-0.391303	-3.482211	-1.445373

H	-0.128441	-0.435758	2.090682
H	0.762870	0.570664	1.346665
H	0.995347	-2.087262	3.484174
H	0.306394	-2.393285	2.130367
H	2.602183	-3.493629	4.135958
H	3.294799	-2.171168	4.614471
H	4.779966	-2.300639	6.306996
H	5.400550	-2.228745	4.882891
H	-1.368716	-4.658494	1.828394
H	-0.549074	-3.886544	0.746008
H	6.311978	-4.042254	4.081724
H	5.780258	-3.110105	2.970345
H	1.713882	-6.122958	1.719391
H	0.319221	-5.851662	1.050359
H	-1.146093	-3.444961	3.545172
H	-1.176838	-4.954106	3.961769
H	4.001425	-4.218239	2.076404
H	3.640574	-2.810683	2.481555
H	5.001058	-5.826517	4.443708
H	6.335069	-6.399305	3.966070
H	-0.181338	-7.037702	4.108717
H	0.743284	-5.969775	4.664930
H	1.276468	-8.495137	3.300746
O	0.394392	-8.360920	2.942561
H	0.555345	-7.817699	2.140337

$Cl^-(H_2O)_{17}$

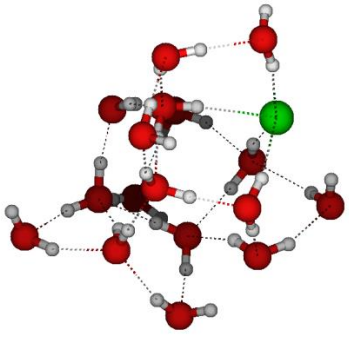

Figure S_{105} : Cl^- optimized structure with 17 water molecules.

E = -1314.103624

H = -1314.102680

O	0.405445	-2.460048	0.282663
O	2.807184	-3.064503	-0.363884
O	1.948582	-5.396432	-1.491946
O	-0.610078	-4.769943	1.323752
O	-2.013804	-3.756781	3.419629
O	1.214795	-6.837750	0.902187
O	-0.165449	-5.802174	4.093558
O	0.689194	-8.270935	3.299637
O	0.032010	0.127241	1.259454
O	0.122607	-1.913985	3.102657
O	2.445912	-2.587593	4.225067
O	4.689746	-1.695183	5.424189
O	6.171667	-3.041802	3.662081
O	3.893408	-3.580635	2.128209
O	6.526373	-5.783778	4.117138
O	-0.652091	-4.320681	-1.605893
Cl	3.589987	-6.611632	3.171666
H	0.218797	-1.502892	0.349098
H	1.378430	-2.599750	0.022520
H	1.799257	-6.062131	-0.799255
H	1.050448	-5.094091	-1.730571
H	3.305946	-3.247146	0.458706
H	2.656253	-3.930491	-0.812142
H	-1.022846	-4.806661	-0.858208
H	-0.386300	-3.481938	-1.190582
H	-0.044838	-0.360015	2.105273
H	0.890241	0.555829	1.298521
H	0.947229	-2.033576	3.636477
H	0.337739	-2.313109	2.241935
H	2.281957	-3.420543	4.747663

H	3.171469	-2.112133	4.699122
H	4.772562	-2.165286	6.256792
H	5.330290	-2.144171	4.808210
H	-1.325585	-4.497189	1.945046
H	-0.237537	-3.925633	0.993519
H	6.379355	-3.960058	3.925238
H	5.503899	-3.148097	2.956689
H	2.002058	-6.633143	1.436184
H	0.562809	-6.131469	1.083206
H	-1.382431	-3.015534	3.501558
H	-1.686076	-4.439153	4.023899
H	3.844705	-4.537795	2.307293
H	3.314323	-3.178636	2.819956
H	5.626481	-6.133188	3.972704
H	7.024354	-6.123541	3.369828
H	-0.005609	-6.764855	3.949056
H	-0.003535	-5.417266	3.219882
H	1.617385	-8.167497	3.554923
H	0.712221	-8.061348	2.347921
H	2.659713	-5.483395	5.004598
O	2.034846	-4.897537	5.462510
H	1.166507	-5.209361	5.127704

Cl^- $(H_2O)_{18}$

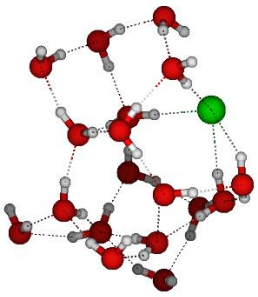

Figure S_{106} : Cl^- optimized structure with 18 water molecules.

E = -1390.512144

H = -1390.511200

O	0.367970	-2.393230	0.295078

O	2.741325	-3.050825	-0.394517
O	1.781388	-5.256041	-1.695216
O	-0.521236	-4.788665	1.291995
O	-1.842884	-3.954725	3.509662
O	3.850735	-3.750570	2.049779
O	2.496243	-2.712456	4.184959
O	1.949404	-4.735768	5.804279
O	0.159114	-1.981821	3.142885
O	4.728037	-1.512319	5.090562
O	6.168628	-2.975186	3.411886
O	0.189455	-5.882125	4.022191
O	0.770135	-8.348081	3.001516
O	0.088139	0.153136	1.408085
O	1.110828	-6.897361	0.592817
O	6.564545	-5.606887	4.279306
O	-0.801649	-4.134767	-1.612563
Cl	3.728059	-6.933177	2.610349
H	0.209905	-1.435966	0.413565
H	1.334224	-2.547342	0.017855
H	1.637331	-5.985245	-1.069132
H	0.883411	-4.914105	-1.872924
H	3.237382	-3.305863	0.410188
H	2.557863	-3.875487	-0.903310
H	-1.126602	-4.673277	-0.880373
H	-0.502806	-3.328011	-1.156222
H	0.010953	-0.374112	2.229634
H	0.961380	0.550019	1.451378
H	1.006219	-2.136542	3.633810
H	0.333002	-2.335191	2.253379
H	2.316556	-3.439209	4.843263
H	3.222251	-2.158191	4.564034
H	4.949177	-1.804245	5.977119
H	5.355976	-1.998777	4.486815
H	-1.199670	-4.578273	1.976519

H	-0.201391	-3.919127	0.977295
H	6.427716	-3.846741	3.771624
H	5.474717	-3.188098	2.757072
H	1.958972	-6.773541	1.051214
H	0.532114	-6.157526	0.872229
H	-1.263789	-3.170601	3.581302
H	-1.416860	-4.634530	4.053587
H	3.841933	-4.719335	2.152190
H	3.292391	-3.401578	2.785729
H	5.860295	-5.811331	4.917699
H	6.295405	-6.095703	3.492726
H	0.285230	-6.837832	3.796632
H	0.340699	-5.437652	3.176616
H	1.732601	-8.277689	3.092869
H	0.646227	-8.119579	2.061884
H	2.722560	-5.321404	5.870585
H	1.294155	-5.219811	5.258408
H	3.953551	-6.688581	4.657850
O	4.183607	-6.460616	5.591407
H	4.206039	-7.297685	6.061583

$Cl^-(H_2O)_{19}$

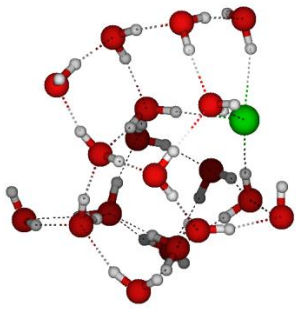

Figure S_{107} : Cl^- optimized structure with 19 water molecules.

E = -1466.922858

H = -1466.921913

O	0.420878	-2.420004	0.259909

O	2.775247	-3.234006	-0.331046
O	1.722584	-5.409969	-1.613242
O	-0.614311	-4.742678	1.301634
O	-1.930871	-3.797205	3.473510
O	0.863800	-6.975286	0.672820
O	3.794302	-3.881910	2.169113
O	2.432089	-2.676072	4.197119
O	1.833674	-4.665070	5.836800
O	0.141453	-1.910283	3.089218
O	4.637850	-1.415270	5.051657
O	6.105261	-3.010853	3.540622
O	0.237804	0.165104	1.286809
O	0.033248	-5.778855	4.066228
O	0.428373	-8.317972	3.124734
O	6.621109	-5.379343	4.818977
O	-0.779393	-4.126664	-1.643412
O	4.051703	-6.412145	5.627820
Cl	3.476219	-7.077427	2.666608
H	0.313134	-1.452193	0.350233
H	1.384780	-2.633949	0.020725
H	1.503035	-6.123120	-0.991342
H	0.857302	-5.010090	-1.829906
H	3.235318	-3.483035	0.496394
H	2.558223	-4.064135	-0.816517
H	-1.174452	-4.632292	-0.922968
H	-0.449901	-3.333532	-1.183035
H	0.104497	-0.327316	2.122710
H	1.124565	0.527451	1.352795
H	0.971146	-2.082232	3.604790
H	0.322209	-2.300316	2.216832
H	2.234936	-3.379470	4.875584
H	3.157019	-2.109147	4.563697
H	4.860397	-1.633013	5.959059
H	5.276835	-1.941667	4.490860

H	-1.292546	-4.481374	1.969122
H	-0.245729	-3.900114	0.968521
H	6.361115	-3.820749	4.037850
H	5.427131	-3.310297	2.906442
H	1.717122	-6.880993	1.127859
H	0.330037	-6.189945	0.917913
H	-1.328862	-3.029204	3.532376
H	-1.534115	-4.472594	4.044355
H	3.711188	-4.840325	2.312739
H	3.238192	-3.457687	2.867841
H	5.791920	-5.669048	5.232040
H	6.764015	-6.008403	4.085195
H	0.067136	-6.744995	3.872642
H	0.199057	-5.371137	3.204762
H	1.390075	-8.344246	3.229616
H	0.335835	-8.101221	2.178194
H	2.596154	-5.265515	5.897072
H	1.163110	-5.135274	5.298355
H	3.838226	-6.672044	4.703016
H	4.073564	-7.233618	6.124691
H	5.730594	-7.252773	2.485272
O	6.677307	-7.030799	2.540899
H	6.814844	-6.413153	1.818019

$Cl^-(H_2O)_{20}$

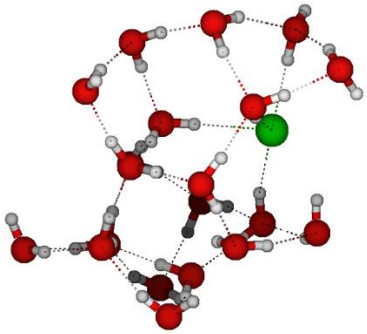

Figure S_{108} : Cl^- optimized structure with 20 water molecules.

E = -1543.331828

H = -1543.330884

O	0.199207	-2.163568	0.385641
O	2.531973	-2.840208	-0.429115
O	1.458005	-4.911691	-1.867293
O	-0.710657	-4.613983	1.228879
O	-1.912322	-3.955931	3.566596
O	0.804536	-6.697672	0.322225
O	3.719614	-3.737235	1.915185
O	2.460752	-2.842232	4.160726
O	1.943093	-4.897898	5.749497
O	0.103690	-1.996365	3.269655
O	4.660891	-1.530675	4.954470
O	6.092842	-2.883035	3.185962
O	6.647206	-5.268021	4.428561
O	0.043743	0.278366	1.724731
O	0.128276	-5.909868	3.906049
O	0.524190	-8.299310	2.631967
O	-1.072847	-3.715094	-1.606502
O	6.468252	-7.670743	2.789444
O	4.217800	-6.436241	5.242984
Cl	3.527539	-6.982978	2.177649
H	0.079692	-1.216381	0.597058
H	1.150298	-2.322552	0.067523

H	1.297554	-5.681140	-1.296523
H	0.570935	-4.518599	-1.987290
H	3.047257	-3.163159	0.337999
H	2.307307	-3.619961	-0.988295
H	-1.396046	-4.300360	-0.910365
H	-0.739551	-2.954739	-1.096750
H	-0.024757	-0.311908	2.503111
H	0.927460	0.650551	1.775214
H	0.964423	-2.214139	3.712899
H	0.235178	-2.276264	2.347748
H	2.308003	-3.582694	4.811291
H	3.186214	-2.273724	4.523788
H	4.972624	-1.822144	5.813781
H	5.278909	-1.955467	4.293844
H	-1.342220	-4.457371	1.970956
H	-0.390858	-3.726117	0.972010
H	6.380735	-3.718948	3.614369
H	5.387255	-3.151281	2.567937
H	1.683114	-6.616243	0.726376
H	0.263346	-5.957796	0.675467
H	-1.324598	-3.181980	3.673085
H	-1.472510	-4.672783	4.048984
H	3.709735	-4.708346	1.939392
H	3.201465	-3.443463	2.704311
H	5.822610	-5.543609	4.871541
H	6.829949	-6.002394	3.824344
H	0.164232	-6.843472	3.591604
H	0.278800	-5.397363	3.101230
H	1.490014	-8.294073	2.694025
H	0.380971	-7.979491	1.721248
H	2.715443	-5.489058	5.794370
H	1.276946	-5.362147	5.203838
H	3.905297	-6.500867	4.321391
H	4.540862	-7.342034	5.425404

H	5.590185	-7.442911	2.410516
H	7.017497	-7.943797	2.051616
H	4.602295	-9.449273	4.509136
O	5.302975	-8.975338	4.964794
H	5.878449	-8.646673	4.248103

$SO_4^{2-}(H_2O)$

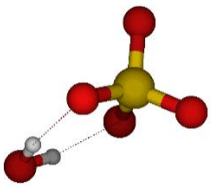

Figure S_{109} : SO_4^{2-} optimized structure with 1 water molecule.

E = -387.174602

H = -387.173658

O	-0.011497	0.913308	0.955240
S	0.243534	-0.321224	-0.118124
O	-0.338896	-1.710314	0.506555
O	1.839495	-0.447506	-0.427575
O	-0.561690	0.029942	-1.521571
H	-1.418389	1.654707	-1.229668
O	-1.650355	2.434814	-0.678348
H	-1.125181	2.122782	0.091877

$SO_4^{2-}(H_2O)_2$

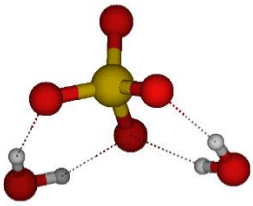

Figure S_{110} : SO_4^{2-} optimized structure with 2 water molecules.

E = -463.608381

H = -463.607437

O	-1.782424	1.791466	-1.034916
O	0.190991	1.199170	0.845337
S	0.502996	-0.330518	0.335935
O	-0.645083	-0.751386	-0.794288
O	0.373662	-1.357349	1.610798
O	1.977995	-0.424247	-0.329643
H	-1.591661	0.844447	-1.193086

H	-1.134601	1.881614	-0.305369
H	-0.803443	-2.723416	1.074061
O	-1.426490	-3.136250	0.440160
H	-1.356717	-2.415558	-0.218563

$SO_4^{2-}(H_2O)_3$

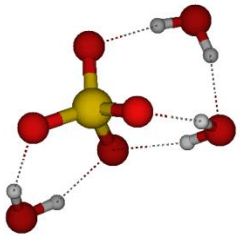

Figure S_{111} : SO_4^{2-} optimized structure with 3 water molecules.

E = -540.037038

H = -540.036094

O	-2.059730	1.714943	-0.866470
O	0.143025	1.428419	0.863504
S	0.629545	-0.028279	0.325415
O	2.147825	0.052881	-0.263863
O	-0.389689	-0.531946	-0.887019
O	0.547910	-1.135435	1.533298
O	0.085611	-3.174763	-0.278531
H	-1.682458	0.847213	-1.112454
H	-1.405046	1.902643	-0.166182
H	0.303371	-2.709222	0.559460
H	-0.214379	-2.372027	-0.760972
H	2.674411	-1.633034	-0.930369
O	2.801557	-2.562290	-1.214444
H	1.941826	-2.942794	-0.964910

$SO_4^{2-}(H_2O)_4$

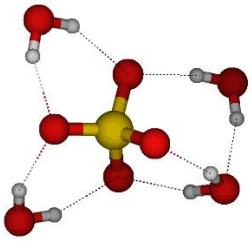

Figure S_{112} : SO_4^{2-} optimized structure with 4 water molecules.

E = -616.462460

H = -616.461516

O	-1.340809	1.992739	-0.502597
O	-0.211512	-0.554310	-0.913611
S	0.966065	-0.433482	0.234973
O	0.631347	-1.485809	1.435712
O	1.007788	1.098262	0.809933
O	2.408908	-0.795651	-0.451917
O	-0.523073	-3.262815	-0.377234
O	2.190599	-3.474006	-1.478883
H	-1.198457	1.095708	-0.858638
H	-0.568317	1.992038	0.091117
H	-0.135493	-2.915144	0.453371
H	-0.603142	-2.398883	-0.833682
H	2.375877	-2.562168	-1.180298
H	1.272922	-3.583415	-1.177331
H	3.637213	0.635605	0.046637
O	3.792905	1.497687	0.473269
H	2.868417	1.652619	0.739722

$SO_4^{2-}(H_2O)_5$

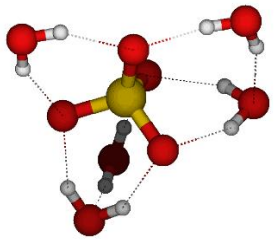

Figure S_{113} : SO_4^{2-} optimized structure with 5 water molecules.

E = -692.885106

H = -692.884161

O	-1.749184	1.810120	-0.963131
O	0.378635	-0.136952	-1.393210
S	1.272018	-0.104398	-0.020322
O	2.630182	-0.978719	-0.202523
O	0.355131	-0.735895	1.196344
O	1.652838	1.439290	0.362552
O	-0.753244	-2.602258	-0.559042
O	4.469210	1.176611	0.165029
O	1.926724	-3.721017	-0.775923
H	-1.044102	1.195286	-1.237347
H	-1.560988	1.904097	-0.014381
H	-0.500020	-2.157389	0.275904
H	-0.520151	-1.874009	-1.166120
H	2.289146	-2.835493	-0.587971
H	0.972409	-3.537077	-0.744683
H	4.155838	0.272877	-0.009490
H	3.591457	1.580191	0.286297
H	0.157280	2.003397	1.341941
O	-0.694747	1.802539	1.781200
H	-0.598927	0.829284	1.785783

$SO_4^{2-}(H_2O)_6$

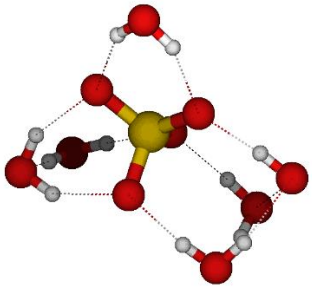

Figure S_{114} : SO_4^{2-} optimized structure with 6 water molecules.

E = -769.611021

H = -769.310077

O	-1.880290	1.684324	-0.987246
O	0.286346	-0.297684	-1.049698
S	1.279834	0.135184	0.172954
O	1.670180	1.710823	0.039196
O	2.633415	-0.771849	0.141155
O	0.502391	-0.090058	1.603018
O	-0.553019	2.517344	1.500006
O	-0.481237	-2.955151	-0.748390
O	4.491359	1.379283	-0.120175
O	2.130762	-3.479334	0.240383
H	-1.197084	1.008081	-1.139896
H	-1.593607	2.063228	-0.139755
H	-0.599948	-2.935849	0.219837
H	-0.254702	-2.019550	-0.949754
H	2.403344	-2.534147	0.214810
H	1.328399	-3.471125	-0.315631
H	4.168301	0.466868	-0.033180
H	3.621565	1.814210	-0.101009
H	0.254028	2.568228	0.949617
H	-0.446033	1.592650	1.794785
H	0.163807	-1.800204	1.973868
O	0.039181	-2.773463	2.057338
H	0.866404	-3.124880	1.678501

$SO_4^{2-}(H_2O)_7$

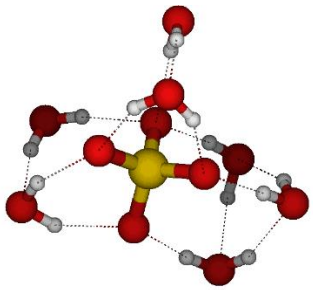

Figure S_{115} : SO_4^{2-} optimized structure with 7 water molecules.

E = -845.729704

H = -845.728760

O	-2.156669	1.543773	-0.563382
O	0.128841	-0.368340	-0.922075
S	1.151903	0.098254	0.272699
O	0.429341	-0.106123	1.719514
O	1.525139	1.673080	0.081512
O	2.521680	-0.783066	0.198968
O	2.071750	-3.500176	0.493225
O	0.020863	-2.777768	2.327479
O	-0.570864	2.527913	1.701152
O	-0.569596	-3.063668	-0.454010
O	3.755363	1.105995	-1.490126
H	-1.478328	0.892434	-0.804144
H	-1.762381	1.974200	0.213228
H	-0.665322	-3.000073	0.514566
H	-0.382478	-2.138139	-0.716419
H	2.334768	-2.558493	0.401319
H	1.262499	-3.536876	-0.051561
H	3.636658	0.270837	-1.001078
H	3.055157	1.621438	-1.044423
H	0.185459	2.566035	1.083617
H	-0.451776	1.607423	1.999895
H	0.123405	-1.809854	2.197315
H	0.842946	-3.130191	1.936879
H	1.089319	0.000473	-2.682865

O	1.709874	0.217362	-3.397187
H	2.482080	0.542962	-2.905977

$SO_4^{2-}(H_2O)_8$

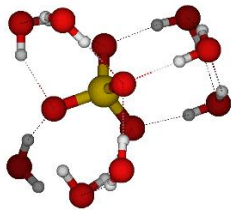

Figure S_{116} : SO_4^{2-} optimized structure with 8 water molecules.

E = -922.143370

H = -922.142426

O	-2.368450	1.347915	-0.817998
O	-1.132260	2.260695	1.666112
O	1.268903	1.632361	0.324245
S	0.936140	0.027672	0.371987
O	2.351108	-0.781433	0.362403
O	0.064185	-0.382151	-0.950066
O	0.091801	-0.296466	1.720027
O	1.996061	-3.539709	0.474995
O	-0.246413	-3.029309	2.137001
O	3.646316	1.178676	-1.109502
O	-0.557930	-3.146696	-0.696095
O	1.804628	0.217732	-3.273139
H	-1.621639	0.755822	-0.999139
H	-2.112397	1.744902	0.030757
H	-0.746815	-3.149802	0.261037
H	-0.401109	-2.200909	-0.889474
H	2.233606	-2.588877	0.462449
H	1.246664	-3.571112	-0.149873
H	3.458319	0.340477	-0.636857
H	2.836896	1.665878	-0.867596
H	-0.313758	2.407313	1.158220
H	-0.965939	1.343281	1.947929
H	-0.175030	-2.053436	2.087294

H	0.626181	-3.322189	1.811585
H	1.143231	-0.004004	-2.596786
H	2.554409	0.519615	-2.741445
H	2.812580	2.335277	1.411983
O	3.730029	2.646314	1.480657
H	4.116956	2.210896	0.710029

$SO_4^{2-}(H_2O)_9$

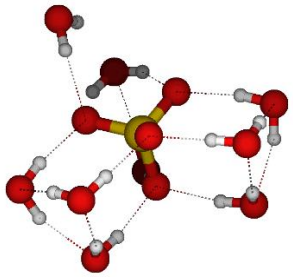

Figure S_{117} : SO_4^{2-} optimized structure with 9 water molecules.

E = -998.565035

H = -998.564091

O	-1.971035	1.563622	-0.940531
O	-1.702850	1.862697	1.879955
O	1.756566	1.618764	0.241682
S	1.186229	0.089879	0.339498
O	0.313963	-0.098485	1.691390
O	2.461410	-0.916240	0.327282
O	0.244721	-0.215500	-0.968927
O	4.052574	0.770212	-1.176290
O	1.822817	-3.614755	0.471372
O	-0.332441	-2.803954	2.116862
O	-0.657471	-2.916237	-0.711933
O	4.347790	2.233539	1.419394
O	2.070237	0.040653	-3.309757
H	-1.243440	0.922940	-1.064185
H	-2.141386	1.519998	0.019320
H	-0.843911	-2.888275	0.245507
H	-0.390188	-1.998593	-0.913884

H	2.161195	-2.695868	0.451639
H	1.079062	-3.568388	-0.158886
H	3.725557	-0.010501	-0.681753
H	3.338050	1.393304	-0.954703
H	-1.200752	2.614340	1.510600
H	-1.032264	1.152611	1.922517
H	-0.142141	-1.845642	2.078368
H	0.498790	-3.204119	1.796943
H	1.387355	-0.068577	-2.628449
H	2.860917	0.237583	-2.788126
H	3.390685	2.090119	1.349276
H	4.658250	1.731187	0.655280
H	0.520897	2.962875	0.174591
O	-0.259959	3.550737	0.124057
H	-0.848950	3.061389	-0.481403

$SO_4^{2-}(H_2O)_{10}$

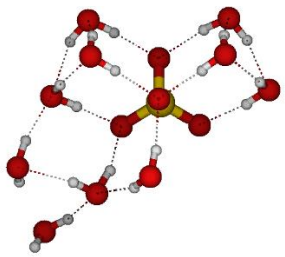

Figure S_{118} : SO_4^{2-} optimized structure with 10 water molecules.

E = -1074.974805

H = -1074.973861

O	-1.448402	1.318643	-0.825433
O	0.285700	2.813799	0.700206
O	2.266524	4.277933	-0.508776
S	1.019519	-0.842343	0.757062
O	0.400557	-0.802433	-0.771573
O	-0.221065	-0.974874	1.805781
O	2.052746	-2.052304	0.927312

O	3.506740	1.706324	-0.655959
O	0.960456	-4.566977	0.418506
O	-1.375566	-3.519400	1.644698
O	-1.847730	1.233771	1.978278
O	-0.988551	-3.253274	-1.165148
O	4.986415	3.663295	0.519041
O	2.497976	-0.182145	-2.742717
H	-0.841430	0.553806	-0.920270
H	-1.872554	1.168421	0.040099
H	-1.402809	-3.293208	-0.282595
H	-0.518631	-2.395804	-1.150847
H	1.444790	-3.741850	0.628011
H	0.415044	-4.294261	-0.343806
H	2.951857	1.162995	-0.037665
H	2.927657	2.452035	-0.898860
H	-1.197511	1.945918	1.884607
H	-1.289505	0.423996	2.001401
H	-1.024271	-2.617219	1.792858
H	-0.570329	-4.039939	1.461788
H	1.784945	-0.492412	-2.160451
H	2.998318	0.413655	-2.168395
H	5.230736	4.047815	-0.326174
H	4.575640	2.808188	0.246921
H	1.496567	3.875111	-0.044037
H	-0.303846	2.472841	-0.011375
H	2.986285	4.285490	0.137364
O	1.771994	0.588112	1.027475
H	0.825988	2.012951	0.914259

$SO_4^{2-}(H_2O)_{11}$

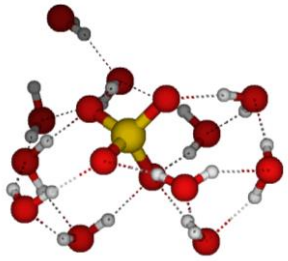

Figure S_{119} : SO_4^{2-} optimized structure with 11 water molecules.

E = -1151.391191

H = -1151.390247

O	-1.439600	1.255698	-0.921862
O	0.159379	2.990941	0.483116
O	1.536713	0.848644	1.378635
S	0.861624	-0.636745	1.201893
O	1.907766	-1.763209	1.634944
O	0.435405	-0.776905	-0.393092
O	-0.487623	-0.753334	2.090687
O	3.460951	1.444803	-0.388311
O	4.929552	3.611066	0.381783
O	2.301660	3.968938	-0.943467
O	-2.090603	1.468724	1.822212
O	0.753639	-4.820912	-0.051277
O	-1.047852	-3.617478	1.880884
O	-1.271439	-3.006128	-0.865848
O	2.756806	-0.989342	-1.902170
H	-0.813155	0.504970	-0.852919
H	-1.947324	1.201025	-0.090623
H	-1.504189	-3.192752	0.063316
H	-0.710828	-2.210857	-0.784297
H	1.607916	-4.359974	-0.178777
H	0.113904	-4.293216	-0.564032
H	2.840649	1.124328	0.317510
H	2.939719	2.127762	-0.852691

H	-1.427876	2.165981	1.721404
H	-1.555877	0.662633	2.003275
H	-0.783493	-2.705093	2.095114
H	-0.260778	-4.037639	1.485603
H	1.872984	-0.944524	-1.481512
H	3.216157	-0.238871	-1.492289
H	5.269996	3.768217	-0.502099
H	4.516200	2.720156	0.292862
H	1.488068	3.748218	-0.432730
H	-0.390986	2.532811	-0.193447
H	2.986077	4.146490	-0.283118
H	0.651664	2.235680	0.886952
H	2.788237	-2.777422	0.467819
O	3.132187	-3.295712	-0.287041
H	3.115852	-2.627527	-0.998369

$SO_4^{2-}(H_2O)_{12}$

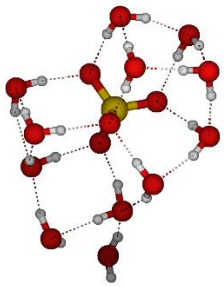

Figure S_{120} : SO_4^{2-} optimized structure with 12 water molecules.

E = -1227.817332

H = -1227.816388

O	-1.455601	1.311474	-0.922607
O	0.194336	3.011425	0.467579
O	1.575818	0.834777	1.309777
S	0.821236	-0.610577	1.173881
O	-0.505689	-0.619685	2.099897
O	1.830831	-1.788513	1.601613
O	0.366159	-0.780570	-0.403107
O	3.447508	1.510008	-0.485587

O	4.940514	3.642076	0.360963
O	3.290614	-3.045774	-0.459454
O	-2.075630	1.638259	1.817939
O	2.316855	4.048423	-0.934360
O	2.647785	-0.814654	-2.029927
O	1.247677	-4.970608	-0.344116
O	-0.946053	-3.301846	-0.744160
O	-1.643952	-3.246656	1.954448
H	-0.865691	0.532541	-0.854644
H	-1.957534	1.293557	-0.086368
H	-1.344729	-3.352369	0.151463
H	-0.508437	-2.431179	-0.733816
H	2.008271	-4.371458	-0.498322
H	0.460946	-4.440719	-0.600761
H	2.847580	1.157857	0.220701
H	2.928562	2.230149	-0.896012
H	-1.400829	2.319473	1.684313
H	-1.551650	0.831254	2.013768
H	-1.365232	-2.319614	2.069932
H	-0.837006	-3.753136	2.199256
H	1.783139	-0.814895	-1.572144
H	3.104393	-0.056731	-1.627614
H	5.301603	3.821537	-0.510360
H	4.530463	2.754585	0.241949
H	1.507103	3.818659	-0.422249
H	-0.360382	2.561737	-0.211455
H	3.008265	4.215259	-0.278057
H	0.686561	2.252805	0.862280
H	2.898868	-2.603785	0.316442
H	3.180226	-2.367947	-1.155447
H	1.222893	-3.446502	2.245642
O	0.860616	-4.347622	2.324441
H	1.018233	-4.718767	1.425352

$SO_4^{2-}(H_2O)_{13}$

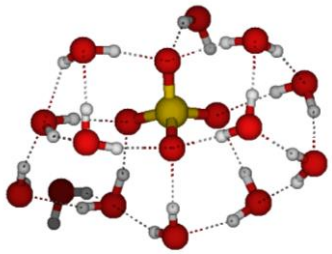

Figure S_{121} : SO_4^{2-} optimized structure with 13 water molecules.

E = -1304.225205

H = -1304.224260

O	-1.380228	1.385859	-1.300812
O	0.144383	3.097572	0.248338
O	1.462385	0.894344	1.081299
S	0.736035	-0.562618	1.025633
O	0.253683	-0.835841	-0.515531
O	-0.569846	-0.556454	1.996515
O	1.782300	-1.690274	1.520712
O	3.456964	1.495827	-0.596316
O	4.912682	3.444976	0.697166
O	2.481224	4.113219	-0.830446
O	-2.204507	1.634366	1.369188
O	2.514967	-0.726928	-2.221497
O	3.157106	-2.958962	-0.647234
O	1.203011	-4.959285	-0.437476
O	1.109427	-4.379099	2.252382
O	-1.447623	-3.334349	2.201721
O	-1.084675	-3.382796	-0.557457
H	-0.829156	0.589312	-1.179608
H	-1.947236	1.378342	-0.505804
H	-1.360918	-3.431995	0.383605
H	-0.680289	-2.500339	-0.628053
H	1.918491	-4.323453	-0.648261
H	0.370488	-4.461108	-0.593790

H	2.805254	1.159045	0.067401
H	3.024737	2.297255	-0.955796
H	-1.534942	2.332453	1.328900
H	-1.701553	0.843247	1.654684
H	-1.212043	-2.392986	2.261712
H	-0.599001	-3.807017	2.357405
H	1.658527	-0.748430	-1.754085
H	2.986727	0.011851	-1.800086
H	5.438698	3.690223	-0.067398
H	4.507189	2.594922	0.415486
H	1.606131	3.902735	-0.433500
H	-0.336808	2.665855	-0.492732
H	3.104424	4.178823	-0.091967
H	0.598725	2.327985	0.662659
H	2.803367	-2.518105	0.145173
H	3.036982	-2.280425	-1.340437
H	1.415238	-3.464508	2.137172
H	1.170447	-4.742993	1.337930
H	0.289054	-0.690513	3.825603
O	1.035457	-0.919333	4.398551
H	1.661303	-1.251313	3.744010

$SO_4^{2-}(H_2O)_{14}$

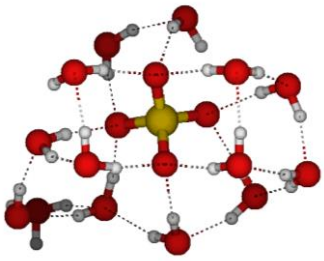

Figure S_{122} : SO_4^{2-} optimized structure with 14 water molecules.

E = -1380.640360

H = -1380.639415

O	-1.440615	1.319131	-0.926902
O	0.186164	2.869045	0.648291

O	1.556446	0.591497	1.431159
S	0.784522	-0.813825	1.105456
O	1.743693	-2.060676	1.485479
O	0.395547	-0.815767	-0.478795
O	-0.575814	-0.905357	1.997091
O	3.463112	1.425532	-0.351964
O	4.974820	3.594356	0.442836
O	2.314045	3.924227	-0.732982
O	-2.155373	1.376303	1.784813
O	2.749850	-0.750566	-2.059052
O	3.252474	-3.134560	-0.708129
O	1.173736	-4.973732	-1.084528
O	0.564430	-4.697862	1.572027
O	-1.859365	-3.454368	1.228323
O	-0.939242	-3.185710	-1.384146
O	2.252040	0.775807	4.332737
H	-0.863805	0.532435	-0.909888
H	-1.973883	1.232616	-0.113572
H	-1.426507	-3.349667	-0.548364
H	-0.470363	-2.357061	-1.187772
H	1.957643	-4.384215	-1.074537
H	0.423059	-4.389818	-1.329164
H	2.882196	1.033103	0.338455
H	2.937909	2.171283	-0.713163
H	-1.485642	2.074561	1.780306
H	-1.642263	0.559874	1.955113
H	-1.581512	-2.571543	1.522314
H	-1.084782	-4.021836	1.447724
H	1.864930	-0.764550	-1.651188
H	3.190206	-0.019244	-1.591158
H	5.297551	3.759336	-0.446290
H	4.588952	2.695292	0.366329
H	1.510261	3.710652	-0.206677
H	-0.354257	2.469405	-0.072504

H	3.012239	4.135379	-0.096495
H	0.665638	2.094772	1.012345
H	2.859200	-2.781962	0.108180
H	3.208494	-2.366866	-1.313635
H	0.994188	-3.831326	1.659891
H	0.790520	-4.960536	0.647929
H	2.132778	0.827518	3.374263
H	1.820736	-0.068625	4.542224
H	1.499005	-2.111306	3.618058
O	0.913373	-1.774632	4.311140
H	0.164443	-1.464995	3.775718

$SO_4^{2-}(H_2O)_{15}$

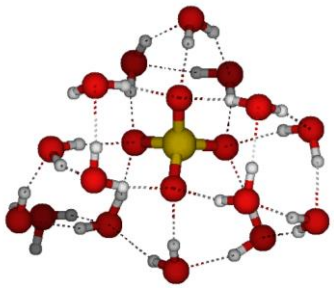

Figure S_{123} : SO_4^{2-} optimized structure with 15 water molecules.

E = -1457.059131

H = -1457.058186

O	-1.429150	1.343053	-0.938344
O	0.218253	2.781908	0.711426
O	2.337872	3.891756	-0.642580
O	1.591991	0.472708	1.420126
S	0.802361	-0.913842	1.035058
O	-0.530738	-1.035333	1.956296
O	1.780046	-2.173833	1.300951
O	0.375943	-0.821076	-0.531711
O	3.456738	1.370024	-0.396536
O	4.997475	3.484071	0.495408
O	-2.139961	1.267661	1.767001

O	2.667127	-0.694821	-2.204842
O	3.171252	-3.169313	-1.031415
O	1.038810	-4.952658	-1.384693
O	0.518943	-4.808209	1.301066
O	-1.883275	-3.516620	1.077235
O	-1.047016	-3.114465	-1.539594
O	0.246253	-1.271042	4.731032
O	2.282799	0.598935	4.185352
H	-0.861409	0.550345	-0.946082
H	-1.971004	1.225774	-0.134685
H	-1.508983	-3.313134	-0.696290
H	-0.550258	-2.310368	-1.316308
H	1.833204	-4.378232	-1.391227
H	0.289468	-4.349099	-1.580264
H	2.886525	0.956992	0.289133
H	2.938312	2.141805	-0.711499
H	-1.462322	1.957960	1.794496
H	-1.640341	0.441200	1.917077
H	-1.590300	-2.659699	1.425556
H	-1.111824	-4.105907	1.247702
H	1.798769	-0.723887	-1.764979
H	3.135095	-0.000244	-1.708748
H	5.338650	3.690094	-0.378100
H	4.607086	2.592898	0.369446
H	1.539258	3.665403	-0.114796
H	-0.328182	2.424691	-0.027524
H	3.047505	4.071043	-0.008648
H	0.697964	1.989394	1.031650
H	2.822364	-2.860246	-0.179545
H	3.120364	-2.364588	-1.585962
H	0.983358	-3.969019	1.445944
H	0.720966	-5.016087	0.357296
H	2.105722	0.656999	3.229986
H	1.469221	0.186091	4.534259

H	1.033570	-1.837107	4.614659
H	-0.141137	-1.236400	3.839604
H	2.577814	-2.252997	3.051104
O	2.823148	-2.158944	3.987306
H	2.943373	-1.195796	4.092374

$SO_4^{2-}(H_2O)_{16}$

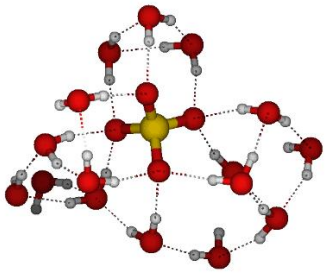

Figure S_{124} : SO_4^{2-} optimized structure with 16 water molecules.

E = -1533.464941

H = -1533.463997

O	-1.341994	1.607077	-1.074981
O	0.253975	3.046856	0.645428
O	2.595209	3.947317	-0.516087
O	3.411223	1.299864	-0.350341
O	1.425276	0.685446	1.453703
S	0.594101	-0.691849	1.133249
O	0.217182	-0.700685	-0.451851
O	-0.776398	-0.731266	2.003184
O	1.491013	-1.965802	1.525355
O	5.106421	3.174041	0.768754
O	-2.249638	1.628230	1.567077
O	2.401151	-0.626665	-2.225898
O	3.254059	-3.222952	-2.558040
O	1.199763	-4.833042	-1.462824
O	1.081110	-5.533556	1.468376
O	-1.183041	-3.820940	1.729536
O	-0.946681	-3.275860	-0.969965
O	1.978305	0.736362	4.286679

O	2.139949	-2.083267	4.289893
O	-0.317194	-0.824500	4.807540
H	-0.826999	0.781070	-1.012552
H	-1.943358	1.550240	-0.307934
H	-1.179976	-3.523036	-0.047416
H	-0.603206	-2.369358	-0.882025
H	1.781468	-4.368979	-2.096840
H	0.391954	-4.268242	-1.360508
H	2.779622	0.970214	0.327221
H	3.007911	2.138199	-0.662164
H	-1.538974	2.280777	1.636607
H	-1.814811	0.778318	1.781202
H	-0.958697	-2.926244	2.020573
H	-0.364057	-4.348464	1.805907
H	1.591534	-0.673900	-1.685091
H	2.964554	-0.017006	-1.719440
H	5.555874	3.390460	-0.051473
H	4.638378	2.340613	0.546618
H	1.737445	3.797726	-0.060037
H	-0.251128	2.700447	-0.126032
H	3.273265	4.000540	0.173476
H	0.657199	2.234302	1.017146
H	3.591750	-3.352660	-1.658999
H	2.953671	-2.286942	-2.545586
H	1.895910	-5.009805	1.521547
H	0.988480	-5.642526	0.511197
H	1.879428	0.805756	3.321498
H	1.094073	0.449252	4.585844
H	0.400586	-1.487706	4.789525
H	-0.605783	-0.795786	3.878176
H	1.970731	-2.174274	3.335313
H	2.401141	-1.146553	4.368197
H	2.684960	-3.006837	0.642869
O	3.094299	-3.823170	0.299522

H	2.390517	-4.191529	-0.275030

$SO_4^{2-}(H_2O)_{17}$

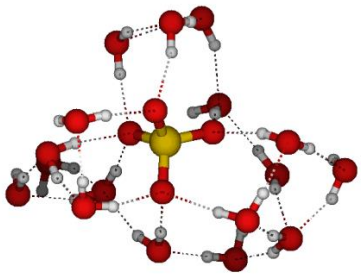

Figure S_{125} : SO_4^{2-} optimized structure with 17 water molecules.

E = -1609.871986

H = -1609.871042

O	-1.424496	1.869140	-1.004714
O	0.441264	3.010838	0.637530
O	1.399746	0.469172	1.429220
S	0.185318	-0.623544	1.178313
O	0.721337	-2.097858	1.573357
O	-0.206799	-0.599089	-0.399324
O	-1.061697	-0.228353	2.114024
O	3.285524	-4.228470	0.376219
O	3.298867	1.160325	-0.408777
O	5.280476	2.867860	0.470763
O	2.722430	3.832021	-0.619321
O	1.172842	-4.684602	-1.625221
O	-1.100605	-3.267637	-1.183522
O	-0.899232	-4.411599	1.330179
O	-2.259426	2.231453	1.630448
O	2.080249	-0.611024	-2.174290
O	3.289872	-3.046936	-2.308806
O	2.278283	-1.624083	5.128463
O	-0.409251	-0.611059	4.891268
O	1.784974	0.988212	4.238631
O	1.137477	-6.280543	0.578046
H	-1.078625	0.959211	-0.931666

H	-2.010849	1.957438	-0.228382
H	-1.217250	-3.710446	-0.314186
H	-0.853924	-2.355155	-0.957274
H	1.877155	-4.175041	-2.078405
H	0.363069	-4.121430	-1.589999
H	2.652553	0.834763	0.258352
H	2.959905	2.040572	-0.687615
H	-1.449750	2.761579	1.646875
H	-1.941854	1.338023	1.870994
H	-0.393375	-3.619773	1.581508
H	-0.231671	-5.108437	1.175929
H	1.277186	-0.633998	-1.624621
H	2.652031	0.038547	-1.726518
H	5.637461	3.022806	-0.406996
H	4.704919	2.086373	0.334941
H	1.884951	3.725890	-0.112342
H	-0.137083	2.710493	-0.104745
H	3.441232	3.877535	0.026839
H	0.767549	2.173442	1.023995
H	3.631918	-3.221118	-1.419984
H	2.868368	-2.156106	-2.275636
H	1.973696	-5.927480	0.908839
H	1.118251	-5.904628	-0.328855
H	1.714314	0.856749	3.276878
H	0.904657	0.712599	4.562707
H	0.329299	-1.240851	4.971229
H	-0.704579	-0.655054	3.965595
H	2.629890	-2.066380	4.339136
H	2.342075	-0.674730	4.904068
H	3.294340	-3.591255	1.114403
H	2.419596	-4.147354	-0.054711
H	2.207221	-2.173577	2.177894
O	3.148361	-2.326337	2.465276
H	3.596509	-1.512015	2.219527

$SO_4^{2-}(H_2O)_{18}$

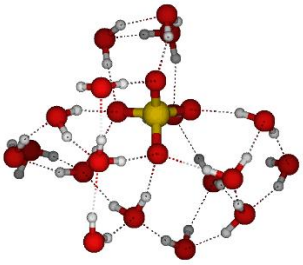

Figure S_{126} : SO_4^{2-} optimized structure with 18 water molecules.

E = -1686.282243

H = -1686.281299

O	-0.500740	1.647566	-1.564160
O	0.776625	2.965359	0.499433
O	3.351619	3.614763	-0.209163
O	3.560687	0.874243	-0.118403
O	1.431422	0.424223	1.518290
S	0.218983	-0.644232	1.170988
O	-1.154258	-0.095184	1.798005
O	0.600477	-2.073693	1.814125
O	0.123840	-0.785743	-0.451221
O	3.067973	-2.244684	2.686935
O	5.509140	2.316056	1.256250
O	-2.098218	2.272780	0.622009
O	2.472046	-0.833276	-2.022382
O	3.751822	-3.302217	-2.224863
O	1.542685	-4.746404	-1.407774
O	-0.789329	-3.411807	-1.239557
O	1.405823	-6.241969	0.855472
O	-0.801357	-4.474332	1.306214
O	3.495079	-4.115780	0.576989
O	-0.854204	-0.433631	4.674545
O	1.421423	1.131561	4.309481
O	1.795438	-1.477483	5.263236
H	-0.310760	0.737951	-1.251550
H	-1.313622	1.884349	-1.075787

H	-0.972041	-3.840740	-0.373587
H	-0.579358	-2.490936	-1.010261
H	2.247178	-4.330500	-1.944404
H	0.714735	-4.212513	-1.489960
H	2.804194	0.652404	0.471616
H	3.399120	1.801765	-0.403478
H	-1.324828	2.805155	0.858525
H	-1.908305	1.413176	1.047099
H	-0.390825	-3.649936	1.618439
H	-0.075511	-5.127383	1.265304
H	1.660385	-0.956847	-1.494568
H	3.007402	-0.223230	-1.475902
H	6.065954	2.500834	0.496200
H	4.916847	1.608715	0.929555
H	2.426078	3.591534	0.117707
H	0.467151	2.608751	-0.363870
H	3.928600	3.535145	0.564017
H	0.960246	2.153506	1.012551
H	4.015701	-3.452992	-1.303574
H	3.346946	-2.409412	-2.229008
H	2.206455	-5.827866	1.203220
H	1.425444	-5.934179	-0.074948
H	1.485332	0.943632	3.357112
H	0.504387	0.865919	4.520673
H	-0.146342	-1.082866	4.832494
H	-1.059799	-0.485107	3.726160
H	2.261166	-1.926254	4.542416
H	1.886722	-0.528826	5.046099
H	3.412861	-3.473695	1.306248
H	2.649233	-4.115358	0.095624
H	2.128605	-2.144719	2.383701
H	3.461381	-1.390112	2.487607
H	1.666963	0.394395	-3.455756
O	1.175129	1.058874	-3.960801

H 0.536117 1.407736 -3.325628

$LiCl(H_2O)_1$

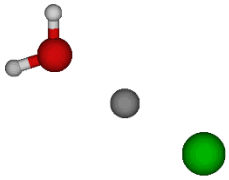

Figure S_{127} : LiCl optimized structure with 1 water molecule.

E = -91.731214

H = -91.730270

Li	0.506097	0.000000	0.652537
Cl	-0.844298	0.000000	2.301953
O	1.783250	0.000000	-0.809230
H	1.587068	0.000000	-1.751535
H	2.742032	0.000000	-0.723235

$LiCl(H_2O)_2$

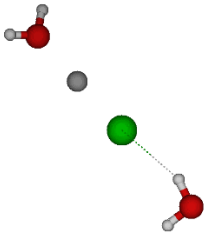

Figure S_{128} : LiCl optimized structure with 2 water molecules.

E = -168.106856

H = -168.105912

O	2.378238	-0.021140	-1.132596
Li	0.855712	-0.006077	0.055058
Cl	-0.808585	0.030516	1.398144
H	2.384229	0.205979	-2.068072
H	3.289820	-0.211762	-0.888356

H	-2.506577	0.169861	3.108249
O	-3.393936	0.087413	3.484410
H	-3.899470	-0.254790	2.741134

$LiCl(H_2O)_3$

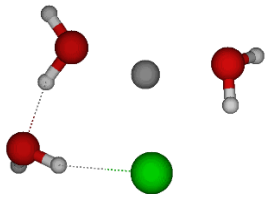

Figure S_{129} : LiCl optimized structure with 3 water molecules.

E = -244.527277

H = -244.526333

O	1.225034	0.690723	0.547026
Li	0.359457	-0.601363	-0.522393
Cl	-1.610509	-1.400868	0.376211
O	-0.479456	0.562989	2.521393
H	1.997885	1.253710	0.613019
H	0.686002	0.768877	1.385879
H	-0.930462	-0.193636	2.082112
H	-1.135604	1.268041	2.483684
O	0.151205	-1.683991	-2.156745
H	-0.134623	-1.345743	-3.011390
H	-0.639243	-2.092092	-1.756311

$LiCl(H_2O)_4$

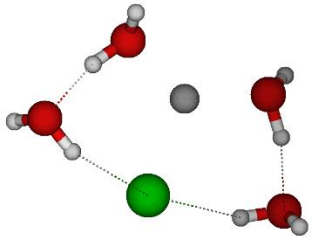

Figure S_{130}: LiCl optimized structure with 4 water molecules.

E = -320.919230

H = -320.918286

O	1.332081	0.549182	0.285226
Li	-0.235635	-0.464490	-0.188455
O	-0.577003	-1.798787	-1.535576
Cl	-1.935387	-0.291120	1.381376
O	0.384646	1.409543	2.590027
H	2.213471	0.174478	0.367133
H	1.110290	0.958662	1.168281
H	-0.409704	0.840239	2.497200
H	0.034774	2.306015	2.535803
H	-0.659589	-1.633428	-2.478845
H	-1.431026	-2.227453	-1.244579
H	-2.833705	-1.889541	0.171519
O	-2.835784	-2.633746	-0.469286
H	-2.727574	-3.416679	0.082197

$LiCl(H_2O)_5$

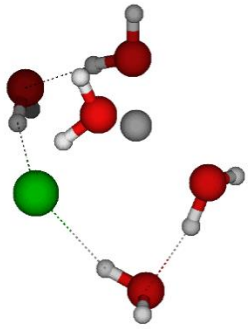

Figure S_{131}: LiCl optimized structure with 5 water molecules.

E = -397.309407

H = -397.308462

O	1.225334	0.833070	0.022525
Li	0.459615	-0.969602	0.056138
O	-0.574563	-1.438945	-1.534124
Cl	-1.185555	-1.007888	2.055609
O	-2.906022	-1.968307	-0.371179
O	-0.043434	1.876260	2.090639
H	2.163123	1.039662	0.060076
H	0.797066	1.339861	0.767242
H	-0.467276	1.015957	2.307822
H	-0.780492	2.447369	1.847729
H	-0.695192	-0.753971	-2.198332
H	-1.486736	-1.688471	-1.227878
H	-2.589353	-1.617676	0.489047
H	-3.038830	-2.908694	-0.208668
O	1.321563	-2.444526	1.108239
H	0.628800	-2.332806	1.789508
H	2.161660	-2.398051	1.574393

$LiCl(H_2O)_6$

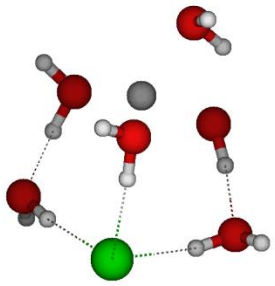

Figure S_{132}: LiCl optimized structure with 6 water molecules.

E = -473.695741

H = -473.694796

O	1.390657	1.059654	0.364508
Li	1.262357	-0.868208	0.109131
O	-0.089021	-1.253489	-1.374067
O	0.970033	-2.028512	1.666885
Cl	-1.759543	-1.002318	2.451299
O	-0.446802	1.770500	2.101020
O	-2.364619	-2.038461	-0.375092
H	2.213754	1.497624	0.597630
H	0.701567	1.396348	1.007574
H	-0.884194	0.914913	2.329428
H	-1.162729	2.310381	1.749549
H	-0.322078	-0.468216	-1.880188
H	-0.961696	-1.624000	-1.039746
H	-2.313936	-1.665147	0.539219
H	-2.482011	-2.984530	-0.237863
H	0.062519	-1.795717	2.001363
H	1.528038	-2.007935	2.450447
O	2.528451	-1.863987	-1.162369
H	1.709446	-1.999876	-1.670102
H	2.782341	-2.736591	-0.843968

$LiCl(H_2O)_7$

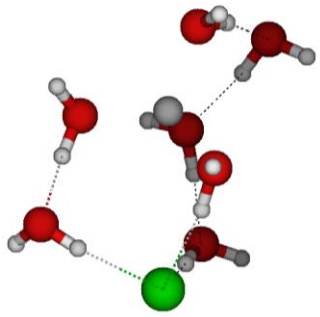

Figure S_{133}: LiCl optimized structure with 7 water molecules.

E = -550.083168

H = -550.082224

O	1.208919	1.059436	0.854526
Li	1.367601	-0.899003	0.794351
O	0.520096	-1.977311	2.204680
O	0.411576	-1.273578	-0.980684
O	2.393886	-3.044846	-1.565317
O	-2.131604	-1.681524	-0.699746
O	-0.925764	1.840302	2.188111
Cl	-2.319062	-0.914865	2.245959
H	1.958542	1.576690	1.162135
H	0.409701	1.409393	1.341662
H	-1.413140	0.992795	2.325568
H	-1.542965	2.381250	1.683996
H	0.453653	-0.432518	-1.450802
H	-0.572528	-1.487598	-0.900745
H	-2.311513	-1.382722	0.228072
H	-2.440719	-2.593468	-0.718658
H	-0.439418	-1.724389	2.256904
H	0.816164	-1.966362	3.120010
H	1.584611	-2.487027	-1.552887
H	2.102997	-3.908539	-1.253856
O	3.237120	-1.501208	0.445451
H	3.743580	-1.972155	1.112887
H	3.115108	-2.134599	-0.306811

$LiCl(H_2O)_8$

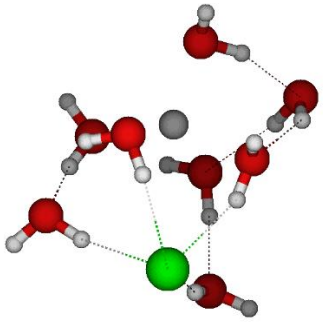

Figure S_{134}: LiCl optimized structure with 8 water molecules.

E = -626.465516

H = -626.464572

O	1.191611	1.153015	0.194182
Li	1.469069	-0.892445	0.876444
O	0.724564	-2.871525	1.546670
O	3.317885	-1.366792	0.268599
O	0.383380	-1.167536	-0.936786
O	-2.267889	-1.345940	-0.585974
O	-0.543751	1.728191	2.181790
O	2.051599	-3.363071	-0.951913
Cl	-1.728596	-1.155813	2.489221
H	1.971086	1.714310	0.243150
H	0.527868	1.526305	0.818469
H	-1.068877	0.898343	2.260490
H	-1.174359	2.447940	2.283945
H	0.542562	-0.235393	-1.144467
H	-0.601662	-1.270371	-0.887291
H	-2.276973	-1.254368	0.390841
H	-2.658322	-2.210151	-0.753432
H	-0.182925	-2.565101	1.763511
H	1.096658	-3.125172	2.398741
H	1.465121	-2.679390	-1.329105
H	1.565294	-3.592137	-0.142122
H	3.979857	-1.644534	0.908019
H	3.061987	-2.179237	-0.244288

O	1.289190	-0.344458	2.865795
H	0.400163	-0.710708	3.044130
H	1.137581	0.605616	2.965807

$LiCl(H_2O)_9$

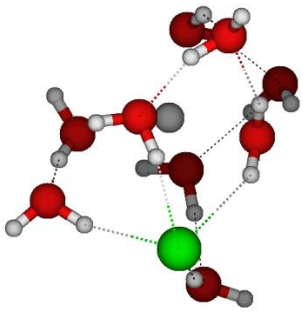

Figure S_{135}: LiCl optimized structure with 9 water molecules.

E = -702.852976

H = -702.852032

O	0.982042	1.219203	-0.076096
Li	1.325228	-0.792090	0.515238
O	3.262975	-1.184448	0.145777
O	1.357353	-0.140780	2.669186
O	0.181217	-1.165431	-1.183239
O	0.914100	-2.732983	1.363954
O	2.079346	-3.233617	-1.194910
O	-2.339641	-1.544438	-0.373368
O	-0.501762	1.880565	2.099543
Cl	-1.560296	-1.014061	2.628512
H	1.804003	1.719741	-0.079625
H	0.406766	1.622487	0.611764
H	-1.029094	1.061746	2.249132
H	-1.103450	2.614684	2.258609
H	0.208946	-0.240972	-1.462420
H	-0.768789	-1.355749	-0.969102
H	-2.235601	-1.356538	0.583742
H	-2.664575	-2.450190	-0.409865
H	0.073272	-2.602902	1.835310
H	1.613913	-2.795079	2.043356
H	1.438277	-2.607842	-1.576267
H	1.630947	-3.476438	-0.367831

H	3.598203	-1.551691	0.979149
H	3.080197	-1.968914	-0.425909
H	0.462234	-0.514290	2.855442
H	1.215311	0.811851	2.764730
O	3.137219	-2.111892	2.859054
H	3.559662	-2.393824	3.675509
H	2.654990	-1.277827	3.045917

$LiCl(H_2O)_{10}$

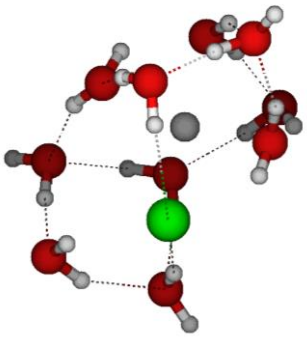

Figure S_{136}: LiCl optimized structure with 10 water molecules.

E = -779.247697

H = -779.246753

O	0.579707	1.862830	-0.666676
Li	1.343050	-1.159928	0.749825
O	3.351536	-1.648027	0.143649
O	0.279943	-0.854265	-0.944863
O	0.998409	-3.067267	1.420346
O	2.355322	-0.394295	3.584658
O	3.313358	-2.688942	2.737195
O	-2.264715	-0.734207	0.073763
O	-1.552356	1.858154	0.847155
O	1.772602	-3.268314	-1.346043
Cl	-0.719340	-0.793409	2.673436
H	0.635333	2.653298	-1.211915
H	-0.240789	1.954061	-0.091738
H	-1.259897	1.463532	1.686623
H	-2.078238	1.135784	0.455600
H	0.412627	0.096427	-1.141287
H	-0.679283	-0.932684	-0.753194
H	-1.919069	-0.917754	0.982831
H	-3.056316	-1.271544	-0.034202
H	0.253648	-2.824915	1.997813
H	1.774322	-3.186952	2.012928
H	1.211414	-2.509497	-1.581248
H	1.358346	-3.591365	-0.529068

H	3.642202	-2.140262	0.933129
H	3.018095	-2.313855	-0.503406
H	1.389119	-0.494695	3.660544
H	2.447801	0.217542	2.829224
H	3.846611	-3.162946	3.381774
H	3.023056	-1.827098	3.159755
O	2.313782	0.666356	1.019930
H	3.020342	0.257242	0.492675
H	1.832569	1.299175	0.442862

$LiCl(H_2O)_{11}$

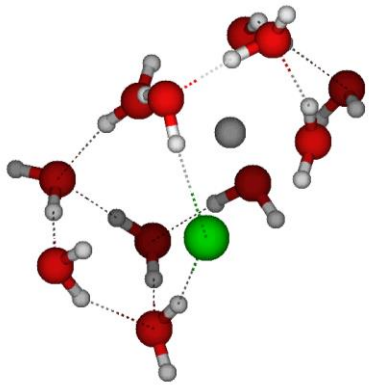

Figure S_{137}: LiCl optimized structure with 11 water molecules.

E = -855.632056

H = -855.632056

O	0.499879	2.043950	-0.476550
O	-1.340182	2.100177	1.378728
O	2.162363	0.307000	0.696512
Li	1.480604	-1.620179	0.615711
O	-0.820765	0.022104	-1.899364
O	1.302297	-3.394160	1.674253
O	3.557402	-1.942033	0.270521
O	3.460238	-2.526164	3.021082
O	2.197960	-0.258268	3.397204
O	2.419666	-4.108150	-0.905245
O	-2.682932	-0.012571	0.209754
Cl	-0.744581	-1.110588	2.294627
H	0.713963	2.932119	-0.779115
H	-0.189169	2.142165	0.251665
H	-1.012440	1.507717	2.073776
H	-2.031484	1.552098	0.954004
H	-0.319122	0.795668	-1.573833
H	-1.616049	0.007586	-1.333379
H	-2.159212	-0.524841	0.874191
H	-3.599750	-0.284054	0.323211
H	0.487798	-3.149130	2.144819
H	2.035720	-3.302322	2.323198

H	1.765591	-3.531429	-1.336245
H	1.989523	-4.304669	-0.057273
H	3.847193	-2.223923	1.157079
H	3.401527	-2.770184	-0.241235
H	1.247992	-0.470135	3.428922
H	2.287819	0.164017	2.518570
H	3.997760	-2.824374	3.760384
H	3.046205	-1.650460	3.280086
H	2.961674	0.056001	0.211004
H	1.679894	1.020493	0.214523
O	0.402928	-2.104180	-1.000444
H	-0.347189	-2.595658	-0.645966
H	-0.013493	-1.301477	-1.444199

$LiCl(H_2O)_{12}$

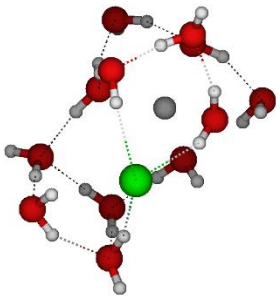

Figure S_{138}: LiCl optimized structure with 12 water molecules.

E = -932.020813

H = -932.019869

O	0.254137	1.943355	-0.414305
O	-1.519459	2.114985	1.497310
O	2.143695	0.204004	0.440558
Li	1.584877	-1.702929	0.407001
O	0.217302	-2.202953	-0.957885
O	1.067715	-3.214933	1.725705
O	3.500360	-2.500205	0.148552
O	-1.083343	-0.093995	-1.769952
O	3.420608	-2.609456	2.893762
O	2.347870	-0.249150	3.138896

O	1.911001	-4.505438	-0.667261
O	-2.837253	-0.088481	0.427654
Cl	-0.824093	-0.934099	2.565208
H	0.472074	2.821923	-0.741195
H	-0.398954	2.072182	0.341605
H	-1.176503	1.538410	2.200675
H	-2.221925	1.558403	1.106570
H	-0.578385	0.686319	-1.462897
H	-1.850106	-0.117130	-1.165365
H	-2.271051	-0.524689	1.111044
H	-3.735709	-0.392387	0.593703
H	0.327634	-2.769817	2.187806
H	1.820220	-3.219528	2.355020
H	1.353983	-3.911211	-1.197402
H	1.474087	-4.472782	0.201349
H	3.741907	-2.651283	1.086418
H	3.154340	-3.355291	-0.209472
H	1.392144	-0.375279	3.278915
H	2.388123	0.111821	2.226547
H	3.972661	-2.883350	3.631810
H	3.089834	-1.677629	3.086031
H	2.959543	0.253359	-0.118601
H	1.514003	0.898321	0.136211
H	-0.478014	-2.614240	-0.430667
H	-0.238036	-1.405752	-1.376884
O	4.354135	-0.207021	-1.011398
H	4.209983	-0.245937	-1.962604
H	4.263139	-1.134080	-0.699355

$LiCl(H_2O)_{13}$

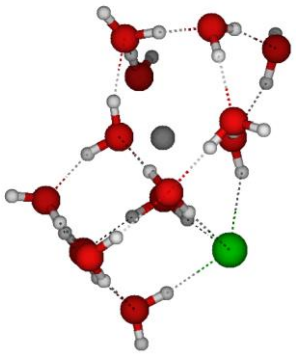

Figure S_{139}: LiCl optimized structure with 13 water molecules.

E = -1008.410925

H = -1008.409981

O	0.200349	2.017688	-0.556036
O	-0.578886	2.098967	1.914284
O	1.747403	-0.094475	-0.099179
Li	1.008189	-1.855819	-0.790574
O	-0.907427	-1.953459	-1.068156
O	1.293458	-3.150801	0.791014
O	4.775584	-2.566829	0.879957
O	-2.035523	0.467227	-1.336394
O	4.226450	-0.828557	-0.916558
O	3.375106	-4.864989	0.355777
O	2.808947	-2.084738	2.830540
O	1.035234	-0.148797	2.519381
O	-2.750705	0.450781	1.415522
Cl	-1.340122	-2.180048	2.160907
H	0.417299	2.890741	-0.896756
H	-0.096368	2.139459	0.405050
H	0.019910	1.467505	2.360046
H	-1.435219	1.623432	1.865691
H	-1.282808	1.080276	-1.240727
H	-2.477283	0.510481	-0.468410
H	-2.385536	-0.429986	1.676019
H	-3.624671	0.494944	1.817387

H	0.395086	-3.183264	1.183624
H	1.844067	-2.794078	1.527523
H	3.381198	-5.318480	-0.491875
H	2.480333	-4.476225	0.447231
H	4.274910	-2.323229	1.681126
H	4.406183	-3.445470	0.630123
H	0.259265	-0.757414	2.495227
H	1.320379	-0.095101	1.573848
H	2.709493	-2.566562	3.658346
H	2.236600	-1.272255	2.902367
H	2.697408	-0.097653	-0.348559
H	1.315646	0.734434	-0.424645
H	-1.301840	-2.198580	-0.214053
H	-1.348086	-1.092945	-1.297386
H	5.019484	-0.339000	-1.153548
H	4.491576	-1.512989	-0.207889
O	2.274975	-2.006878	-2.309005
H	2.451228	-2.755736	-2.882914
H	3.135291	-1.630427	-2.017003

$NaCl(H_2O)_1$

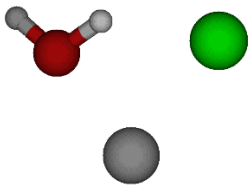

Figure S_{140} : NaCl optimized structure with 1 water molecule.

E = -91.717663

H = -91.716719

Na	-0.410428	-0.382807	-0.153357
Cl	0.692933	0.324101	2.007337
O	1.624558	0.148962	-0.875909
H	2.421611	0.325446	-1.375549
H	1.801481	0.359970	0.067969

$NaCl(H_2O)_2$

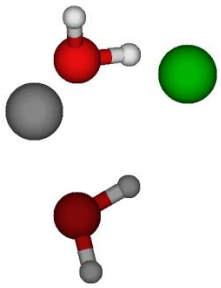

Figure S_{141} : NaCl optimized structure with 2 water molecules.

E = -168.088613

H = -168.087669

Na	0.204280	0.995867	0.733156
Cl	0.816195	-1.556512	0.238895
O	1.053614	0.284889	2.682056
H	1.141875	-0.584195	2.229604
H	1.764858	0.327097	3.326513

H	-1.053175	-0.575821	-0.525254
O	-1.537156	0.279975	-0.496464
H	-2.464966	0.053028	-0.388661

$NaCl(H_2O)_3$

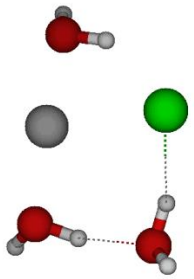

Figure S_{142} : NaCl optimized structure with 3 water molecules.

E = -244.481600

H = -244.480656

Na	0.454281	0.939294	1.148771
Cl	0.435126	0.367210	3.743846
O	2.453969	-0.062470	1.456972
H	2.186441	-0.149520	2.396428
H	2.942139	-0.862120	1.243203
O	-1.600653	0.530671	0.415643
H	-2.004908	0.041477	-0.305153
H	-2.045607	0.211597	1.250086
O	-2.433138	-0.305892	2.779216
H	-1.553028	-0.267042	3.224022
H	-2.963888	0.332467	3.268295

$NaCl(H_2O)_4$

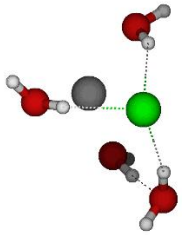

Figure S_{143} : NaCl optimized structure with 4 water molecules.

E = -320.873902

H = -320.872958

O	2.218661	-0.184721	1.455827
Na	0.360919	1.074610	1.054658
O	-1.554340	0.205669	0.287019
O	-2.411185	-0.595262	2.669728
Cl	0.335361	0.274187	3.865468
H	1.919373	-0.269214	2.386426
H	2.581894	-1.042614	1.219718
H	-1.802837	-0.414574	-0.402742
H	-1.991719	-0.121000	1.118663
H	-1.569801	-0.480440	3.168214
H	-3.018918	0.017193	3.098258
O	0.426606	2.958185	2.340201
H	1.069771	3.643599	2.541546
H	0.396448	2.381716	3.133445

$NaCl(H_2O)_5$

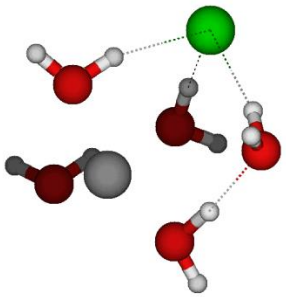

Figure S_{144} : NaCl optimized structure with 5 water molecules.

E = -397.261393

H = -397.260448

O	1.638980	0.089099	0.789799
Na	-0.341041	1.543629	0.607619
O	-2.151049	0.211406	0.636929
O	-0.285702	2.863719	2.455803
O	-1.932276	-0.819921	3.078605
Cl	0.895558	0.343700	3.713545
H	1.609876	0.142276	1.780352
H	1.706814	-0.851173	0.597716
H	-2.501107	-0.447019	0.031856
H	-2.161656	-0.212284	1.536712
H	-1.010992	-0.589022	3.341547
H	-2.477273	-0.362938	3.728267
H	0.052788	3.714980	2.744969
H	0.104237	2.198887	3.071668
O	1.256853	2.077882	-0.972450
H	1.835863	2.821881	-1.157481
H	1.797199	1.409887	-0.509405

$NaCl(H_2O)_6$

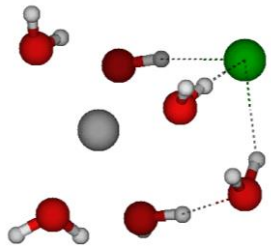

Figure S_{145} : NaCl optimized structure with 6 water molecules.

E = -473.664997

H =-473.646425

O	1.332449	0.109464	0.362037
Na	-0.400252	1.855988	0.639099
O	-2.279001	0.276527	0.846660
O	-0.166597	2.206552	2.949469
O	1.514543	2.631627	-0.465901
O	-1.965621	0.057903	3.443845
Cl	1.204282	-0.437646	3.325318
H	1.423273	-0.136008	1.322771
H	1.402949	-0.722403	-0.115400
H	-2.385187	-0.594103	0.453420
H	-2.265641	0.128888	1.838866
H	-1.122122	-0.430860	3.529772
H	-1.670150	0.972453	3.589846
H	0.144618	2.947059	3.479183
H	0.411946	1.433687	3.195564
H	2.220818	3.244300	-0.244673
H	1.858827	1.733936	-0.290901
O	-2.388611	2.748290	-0.155999
H	-2.779261	1.884860	0.078575
H	-2.787296	3.026261	-0.984075

$NaCl(H_2O)_7$

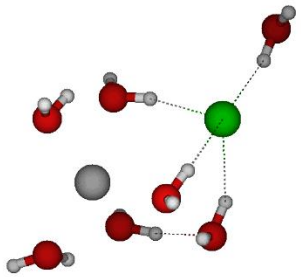

Figure S_{146} : NaCl optimized structure with 7 water molecules.

E = -550.020979

H =-550.020035

O	1.289235	0.173890	0.448492
Na	-0.458821	1.929259	0.584240
O	-2.409295	2.796413	-0.317314
O	1.491676	2.664314	-0.469737
O	-0.318160	2.389366	2.895989
O	-2.345916	0.367779	0.792055
O	-2.169860	0.297276	3.417254
Cl	1.032137	-0.249166	3.439566
H	1.350064	-0.033848	1.416208
H	1.388836	-0.674175	0.005265
H	-2.445842	-0.520341	0.437873
H	-2.389640	0.272229	1.787926
H	-1.352778	-0.212298	3.576929
H	-1.851983	1.210761	3.519487
H	-0.037766	3.163943	3.393377
H	0.254220	1.642012	3.208453
H	2.195871	3.294474	-0.297368
H	1.843960	1.780262	-0.251010
H	-2.818096	1.945608	-0.069582
H	-2.779311	3.055778	-1.164484
H	1.931034	-2.434459	3.706620
O	2.568273	-3.161368	3.764086
H	3.290046	-2.767417	4.262887

$NaCl(H_2O)_8$

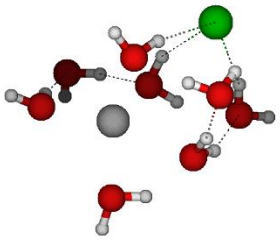

Figure S_{147} : NaCl optimized structure with 8 water molecules.

E = -626.421253

H =-626.420309

O	1.450335	0.486524	0.823942
Na	-0.650486	1.733972	0.521767
O	-2.619128	1.188113	-0.581348
O	2.888182	1.930619	-0.973041
O	-0.640037	2.608362	2.739188
O	-1.842458	-0.338007	1.417720
O	-2.240505	0.580855	3.941583
Cl	1.108331	0.410303	3.944459
O	0.464874	-1.824484	1.924241
H	1.626721	0.677493	1.770009
H	1.268866	-0.472150	0.860307
H	-1.202595	-1.065155	1.516101
H	-2.118036	-0.103683	2.337184
H	-1.411478	0.266180	4.337515
H	-2.002346	1.485375	3.674860
H	-0.444266	3.493960	3.061849
H	0.010433	2.013859	3.191892
H	3.004803	1.410476	-1.774514
H	2.551952	1.296568	-0.300721
H	-2.640148	0.405390	0.007106
H	-2.938086	0.910935	-1.443094
H	0.668214	-1.278041	2.721960
H	0.728120	-2.724383	2.141502
O	0.500518	3.153675	-0.881614

H	0.528326	4.102797	-1.023446
H	1.423837	2.825487	-1.007992

$NaCl(H_2O)_9$

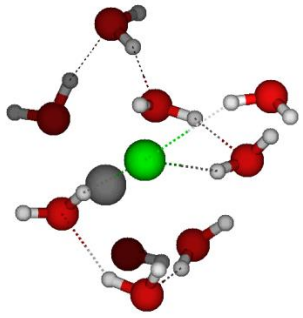

Figure S_{148} : NaCl optimized structure with 9 water molecules.

E = -702.801495

H =-702.800551

O	1.380900	0.626318	1.153288
Na	-0.673751	1.750693	0.446822
O	0.596972	2.866412	-1.114227
O	-2.617428	1.154744	-0.683085
O	-0.865394	2.921841	2.518777
O	-1.937705	-0.232056	1.456554
O	2.901772	1.514059	-0.903413
O	-2.566129	1.022417	3.777392
O	0.339248	-1.439080	2.523787
Cl	0.804076	1.087636	4.321328
H	1.595093	1.046231	2.005161
H	1.125839	-0.282185	1.447372
H	-1.361443	-0.980848	1.677858
H	-2.282934	0.104198	2.319334
H	-1.835037	0.789990	4.369698
H	-2.272426	1.877436	3.416181
H	-0.791631	3.859228	2.725518
H	-0.237720	2.466276	3.132564
H	2.998062	0.824418	-1.567922

H	2.522341	1.063292	-0.115179
H	-2.673498	0.405204	-0.056985
H	-2.869360	0.824872	-1.548725
H	0.222540	-0.690919	3.147121
H	1.014899	-1.959487	3.007192
H	0.681557	3.764671	-1.442083
H	1.500620	2.467568	-1.152123
H	2.190913	-0.918799	4.515095
O	2.300935	-1.875963	4.378219
H	1.993319	-2.264426	5.204273

$NaCl(H_2O)_{10}$

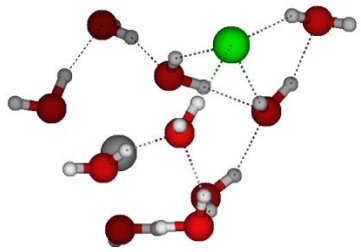

Figure S_{149} : NaCl optimized structure with 10 water molecules.

E = -779.186228

H =-779.185284

O	1.340884	0.679964	1.320821
Na	-0.646623	1.812116	0.536022
O	0.648175	2.796341	-1.105086
O	-2.527114	1.055114	-0.627203
O	-1.266814	3.372134	2.196208
O	-1.871733	-0.181360	1.601728
O	2.864327	1.327362	-0.814154
O	0.340182	-1.442729	2.703893
O	-2.868758	1.360008	3.595252
O	2.628188	-2.362142	3.839563
Cl	1.831279	0.741259	4.444180
H	1.706434	1.013947	2.164928
H	1.046840	-0.220782	1.593846

H	-1.285189	-0.889756	1.917706
H	-2.296364	0.216165	2.398324
H	-2.139962	1.566625	4.208395
H	-2.868453	2.142017	3.023718
H	-1.312645	4.323366	2.063465
H	-0.891534	3.233655	3.098008
H	2.914054	0.580210	-1.418838
H	2.467310	0.966299	0.012626
H	-2.547733	0.339401	0.041548
H	-2.689620	0.650330	-1.482485
H	0.452207	-0.780590	3.414563
H	1.060247	-2.070886	2.934345
H	0.790772	3.667197	-1.482663
H	1.525909	2.340824	-1.118275
H	2.716287	-1.421865	4.083880
H	2.469756	-2.803456	4.681183
H	0.242956	1.975068	4.637207
O	-0.554847	2.568204	4.665050
H	-0.455081	3.088944	5.468561

$NaCl(H_2O)_{11}$

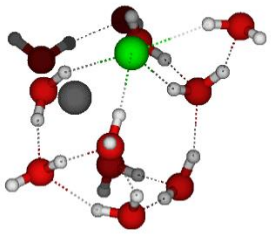

Figure S_{150} : NaCl optimized structure with 11 water molecules.

E = -855.574446

H =-855.573502

O	1.931053	0.365874	0.711572
Na	0.371718	2.099350	0.104713
O	1.483406	2.712648	-1.799359
O	-1.522517	0.986807	-0.333308
O	-1.874539	3.672441	3.469880

O	-2.202794	-0.663057	1.572792
O	2.644188	0.289320	-1.925150
O	-1.215249	2.022249	5.492508
O	-3.087256	1.065779	3.519778
O	0.468524	-1.028507	2.436047
O	2.264865	-1.936574	4.258355
Cl	1.479589	1.206022	4.335920
H	2.626191	0.670967	1.306932
H	1.417845	-0.291879	1.255816
H	-1.350668	-1.001449	1.901802
H	-2.557740	-0.100069	2.298706
H	-2.574935	1.050645	4.343244
H	-2.930882	1.969680	3.202201
H	-2.264585	4.524649	3.686843
H	-1.612147	3.253517	4.323367
H	2.086557	-0.347067	-2.384539
H	2.482503	0.130599	-0.969390
H	-1.831954	0.324496	0.354969
H	-2.236136	1.068208	-0.969673
H	0.513091	-0.241980	3.023403
H	1.019759	-1.660072	2.951582
H	2.084693	3.439578	-1.980234
H	1.979804	1.885239	-2.009594
H	2.311599	-0.986611	4.476558
H	1.900680	-2.344343	5.051281
H	-0.316942	1.716163	5.209595
H	-1.144050	2.194614	6.436720
O	0.487329	3.317572	2.023982
H	-0.345255	3.577634	2.464549
H	0.974674	2.841950	2.718871

$NaCl(H_2O)_{12}$

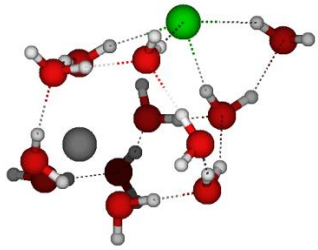

Figure S_{151} : NaCl optimized structure with 12 water molecules.

E = -931.960284

H =-931.959340

O	2.042296	0.467850	0.640076
Na	0.642343	2.474763	0.175287
O	-1.475256	1.385461	-0.114118
O	1.424812	3.152572	2.261575
O	1.671964	2.671189	-1.868462
O	-2.087094	-0.617596	1.421602
O	0.539188	-1.012697	2.273057
O	2.991408	0.324668	-1.905448
O	1.839770	-2.221182	4.328353
O	-3.313640	0.512886	3.622732
O	-0.867071	4.505526	3.209557
O	-1.567130	2.374565	4.793264
Cl	1.079186	0.940819	4.609630
H	2.718805	0.796302	1.243293
H	1.531994	-0.201313	1.168666
H	-1.221913	-0.958299	1.721588
H	-2.534324	-0.285484	2.231425
H	-2.704944	1.161093	4.031109
H	-4.044192	1.036619	3.279238
H	-0.855996	5.335279	3.695336
H	-1.183708	3.812838	3.831692
H	2.495106	-0.335772	-2.399594
H	2.723505	0.197734	-0.967601
H	-1.745302	0.615492	0.478359

H	-1.802238	1.162356	-0.990638
H	0.516334	-0.287930	2.938025
H	0.978610	-1.715732	2.803894
H	2.136738	3.415474	-2.258449
H	2.226719	1.872257	-2.033734
H	1.869242	-1.309111	4.670761
H	1.239600	-2.676032	4.929305
H	-0.702103	1.878863	4.771201
H	-1.754874	2.485656	5.732424
H	0.776118	3.791239	2.609127
H	1.526551	2.514647	2.989183
O	-1.127066	4.067948	0.396480
H	-1.214840	4.325263	1.329126
H	-1.660243	3.261282	0.293322

$KCl(H_2O)_1$

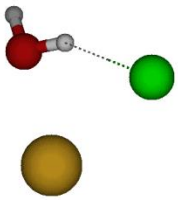

Figure S_{152} : KCl optimized structure with 1 water molecule.

E = -119.831948

H =-119.831003

K	-0.534375	0.181427	-0.308108
Cl	1.167587	-0.146208	2.066631
O	2.002152	0.113976	-0.899777
H	2.839304	-0.181543	-1.267215
H	2.101191	0.032348	0.078965

$KCl(H_2O)_2$

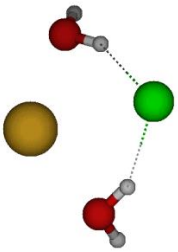

Figure S_{153} : KCl optimized structure with 2 water molecules.

E = -196.223913

H =-196.222969

O	1.860043	-0.039500	-0.727310
K	-0.436755	1.176040	-1.172249
Cl	0.126805	0.548752	1.789139
H	2.391958	-0.837999	-0.780719
H	1.593929	0.024842	0.218182
O	-2.493120	0.193487	0.150878
H	-3.093166	-0.535162	0.330750

H	-1.876524	0.209834	0.918092

$KCl(H_2O)_3$

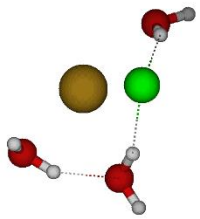

Figure S_{154} : KCl optimized structure with 3 water molecules.

E = -272.613316

H =-272.612372

O	2.061413	-0.755827	-0.129906
K	0.333776	-0.152758	-2.048650
O	-2.193633	0.297967	-0.804639
Cl	0.185287	1.659137	0.506918
H	2.334898	-1.357643	0.567559
H	1.686395	0.021762	0.339256
H	-3.013696	0.160844	-0.321166
H	-1.596748	0.798897	-0.190362
O	-1.486091	1.542162	-3.120243
H	-2.020295	1.251738	-2.351815
H	-1.322682	2.476871	-2.955459

$KCl(H_2O)_4$

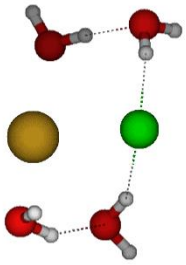

Figure S_{155} : KCl optimized structure with 4 water molecules.

E = -349.002067

H =-349.001122

O	2.859133	-0.459141	-0.216024
K	0.023223	0.313672	-2.902447
O	-1.978753	2.160805	-2.887346
O	-2.184036	0.110336	-1.077690
Cl	0.355014	1.395957	0.008588
H	2.670096	-1.129926	0.448721
H	2.186520	0.237665	-0.038943
H	-2.885214	-0.214905	-0.505189
H	-1.492728	0.483140	-0.476596
H	-2.352467	1.568455	-2.204221
H	-1.699579	2.937549	-2.389562
O	2.216955	-1.129855	-2.732423
H	3.028351	-1.308047	-3.214857
H	2.509255	-0.955953	-1.800212

$KCl(H_2O)_5$

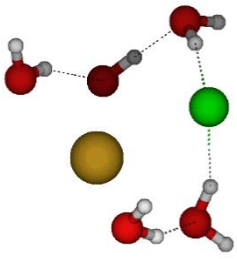

Figure S_{156} : KCl optimized structure with 5 water molecules.

E = -425.387799

H =-425.386855

O	2.958517	-0.211729	-0.574987
O	1.969644	-1.171155	-2.827376
K	-0.223822	0.602892	-3.189996
O	-2.368076	2.221546	-2.653242
O	-2.083254	0.008722	-1.042675
Cl	0.437651	1.536814	-0.247629
H	2.920824	-0.794265	0.191279
H	2.259849	0.461229	-0.386283
H	-2.665214	-0.391687	-0.389862
H	-1.344992	0.420420	-0.531162
H	-2.564298	1.533443	-1.987104
H	-2.047162	2.963276	-2.127682
H	2.278097	-2.068342	-2.982914
H	2.388469	-0.876979	-1.967902
O	1.990062	0.737937	-4.752191
H	2.697989	1.388300	-4.731925
H	2.274963	0.015878	-4.154034

$KCl(H_2O)_6$

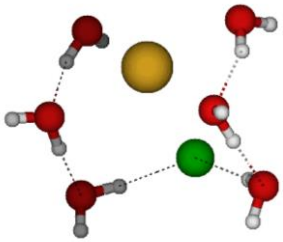

Figure S_{157} : KCl optimized structure with 6 water molecules.

E = -501.773963

H =-501.773018

O	3.511641	-0.303363	-0.899886
O	2.047902	-1.480467	-2.770446
O	1.994612	0.445012	-4.726872
K	-0.163596	0.340845	-3.051273
O	-2.263977	2.070643	-3.317990

O	-2.318096	0.368202	-1.167688
Cl	1.333835	1.889833	-0.814966
H	3.461388	-0.690093	-0.019339
H	2.966709	0.515825	-0.824366
H	-3.158984	-0.018319	-0.906463
H	-1.980308	0.859962	-0.367265
H	-2.512424	1.631664	-2.478462
H	-2.104912	2.990195	-3.081401
H	2.417760	-2.339817	-2.993064
H	2.624375	-1.116692	-2.041118
H	2.590113	1.175504	-4.528956
H	2.276905	-0.280065	-4.132869
H	-0.431591	2.006870	0.381544
O	-1.290963	1.791495	0.815478
H	-1.027324	1.294210	1.597033

$KCl(H_2O)_7$

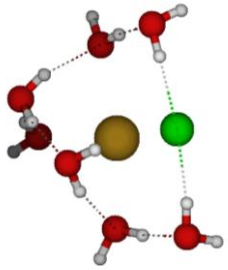

Figure S_{158} : KCl optimized structure with 7 water molecules.

E = -578.164292

H =-578.163347

O	3.793927	0.610241	-0.990809
O	2.643665	-0.963711	-2.815642
O	1.121776	0.309415	-4.816114
K	-0.077774	-1.016816	-2.214175
O	-0.239805	1.906395	-2.986402
O	-2.373570	0.516113	-1.789784
O	-2.105362	1.676398	0.589727
Cl	0.873709	1.019198	0.010594

H	4.159334	0.112874	-0.250794
H	2.961111	0.979423	-0.623555
H	-3.245862	0.691558	-2.155775
H	-2.370439	0.931226	-0.883836
H	-1.108731	1.597797	-2.663433
H	0.264039	2.059066	-2.170427
H	3.302808	-1.523969	-3.236232
H	3.141359	-0.394489	-2.167938
H	0.658298	1.005959	-4.304963
H	1.835945	0.007692	-4.222120
H	-1.123448	1.703578	0.553988
H	-2.289255	1.114019	1.350045
O	-0.463545	-1.838610	-4.709981
H	-1.024230	-2.009782	-5.470242
H	0.104105	-1.064522	-4.957340

$KCl(H_2O)_8$

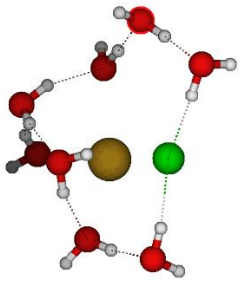

Figure S_{159} : KCl optimized structure with 8 water molecules.

E = -654.548788

H =-654.547844

O	3.911664	-0.067783	-0.673532
O	2.226539	-1.269212	-2.291052
K	-0.519307	-0.908923	-2.143405
O	-0.505607	-1.718767	-4.681604
O	1.348552	0.198425	-4.492599
O	-0.100776	1.946861	-2.851894
O	-2.663484	0.905852	-2.408812

O	-3.067322	1.980560	-0.006520
Cl	-0.144441	0.983397	0.332669
H	3.491347	0.262711	0.165008
H	4.290421	0.717879	-1.080600
H	-3.348279	1.179855	-3.026484
H	-2.912228	1.305975	-1.531475
H	-1.064466	1.788624	-2.804477
H	0.161745	2.029449	-1.920744
H	2.711684	-2.047433	-2.583044
H	2.846982	-0.800797	-1.659509
H	0.908342	0.944525	-4.035674
H	1.866808	-0.240044	-3.787707
H	-2.127471	1.887387	0.265892
H	-3.539414	1.413959	0.613451
H	-0.946230	-1.826906	-5.527723
H	0.185260	-1.021276	-4.820285
H	1.820759	1.098719	1.213229
O	2.740973	0.925438	1.508905
H	2.638225	0.277827	2.214256

$KCl(H_2O)_9$

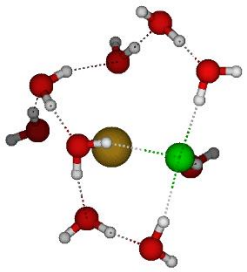

Figure S_{160} : KCl optimized structure with 9 water molecules.

E =-730.933124

H =-730.932180

O	4.146545	0.095477	-0.935288
O	2.440716	-1.197866	-2.474989
O	3.019606	1.305708	1.165407
K	-0.354130	-1.097823	-2.266336

O	-0.299773	-1.551057	-4.908609
O	1.478408	0.410949	-4.537203
O	-0.047691	1.857811	-2.694656
O	-2.552343	0.720240	-2.341643
O	-3.027265	1.588670	0.137952
Cl	-0.004929	0.839112	0.506849
H	3.735505	0.502336	-0.128311
H	4.520841	0.840626	-1.416161
H	-3.256325	0.999598	-2.934792
H	-2.820356	1.032231	-1.436378
H	-1.004128	1.653783	-2.655412
H	0.217695	1.903252	-1.763245
H	2.950465	-1.940752	-2.813314
H	3.065422	-0.711087	-1.865218
H	0.993280	1.064005	-3.992213
H	2.007452	-0.088149	-3.882498
H	-2.087226	1.585577	0.416593
H	-3.434592	0.923946	0.704376
H	-0.762851	-1.563005	-5.749578
H	0.360481	-0.814227	-4.972524
H	2.052831	1.297097	1.001251
H	3.120569	0.835884	1.999693
O	-0.727806	-2.220684	0.191833
H	-0.263632	-2.864556	0.734407
H	-0.495683	-1.352834	0.575981

$KCl(H_2O)_{10}$

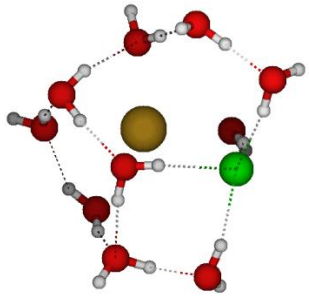

Figure S_{151} : KCl optimized structure with 10 water molecules.

E =-807.320982

H =-807.320038

O	4.064116	0.421800	-1.094695
O	2.660981	-1.192650	-2.618871
O	2.964369	1.143375	1.233636
O	1.376899	0.272605	-4.612941
O	-0.450585	-1.613405	-4.894857
K	-0.061645	-1.482032	-2.096563
O	-0.193210	-2.504123	0.427578
O	-0.121138	1.403999	-2.602637
O	-2.862765	1.519403	-2.502191
O	-3.004685	1.723763	0.141548
Cl	-0.067427	0.665264	0.579873
H	3.664433	0.649711	-0.214797
H	4.222273	1.270687	-1.519522
H	-3.365068	2.238262	-2.897611
H	-2.989306	1.597258	-1.516946
H	-1.088482	1.553723	-2.664316
H	0.085682	1.502697	-1.659275
H	3.298253	-1.859784	-2.892069
H	3.175755	-0.576655	-2.020608
H	0.904592	0.870249	-3.996849
H	1.993786	-0.209365	-4.024376
H	-2.081414	1.537675	0.416662
H	-3.520049	1.026808	0.561474

H	-0.461833	-2.030236	-5.760254
H	0.215781	-0.871892	-4.946363
H	1.992515	1.136429	1.106305
H	3.113590	0.511034	1.944378
H	-0.910565	-2.921452	0.913360
H	-0.156915	-1.590608	0.769428
O	-2.592821	-1.245508	-3.119955
H	-2.092861	-1.293520	-3.954314
H	-2.852525	-0.312954	-3.027476

$KCl(H_2O)_{11}$

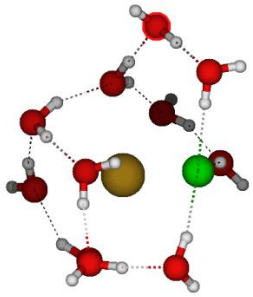

Figure S_{162} : KCl optimized structure with 11 water molecules.

E =-883.704120

H =-883.703176

O	4.203297	0.140922	-0.844371
O	2.493119	-1.095286	-2.521816
O	2.842491	1.415297	1.121707
K	-0.261073	-1.395452	-2.284713
O	0.109500	-2.630941	0.382135
O	-2.794785	-1.061463	-3.250307
O	1.332603	0.208070	-4.648632
O	-0.667326	-1.463163	-5.048118
O	-0.145242	1.506144	-2.679753
O	-2.885761	1.680405	-2.495633
O	-3.012044	1.662485	0.159781
Cl	-0.115373	0.464449	0.523356
H	3.708230	0.591453	-0.117654
H	4.652191	0.852643	-1.311322

H	-3.371049	2.440209	-2.831341
H	-3.003503	1.686082	-1.506877
H	-1.107947	1.689904	-2.692778
H	0.110122	1.556302	-1.747478
H	2.528244	-2.042054	-2.304467
H	3.126635	-0.640969	-1.914170
H	0.897095	0.859748	-4.064224
H	1.923378	-0.279568	-4.035546
H	-2.101019	1.404718	0.415878
H	-3.565646	0.959674	0.516467
H	-0.607188	-1.953498	-5.871747
H	0.087897	-0.808897	-5.052316
H	1.890851	1.257568	0.958265
H	3.002252	1.004681	1.977938
H	-0.536857	-3.041679	0.963256
H	0.130530	-1.682548	0.635463
H	-2.310432	-1.114641	-4.093414
H	-2.997003	-0.117866	-3.128491
O	1.605728	-3.593864	-1.678755
H	2.000216	-4.468767	-1.633684
H	1.233943	-3.405219	-0.793540

$KCl(H_2O)_{12}$

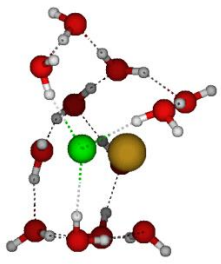

Figure S_{163} : KCl optimized structure with 12 water molecules.

E =-960.100684

H =-960.099740

O	4.169951	0.276065	-0.909467
O	2.618640	-1.139917	-2.595840
O	2.735812	1.430734	1.084273

O	1.429378	0.305677	-4.604570
O	-0.550729	-1.295704	-5.115152
K	-0.176293	-1.485934	-2.373853
O	-3.065697	-0.622648	-4.208065
O	1.529038	-3.461738	-1.426625
O	1.245051	-2.732471	1.138047
O	-0.108876	1.408713	-2.592408
O	-2.820202	1.629109	-2.610752
O	-3.164094	0.186746	-0.475317
Cl	-0.048634	0.049852	0.438451
H	3.653094	0.686118	-0.174242
H	4.559872	1.019686	-1.379458
H	-3.355657	2.428263	-2.615230
H	-3.004356	1.151313	-1.740510
H	-1.052589	1.672437	-2.638477
H	0.112278	1.400637	-1.649103
H	2.549362	-2.038753	-2.231024
H	3.189217	-0.627377	-1.971081
H	0.990624	0.912371	-3.973858
H	2.011265	-0.236182	-4.028289
H	-2.342904	0.225911	0.048740
H	-3.147413	-0.702217	-0.892728
H	-0.491094	-1.724774	-5.973211
H	0.216909	-0.644476	-5.064628
H	1.809466	1.157410	0.929657
H	2.960878	1.021450	1.926664
H	0.545880	-3.186513	1.620377
H	0.906138	-1.816326	1.036153
H	-2.207166	-0.749758	-4.667367
H	-3.048373	0.279115	-3.826534
H	1.929177	-4.331344	-1.514597
H	1.487846	-3.274431	-0.453001
O	-2.867791	-2.059547	-2.056740
H	-3.057899	-1.579253	-2.922953

H	-3.514865	-2.767314	-1.985114

$KCl(H_2O)_{13}$

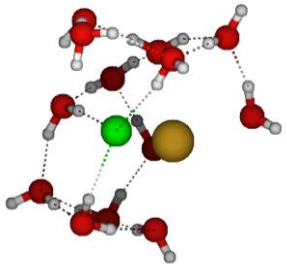

Figure S_{164} : KCl optimized structure with 13 water molecules.

E =-1036.487577

H =-1036.486633

O	3.035003	0.748934	-1.407992
O	2.057469	-1.560684	-2.338510
O	2.624661	0.817332	1.326931
O	1.242750	-0.128873	-4.498978
O	-0.922405	-1.410892	-5.047590
O	-3.148917	0.029829	-4.359043
O	-3.443832	-1.450005	-2.253657
O	0.383362	1.416942	-2.361326
O	-2.252592	2.101140	-2.715923
O	-3.242738	0.808114	-0.678169
K	-0.695401	-1.998596	-2.340344
O	2.523893	-3.686472	-0.522325
O	1.858695	-1.991339	1.479306
Cl	-0.377536	-0.241911	0.324788
H	2.966140	0.834508	-0.430174
H	2.372996	1.360832	-1.762946
H	-2.614238	2.991384	-2.770983
H	-2.649575	1.682253	-1.887496
H	-0.476447	1.860042	-2.526900
H	0.241058	0.931610	-1.526923
H	2.472002	-2.322808	-1.903160
H	2.462903	-0.750126	-1.926999

H	0.964898	0.529160	-3.823319
H	1.761387	-0.765681	-3.965854
H	-2.504179	0.607760	-0.075689
H	-3.424823	-0.053166	-1.116202
H	-0.908961	-1.816153	-5.919422
H	-0.063919	-0.883862	-4.960487
H	1.670616	0.984455	1.287821
H	2.658359	-0.133837	1.520606
H	1.572101	-2.327718	2.335732
H	1.070458	-1.511024	1.119749
H	-2.352359	-0.389897	-4.753407
H	-2.842210	0.865832	-3.951068
H	3.349602	-4.142550	-0.335194
H	2.330868	-3.109588	0.256788
H	-3.446070	-0.910090	-3.107813
H	-4.287332	-1.911330	-2.221340
O	0.080639	-4.464535	-1.550541
H	0.982828	-4.354565	-1.188387
H	-0.304398	-5.199474	-1.066461

$KCl(H_2O)_{14}$

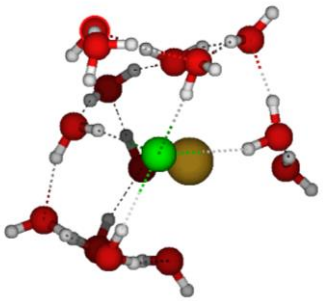

Figure S_{165} : KCl optimized structure with 14 water molecules.

E =-1112.869649

H =-1112.868705

O	2.932196	0.733626	-1.385658
O	2.069914	-1.465570	-2.681585
O	1.333080	0.359891	-4.585137
O	-0.861592	-0.586359	-5.580374

O	-3.100500	0.630256	-4.538422
O	-3.429736	-1.339572	-2.883805
O	-3.300228	0.347490	-0.733019
O	-2.292946	2.138720	-2.326302
O	0.289174	1.308588	-2.189309
O	2.509843	0.669487	1.355386
K	-0.675301	-1.893847	-3.133821
O	0.002094	-4.359055	-0.709146
O	2.681001	-3.571181	-0.852960
O	2.055907	-2.118480	1.367358
Cl	-0.471453	-1.045688	0.011800
H	2.872813	0.733324	-0.405003
H	2.230888	1.340578	-1.667650
H	-2.621371	3.020872	-2.126174
H	-2.706946	1.512893	-1.648823
H	-0.574658	1.777838	-2.221513
H	0.179466	0.626966	-1.502224
H	2.472178	-2.256820	-2.288150
H	2.415934	-0.710202	-2.136348
H	1.003220	0.837172	-3.793349
H	1.840294	-0.376246	-4.189876
H	-2.578964	-0.023926	-0.195476
H	-3.472697	-0.350309	-1.406123
H	-0.840044	-0.739213	-6.529283
H	0.019111	-0.169506	-5.331708
H	1.563829	0.859819	1.374661
H	2.546408	-0.291528	1.511157
H	1.846471	-2.599716	2.175887
H	1.183510	-1.820185	1.006431
H	-2.292461	0.337764	-5.013768
H	-2.815817	1.320053	-3.905367
H	3.419018	-4.180858	-0.755260
H	2.631172	-3.049771	-0.018901
H	-3.422142	-0.605505	-3.575628

H	-4.234044	-1.846813	-3.028802
H	0.964890	-4.199297	-0.785878
H	-0.351173	-3.531800	-0.345688
O	-0.847487	-4.552916	-3.259311
H	-1.458399	-5.272987	-3.433642
H	-0.578143	-4.649142	-2.315552

$KCl(H_2O)_{15}$

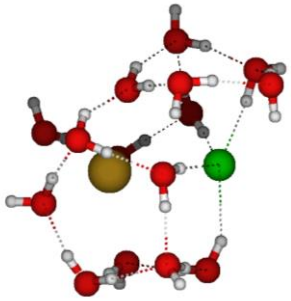

Figure S_{166} : KCl optimized structure with 15 water molecules.

E =-1189.251516

H =-1189.250572

O	2.903474	0.793301	-1.356279
O	2.088389	-1.359104	-2.764669
O	1.337266	0.623312	-4.538256
O	-0.877191	-0.205458	-5.609227
O	-3.155935	0.858746	-4.550267
O	-3.389040	-1.288627	-3.117751
O	-3.329295	0.181394	-0.810006
O	-2.347650	2.153097	-2.199879
O	0.261385	1.381166	-2.098223
O	2.543641	0.612311	1.393805
K	-0.631774	-1.913661	-3.397910
O	-1.249565	-4.738632	-2.882014
O	0.102204	-4.394938	-0.645799
O	2.743680	-3.553872	-1.021974
O	2.077368	-2.160734	1.224365
Cl	-0.477387	-1.183650	-0.145075
H	2.868813	0.749547	-0.376270

H	2.178574	1.392598	-1.593529
H	-2.696177	3.002009	-1.910182
H	-2.751466	1.451838	-1.595283
H	-0.615718	1.825558	-2.116950
H	0.139875	0.616127	-1.508005
H	2.500720	-2.157967	-2.400058
H	2.411136	-0.623823	-2.179804
H	0.987077	1.022267	-3.711456
H	1.844503	-0.141490	-4.207308
H	-2.601155	-0.217809	-0.302579
H	-3.466784	-0.448698	-1.554898
H	-0.806404	-0.425771	-6.542252
H	0.009813	0.170250	-5.328322
H	1.609118	0.843456	1.452530
H	2.545900	-0.357391	1.490252
H	1.858022	-2.695586	1.995968
H	1.206033	-1.866841	0.855912
H	-2.335673	0.628811	-5.040390
H	-2.884053	1.485816	-3.850432
H	3.522690	-4.112375	-0.935458
H	2.679536	-3.034606	-0.186766
H	-3.397980	-0.480413	-3.724734
H	-4.189199	-1.783549	-3.318402
H	1.050011	-4.246632	-0.840019
H	-0.222668	-3.520493	-0.366065
H	-2.026023	-5.285339	-2.737151
H	-0.743766	-4.727191	-2.024598
O	0.033093	-3.980885	-5.125691
H	-0.399354	-4.515171	-4.428853
H	0.857559	-4.430627	-5.328893

$KCl(H_2O)_{16}$

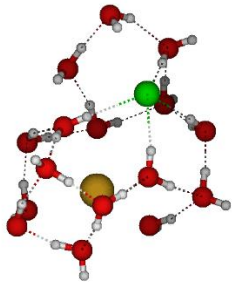

Figure S_{167} : KCl optimized structure with 16 water molecules.

E =-1265.635946

H =-1265.635001

O	2.596131	0.766392	-1.201452
O	1.886980	-1.283390	-2.827860
O	1.465621	1.032092	-4.215435
O	-0.502631	0.404423	-5.778005
O	-2.884834	1.532021	-4.986939
O	-3.631523	-0.925602	-4.534304
O	-4.175864	-0.356838	-1.933695
O	-2.733399	1.769096	-2.183056
O	-0.192625	0.906875	-1.857969
O	2.921932	0.376122	1.525785
K	-0.890663	-1.382968	-3.624914
O	-0.916719	-4.017141	-4.299882
O	-1.618771	-4.857517	-1.780439
O	0.551988	-4.472177	-0.389732
O	2.963768	-3.586053	-1.508502
O	2.972101	-2.438634	0.951982
Cl	0.104525	-1.381767	0.612008
H	2.779746	0.666767	-0.241503
H	1.762345	1.255533	-1.244695
H	-3.142552	2.511901	-1.728019
H	-3.327491	0.961444	-2.010146
H	-1.078713	1.333664	-1.816999
H	-0.138595	0.286403	-1.109645
H	2.385467	-2.089616	-2.618167

H	2.151083	-0.638598	-2.123067
H	0.977914	1.241337	-3.398294
H	1.905260	0.192252	-3.972906
H	-3.618066	-1.060704	-1.538172
H	-4.208484	-0.620774	-2.880148
H	-0.315225	0.488420	-6.717187
H	0.313349	0.723996	-5.289357
H	1.981353	0.283244	1.732538
H	3.227344	-0.545309	1.480085
H	2.956002	-3.083657	1.668840
H	2.031951	-2.140703	0.864886
H	-1.980837	1.310865	-5.298933
H	-2.792475	1.809242	-4.053037
H	3.730214	-4.136546	-1.697354
H	3.141691	-3.151545	-0.639994
H	-3.451381	0.020662	-4.816696
H	-4.233977	-1.300618	-5.182808
H	1.362133	-4.304573	-0.912723
H	0.349463	-3.605003	0.009858
H	-2.084995	-5.639640	-1.470194
H	-0.762243	-4.799918	-1.258845
H	-1.225860	-4.465058	-3.485765
H	-0.277928	-4.615399	-4.695851
O	-2.265912	-2.206173	-1.314047
H	-1.675232	-1.991926	-0.568279
H	-2.258814	-3.180995	-1.387721

$KCl(H_2O)_{17}$

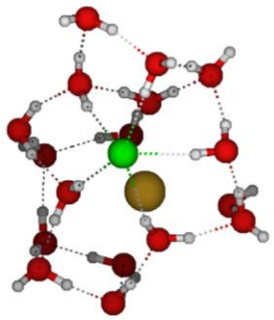

Figure S_{168} : KCl optimized structure with 17 water molecules.

E =-1342.029065

H =-1342.028120

O	2.467392	0.233116	-1.672492
O	1.867304	-1.966996	-3.210315
O	1.015042	2.160249	-3.069712
O	0.207316	1.370887	-5.409809
O	-2.578812	1.350135	-5.225977
O	-3.278989	-1.147238	-5.018984
O	-4.470904	-0.824163	-2.583887
O	-3.406744	1.521856	-2.539872
O	-0.956645	0.604304	-2.049930
O	-2.470759	-2.254711	-1.289310
O	-1.877324	-4.935650	-1.098053
O	0.353070	-4.394449	0.140281
O	-1.389643	-4.524691	-3.779215
K	-0.941722	-1.825695	-3.683444
O	4.538966	0.005713	0.076331
O	2.735515	-3.902234	-1.231586
O	3.096275	-2.219624	0.919311
Cl	0.255590	-1.145004	0.426603
H	3.294668	0.237083	-1.135655
H	1.762177	0.014937	-1.038453
H	-3.945563	2.182254	-2.095030
H	-3.912987	0.642231	-2.511322
H	-1.851659	1.016883	-2.042731

H	-0.765709	0.280082	-1.155719
H	2.214665	-2.714032	-2.697063
H	2.188447	-1.171133	-2.735956
H	0.242380	1.757492	-2.611230
H	1.750686	1.635491	-2.699759
H	-3.878461	-1.371497	-2.027483
H	-4.218067	-1.056551	-3.505617
H	0.490084	1.999996	-6.081218
H	0.601765	1.697201	-4.539767
H	4.460606	0.706018	0.732571
H	4.178834	-0.794239	0.506996
H	3.117755	-2.662491	1.775356
H	2.186831	-1.831907	0.853565
H	-1.599835	1.407814	-5.282748
H	-2.829840	1.636192	-4.326761
H	3.452391	-4.528739	-1.372826
H	3.017161	-3.318750	-0.491444
H	-3.046387	-0.189116	-5.217252
H	-3.670739	-1.511845	-5.817418
H	1.145149	-4.404246	-0.433519
H	0.227513	-3.446371	0.334821
H	-2.391029	-5.581336	-0.604000
H	-1.003930	-4.819958	-0.617117
H	-1.612947	-4.855887	-2.888153
H	-0.918237	-5.236833	-4.218582
H	-1.894416	-1.864683	-0.615136
H	-2.425391	-3.223267	-1.147222
O	0.825739	-1.388709	-5.767490
H	1.466563	-1.601154	-5.067662
H	0.746130	-0.417567	-5.753694

$KCl(H_2O)_{18}$

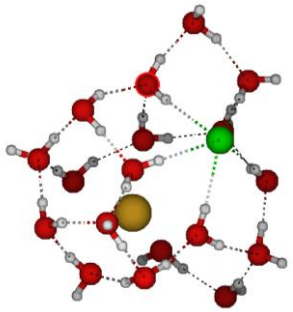

Figure S_{169} : KCl optimized structure with 18 water molecules.

E =-1418.409864

H =-1418.408920

O	2.527783	0.469799	-1.497644
O	4.521979	0.135166	0.322532
O	2.091237	-1.614778	-3.246148
O	3.093263	-2.191185	0.886293
O	2.772903	-3.727803	-1.379395
O	1.019710	2.373899	-2.883397
O	0.341592	1.723886	-5.308180
O	-0.910311	0.659257	-2.046432
O	-3.378685	1.500607	-2.588977
O	-4.281329	-0.902754	-2.792603
O	-3.002982	-1.036441	-5.202034
O	-2.433933	1.501273	-5.238950
K	-0.673435	-1.681328	-3.810017
O	-1.941555	-6.303697	-3.290103
O	-1.914438	-4.978443	-0.882058
O	0.438818	-4.326398	0.031010
O	-2.249332	-2.307626	-1.527900
O	1.112131	-0.972253	-5.819402
Cl	0.241995	-1.107422	0.425034
H	3.329298	0.454221	-0.923639
H	1.801533	0.192118	-0.914057
H	-3.970517	2.100998	-2.126870

H	-3.828416	0.591083	-2.624671
H	-1.819558	1.038983	-2.058489
H	-0.739102	0.316733	-1.154746
H	2.381401	-2.408821	-2.769216
H	2.363997	-0.861675	-2.681996
H	0.256467	1.894121	-2.487433
H	1.774476	1.881673	-2.508882
H	-3.669467	-1.441431	-2.247811
H	-3.986574	-1.068300	-3.716498
H	0.608097	2.420020	-5.917068
H	0.689542	1.999316	-4.402295
H	4.392898	0.761580	1.042336
H	4.165293	-0.713247	0.651096
H	3.085105	-2.699568	1.705452
H	2.183121	-1.807376	0.816551
H	-1.459107	1.625526	-5.245121
H	-2.744443	1.732513	-4.342571
H	3.487613	-4.343018	-1.572047
H	3.056211	-3.203381	-0.597716
H	-2.806381	-0.056965	-5.326636
H	-3.389956	-1.345480	-6.025961
H	1.188724	-4.308459	-0.596963
H	0.299300	-3.383120	0.240490
H	-2.414506	-5.320333	-0.133824
H	-0.979751	-4.817197	-0.548732
H	-2.001961	-5.882494	-2.405047
H	-1.336219	-7.041962	-3.168562
H	-1.712713	-1.892387	-0.834775
H	-2.280126	-3.259491	-1.297962
H	1.731765	-1.188877	-5.101697
H	0.974693	-0.010211	-5.750373
O	-0.555820	-4.294302	-4.535930
H	-0.469343	-4.474731	-5.475908
H	-1.086319	-5.035841	-4.170276

$KCl(H_2O)_{19}$

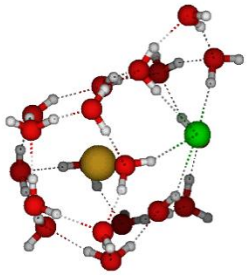

Figure S_{170} : KCl optimized structure with 19 water molecules.

E =-1494.799598

H =-1494.798654

O	2.545348	0.553722	-1.488704
O	4.564684	0.126755	0.271115
O	2.142109	-1.494389	-3.264595
O	3.177197	-2.244424	0.770793
O	2.813999	-3.679182	-1.563509
O	0.479778	-4.330011	-0.162549
O	-1.962802	-4.962461	-0.840368
O	-2.481911	-5.974034	-3.382768
O	-0.432103	-4.260522	-4.245544
K	-0.630277	-1.702927	-3.440132
O	-2.375117	-2.299600	-1.301771
O	-4.255110	-0.973967	-2.796597
O	-3.430998	1.457776	-2.622083
O	-0.954396	0.738417	-1.959903
O	0.981588	2.415032	-2.866576
O	0.303035	1.740638	-5.270251
O	-2.978627	-1.210539	-5.286926
O	-2.429007	1.308453	-5.227026
O	1.065801	-0.900724	-5.728104
Cl	0.317337	-1.112644	0.365607
H	3.356530	0.521813	-0.927485
H	1.832602	0.243902	-0.903245
H	-4.075315	2.065253	-2.247455
H	-3.851232	0.535255	-2.645387

H	-1.873269	1.090059	-1.997411
H	-0.785355	0.408187	-1.063276
H	2.451017	-2.309795	-2.833415
H	2.422112	-0.756118	-2.682683
H	0.222507	1.954881	-2.442069
H	1.744387	1.936724	-2.488544
H	-3.702838	-1.493864	-2.173477
H	-3.909162	-1.198841	-3.685166
H	0.566780	2.425902	-5.892586
H	0.645981	2.031983	-4.363342
H	4.468021	0.707946	1.032644
H	4.225311	-0.741996	0.563412
H	3.188285	-2.771686	1.577882
H	2.265858	-1.863534	0.728105
H	-1.466972	1.511425	-5.238327
H	-2.768839	1.575791	-4.350539
H	3.491885	-4.315366	-1.812795
H	3.126849	-3.226137	-0.750668
H	-2.765961	-0.221402	-5.356981
H	-3.662871	-1.383155	-5.943151
H	1.199870	-4.304772	-0.822924
H	0.357652	-3.392139	0.074211
H	-2.352462	-5.361525	-0.055851
H	-0.990515	-4.826641	-0.633466
H	-2.345557	-5.694836	-2.455139
H	-2.070753	-6.842075	-3.443586
H	-1.858484	-1.889128	-0.592155
H	-2.368276	-3.264333	-1.112317
H	1.671707	-1.129587	-4.997261
H	0.895919	0.058626	-5.658096
H	-0.542413	-3.941309	-5.166248
H	-1.182344	-4.862297	-4.079147
O	-0.805758	-2.753417	-6.534671
H	-0.065973	-2.120106	-6.419626

H	-1.583597	-2.251265	-6.242009

$KCl(H_2O)_{20}$

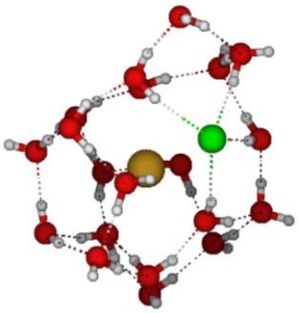

Figure S_{171} : KCl optimized structure with 20 water molecules.

E =-1571.185030

H =-1571.184086

O	2.557383	0.705251	-1.423834
O	4.577983	0.266588	0.332621
O	2.354215	-1.361664	-3.195016
O	1.451206	-0.852566	-5.754408
O	-0.339946	-2.806887	-6.387596
O	-0.157570	-4.275771	-4.109382
K	-0.371021	-1.681483	-3.284593
O	0.217304	1.617181	-5.280621
O	0.900165	2.435866	-2.901505
O	-1.009482	0.772153	-1.896800
O	-3.505860	1.393385	-2.668633
O	-4.092238	-1.149195	-2.706244
O	-2.250234	-2.275199	-1.082387
O	-1.889729	-4.986243	-0.998527
O	0.562962	-4.354120	-0.408885
O	-2.562570	1.112879	-5.370893
O	-2.543489	-1.499861	-4.981262
O	-2.830515	-5.232453	-3.554525
O	3.347342	-2.216446	0.772141
O	2.994491	-3.608314	-1.592755
Cl	0.465406	-1.160148	0.357930

H	3.362943	0.688330	-0.854208
H	1.854534	0.344819	-0.855325
H	-4.167401	2.002736	-2.328269
H	-3.889645	0.468330	-2.623884
H	-1.933256	1.093354	-2.008538
H	-0.885458	0.510774	-0.973752
H	2.684756	-2.168315	-2.761810
H	2.575950	-0.611051	-2.602505
H	0.158668	1.984309	-2.442041
H	1.682628	2.010924	-2.503127
H	-3.562491	-1.538741	-1.974805
H	-3.503808	-1.272684	-3.486718
H	0.459354	2.279945	-5.935882
H	0.545257	1.969941	-4.394937
H	4.458297	0.796505	1.127478
H	4.290718	-0.634975	0.577157
H	3.403416	-2.720894	1.591751
H	2.420118	-1.875224	0.742836
H	-1.608938	1.337436	-5.350868
H	-2.916096	1.405977	-4.512083
H	3.682792	-4.218823	-1.875504
H	3.294713	-3.199574	-0.752530
H	-2.671163	-0.569428	-5.315497
H	-3.302413	-2.082681	-5.218392
H	1.312720	-4.304255	-1.032905
H	0.471165	-3.438074	-0.090269
H	-2.176138	-5.519307	-0.250100
H	-0.900593	-4.847344	-0.880123
H	-2.559767	-5.222716	-2.609349
H	-2.948379	-6.156751	-3.794227
H	-1.649158	-1.898135	-0.420151
H	-2.249146	-3.244849	-0.940114
H	1.971153	-1.037632	-4.949034
H	1.083036	0.045535	-5.642184

H	-0.128319	-3.896882	-5.020419
H	-1.034412	-4.689570	-4.062151
H	0.360989	-2.121568	-6.295344
H	-1.155068	-2.345319	-6.128447
O	-4.562826	-3.282495	-4.731827
H	-4.884951	-2.781206	-3.968316
H	-4.018497	-3.992141	-4.339481

$KCl(H_2O)_{21}$

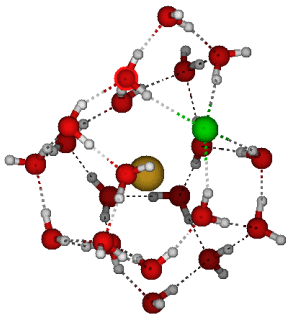

Figure S_{172} : KCl optimized structure with 21 water molecules.

E =-1647.583194

H =-1647.582250

O	2.489244	0.829657	-1.365393
O	4.470607	0.238772	0.391399
O	2.467541	-0.984366	-3.400612
K	-0.207623	-1.721359	-3.171487
O	-0.073270	-5.031493	-4.717405
O	-0.178793	-2.623875	-5.936491
O	1.535686	-0.557689	-5.950176
O	-2.480337	-1.388784	-4.916911
O	-2.611975	1.205864	-5.337694
O	-4.473637	-3.204131	-4.754933
O	-4.092240	-1.101446	-2.693560
O	-3.513046	1.436362	-2.615718
O	-1.026490	0.739214	-1.859961
O	-2.291123	-2.314182	-1.121719
O	0.787277	2.500644	-2.875744

O	0.129723	1.801998	-5.308558
O	-2.340898	-5.031249	-0.979883
O	0.085355	-4.749233	-0.232944
O	-2.748505	-5.216575	-3.664602
O	3.709442	-3.229014	-2.262969
O	3.423023	-2.356420	0.337450
Cl	0.499914	-1.361585	0.243317
H	3.284112	0.765036	-0.783888
H	1.792262	0.378422	-0.858876
H	-4.153747	2.043865	-2.234534
H	-3.907591	0.514871	-2.585470
H	-1.947688	1.067753	-1.975049
H	-0.911585	0.473388	-0.937642
H	3.021428	-1.736378	-3.123300
H	2.602566	-0.281707	-2.727577
H	0.080338	1.994755	-2.418215
H	1.594939	2.135041	-2.472606
H	-3.570029	-1.498467	-1.959163
H	-3.469621	-1.190082	-3.452758
H	0.334817	2.530224	-5.904193
H	0.454974	2.091047	-4.400965
H	4.249979	0.626451	1.244842
H	4.237219	-0.707313	0.472189
H	3.492828	-3.001529	1.050439
H	2.474635	-2.071649	0.342260
H	-1.666666	1.467582	-5.338997
H	-2.958068	1.488733	-4.472328
H	4.600922	-3.532773	-2.457983
H	3.689750	-2.981569	-1.311890
H	-2.621697	-0.454538	-5.245042
H	-3.225912	-1.977421	-5.182731
H	0.536288	-4.612521	-1.117196
H	0.127576	-3.866978	0.169436
H	-2.850821	-5.528995	-0.333246

H	-1.371720	-5.016580	-0.654812
H	-2.622492	-5.210207	-2.685112
H	-3.077990	-6.094514	-3.883838
H	-1.645764	-2.004301	-0.465506
H	-2.423741	-3.272859	-0.962054
H	2.042249	-0.672985	-5.120851
H	1.052436	0.282234	-5.824982
H	-0.061069	-4.221641	-5.282413
H	-1.003776	-5.130684	-4.444734
H	0.488565	-1.904699	-6.075393
H	-1.037624	-2.176957	-5.831048
H	-4.793129	-2.718900	-3.979087
H	-3.915742	-3.915329	-4.384067
O	1.079523	-4.138963	-2.566160
H	2.045383	-4.043956	-2.627200
H	0.733213	-4.588810	-3.395311

$KCl(H_2O)_{22}$

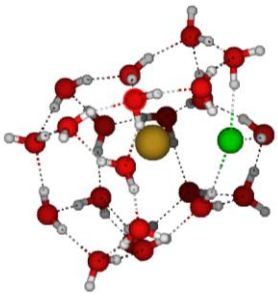

Figure S_{173} : KCl optimized structure with 22 water molecules.

E =-1723.963307

H =-1723.962363

O	2.467168	0.895766	-1.741356
O	3.265154	0.139931	0.714891
O	2.640151	-1.148467	-3.536876
O	1.724767	-0.660987	-6.079999
O	-0.044293	-2.660536	-5.740487
O	-0.031632	-5.189345	-4.794931
O	1.213148	-4.449315	-2.615570

O	0.161154	-5.215158	-0.322227
O	-2.274057	-5.044207	-1.018184
O	-2.104819	-2.313779	-0.955370
O	-3.814974	-1.049530	-2.574733
O	-3.730441	1.552373	-2.687093
O	-2.026243	1.883023	-0.600653
O	-2.697885	-5.234916	-3.673669
O	1.496445	2.771556	-3.351920
O	0.261952	1.798703	-5.573690
O	-2.332799	-1.391583	-4.837579
O	-2.534770	1.215697	-5.299653
O	-4.368883	-3.131181	-4.608240
K	0.020905	-1.942133	-2.966367
O	3.733560	-2.637274	0.096971
O	3.849197	-3.442500	-2.495813
Cl	0.739773	-2.080821	0.466555
H	2.865040	0.747685	-0.845464
H	1.507310	0.693933	-1.638208
H	-4.612376	1.933600	-2.749867
H	-3.857713	0.558601	-2.592137
H	-2.737595	1.880450	-1.281866
H	-2.334697	1.299087	0.100029
H	3.199842	-1.899661	-3.265296
H	2.779588	-0.422450	-2.891010
H	1.383948	3.619784	-2.913133
H	2.077390	2.222256	-2.766161
H	-3.299063	-1.427448	-1.824766
H	-3.194093	-1.155078	-3.335156
H	0.417315	2.341892	-6.353506
H	0.760594	2.223878	-4.840709
H	2.393443	-0.155870	1.023318
H	3.713742	-0.704839	0.534104
H	4.019890	-3.217637	0.811572
H	2.750415	-2.572193	0.205829

H	-1.597675	1.485161	-5.333782
H	-2.871951	1.495697	-4.428407
H	4.711017	-3.779853	-2.757708
H	3.908104	-3.210262	-1.538850
H	-2.486121	-0.466810	-5.174887
H	-3.098300	-1.973181	-5.066896
H	0.639159	-5.047605	-1.181105
H	0.321526	-4.391929	0.174255
H	-2.826343	-5.521058	-0.390445
H	-1.297540	-5.185310	-0.722171
H	-2.565046	-5.227093	-2.692002
H	-3.068619	-6.098150	-3.885099
H	-1.401639	-2.104469	-0.314233
H	-2.261002	-3.280055	-0.882118
H	2.204662	-0.796318	-5.235684
H	1.214600	0.156588	-5.944824
H	0.009090	-4.338037	-5.290447
H	-0.954725	-5.244263	-4.487175
H	0.624449	-1.982473	-6.009692
H	-0.895578	-2.192442	-5.655949
H	-4.601324	-2.644957	-3.801989
H	-3.832157	-3.886187	-4.293867
H	2.172406	-4.321485	-2.712712
H	0.843450	-4.838292	-3.461443
O	-0.178875	0.743832	-2.170758
H	0.059017	1.514448	-2.711812
H	-0.814767	1.103223	-1.501185

$KCl(H_2O)_{23}$

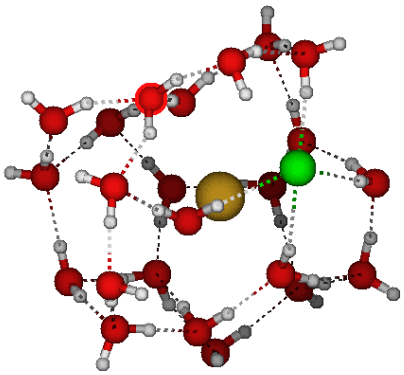

Figure S_{174} : KCl optimized structure with 23 water molecules.

E =-1800.341777

H =-1800.340833

O	2.436545	1.028509	-1.683431
O	1.820056	2.835999	-3.558327
O	0.128069	2.461003	-1.303026
O	-2.434835	2.943362	-0.763745
O	3.492165	0.071844	0.603154
O	-3.680203	1.406853	-2.637193
O	-3.757984	-1.219509	-2.514580
O	-2.204914	-2.824149	-1.007729
O	0.254195	1.692508	-5.502667
O	2.277283	-1.174931	-3.343214
O	-2.324491	-1.567307	-4.868805
O	-2.513516	1.055608	-5.226390
O	-4.390998	-3.256646	-4.521572
O	-2.241608	-5.550289	-1.092338
O	0.206833	-5.427154	-0.390068
O	1.252790	-4.660644	-2.692275
O	-0.013471	-5.306762	-4.894184
O	-2.667844	-5.419254	-3.753736
O	-0.106645	-2.834522	-5.990717
O	1.649365	-0.782026	-5.973026
O	3.767690	-3.384464	-2.517508

O	3.652724	-2.712467	0.105116
K	-0.201936	-2.320715	-3.106606
Cl	0.662432	-2.241209	0.498311
H	2.972669	0.780228	-0.888244
H	1.573171	1.310476	-1.323142
H	-4.597744	1.658235	-2.788551
H	-3.703310	0.422076	-2.447960
H	-2.885653	2.387153	-1.441926
H	-2.634073	2.514439	0.074971
H	2.928924	-1.852778	-3.082657
H	2.353063	-0.421688	-2.719151
H	2.426959	3.562446	-3.728144
H	2.291589	2.209754	-2.957121
H	-3.271284	-1.688557	-1.798236
H	-3.137282	-1.289349	-3.273396
H	0.343191	2.241733	-6.288605
H	0.814324	2.117283	-4.813361
H	2.657426	-0.052603	1.074901
H	3.774043	-0.845537	0.425728
H	3.956775	-3.294932	0.810576
H	2.668836	-2.654204	0.229217
H	-1.578380	1.333059	-5.242710
H	-2.857265	1.315983	-4.350341
H	4.657253	-3.572305	-2.831536
H	3.831017	-3.223943	-1.546805
H	-2.476639	-0.625900	-5.158871
H	-3.123997	-2.118066	-5.049625
H	0.684298	-5.253550	-1.245612
H	0.299901	-4.584901	0.089276
H	-2.728859	-6.133866	-0.502636
H	-1.259915	-5.577925	-0.798988
H	-2.533146	-5.538810	-2.780138
H	-3.062318	-6.239348	-4.069077
H	-1.551356	-2.577691	-0.333830

H	-2.367812	-3.784280	-0.904696
H	2.019259	-0.895074	-5.071273
H	1.131447	0.039723	-5.907062
H	0.002831	-4.472264	-5.420697
H	-0.934714	-5.387113	-4.586448
H	0.575335	-2.127632	-6.109892
H	-0.947961	-2.367123	-5.833632
H	-4.559031	-2.751215	-3.709320
H	-3.841594	-4.011820	-4.234582
H	2.192791	-4.434736	-2.790622
H	0.897227	-5.018002	-3.554972
H	0.382796	2.922261	-2.116272
H	-0.789195	2.751426	-1.057897
O	-0.794098	-0.151918	-1.575315
H	-0.375796	-0.532435	-0.786429
H	-0.506088	0.780081	-1.585359

$KCl(H_2O)_{24}$

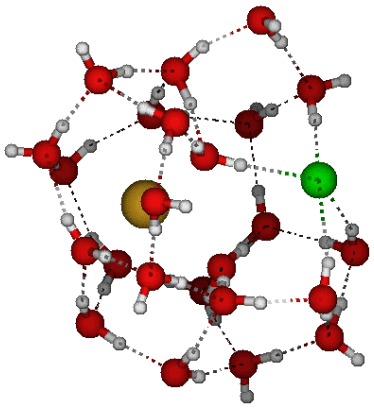

Figure S_{175} : KCl optimized structure with 24 water molecules.

E =-1876.732525

H =-1876.731580

O	2.718691	0.826348	-2.074943
O	1.600460	2.961071	-3.091851
O	3.898194	0.300409	0.287940
O	-0.192932	2.514931	-0.859492

O	-2.857221	2.954021	-1.091025
O	-3.572448	0.782127	-2.586965
O	-3.219005	-1.692521	-1.868343
O	-3.108992	-3.056663	0.397930
O	-2.562930	-5.514583	-0.968150
O	-0.093608	-5.495418	-0.268895
O	0.973806	-4.678434	-2.599718
O	0.038593	-5.340255	-4.956615
O	-2.640682	-5.445487	-3.661933
O	-0.139126	-2.871140	-6.115745
O	1.692704	-0.607653	-6.460408
O	2.952512	-1.062332	-4.028041
K	0.116404	-0.998014	-4.055538
O	0.284673	0.029432	-1.522177
O	0.476523	1.927905	-5.342532
O	-2.571601	-1.799826	-6.192589
O	-1.984282	0.597394	-4.849468
O	-4.069247	-3.017147	-4.204319
O	3.412485	-3.327701	-2.399151
O	3.231191	-2.414954	0.168969
Cl	0.220648	-2.382947	0.582037
H	3.274152	0.770044	-1.257977
H	1.837546	0.440853	-1.792500
H	-4.487578	0.778901	-2.888125
H	-3.411500	-0.142768	-2.221051
H	-3.158586	2.167540	-1.599092
H	-3.220455	2.837666	-0.207241
H	3.216255	-1.881450	-3.571776
H	3.066328	-0.347311	-3.365321
H	2.176008	3.731563	-3.131914
H	2.146440	2.223208	-2.684895
H	-3.337790	-2.089294	-0.961776
H	-2.351903	-2.071028	-2.143627
H	0.442986	2.597181	-6.033690

H	0.911774	2.361444	-4.566655
H	3.309812	0.662505	0.959754
H	3.727407	-0.664322	0.302298
H	3.585752	-2.974075	0.870240
H	2.245507	-2.418371	0.322489
H	-1.332979	1.302490	-5.000759
H	-2.527895	0.821720	-4.067013
H	4.212232	-3.852062	-2.509674
H	3.409555	-3.015281	-1.461971
H	-2.469323	-0.885406	-5.870901
H	-3.151350	-2.237785	-5.528838
H	0.393388	-5.352307	-1.114502
H	0.007838	-4.636784	0.185272
H	-2.981862	-6.257747	-0.520522
H	-1.581387	-5.545764	-0.689529
H	-2.630407	-5.528498	-2.670691
H	-3.135825	-6.201207	-3.994624
H	-2.222411	-2.805566	0.707253
H	-2.978446	-3.925770	-0.031717
H	2.350858	-0.787070	-5.760508
H	1.401650	0.300923	-6.286036
H	0.019783	-4.506163	-5.482722
H	-0.879853	-5.492782	-4.679674
H	0.476696	-2.270924	-6.567560
H	-1.056645	-2.517842	-6.272932
H	-3.965227	-2.560098	-3.346700
H	-3.727234	-3.913709	-4.044759
H	1.856780	-4.259891	-2.604444
H	0.764758	-5.013807	-3.519896
H	0.278059	2.921739	-1.605746
H	-1.143739	2.761729	-0.953257
H	0.165142	-0.629045	-0.809396
H	-0.011366	0.921340	-1.175373
O	-1.132676	-3.032355	-2.890574

H	-0.366363	-3.578461	-2.588654
H	-1.578477	-3.569909	-3.557030

$KCl(H_2O)_{25}$

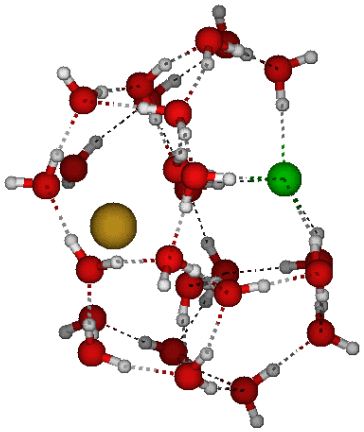

Figure S_{176} : KCl optimized structure with 25 water molecules.

E =-1953.123832

H =-1953.122888

O	2.848134	0.850334	-2.395821
O	1.471281	2.941663	-3.165067
O	0.412917	-0.176174	-2.110280
O	0.301772	2.112741	-0.713508
O	2.878619	1.387029	0.190485
O	-2.303288	2.468647	-0.276467
O	0.185658	1.752495	-5.261647
O	4.123003	-1.375584	-3.321787
O	-3.325721	0.842896	-2.207718
O	-3.198475	-1.705588	-1.780183
O	-2.664718	-3.128428	0.385389
O	-1.462000	-2.786240	-3.481322
K	0.276803	-1.126483	-4.766592
O	0.219605	-4.937361	-3.390993
O	-1.178094	-5.459232	-5.559838
O	-0.077985	-5.818617	-0.897804
O	-2.618843	-5.595698	-1.003277
O	-3.379591	-5.612675	-3.603130

O	-1.037707	-2.897151	-6.662994
O	-3.242835	-1.615359	-6.177157
O	-2.265270	0.559436	-4.820515
O	-4.258870	-3.032851	-4.006369
O	2.895573	-1.275897	-5.831537
O	5.308472	-1.924012	-0.930845
O	3.220236	-1.337942	0.863086
Cl	0.617472	-2.692365	-0.091805
H	3.038398	1.073600	-1.438593
H	1.999390	0.333354	-2.320571
H	-4.257361	1.014343	-2.383954
H	-3.276255	-0.134366	-1.956469
H	-2.698806	1.898551	-0.978380
H	-2.561284	2.058260	0.555219
H	4.687688	-1.678837	-2.573799
H	3.783331	-0.501747	-3.020205
H	1.995072	3.741858	-3.274228
H	2.118650	2.205644	-2.944025
H	-3.105089	-2.148952	-0.891158
H	-2.396894	-2.012746	-2.273585
H	0.416382	2.205689	-6.077642
H	0.610987	2.264837	-4.535327
H	1.940184	1.656443	0.170201
H	2.904307	0.489134	0.573063
H	3.382951	-1.617278	1.770844
H	2.394699	-1.813121	0.600274
H	-1.522199	1.165778	-4.997624
H	-2.562968	0.727809	-3.906197
H	5.954283	-1.241872	-0.721106
H	4.574489	-1.773801	-0.298919
H	-2.962607	-0.777969	-5.746778
H	-3.732262	-2.105575	-5.485486
H	0.140796	-5.640435	-1.846449
H	0.255079	-5.025926	-0.441504

H	-2.992453	-6.297397	-0.458953
H	-1.602448	-5.714253	-0.940913
H	-3.082791	-5.645191	-2.655753
H	-3.944353	-6.381256	-3.731597
H	-1.713576	-2.952297	0.488385
H	-2.702240	-4.008168	-0.043537
H	3.506342	-1.343019	-5.072807
H	3.144941	-2.006259	-6.405113
H	-1.193037	-4.566626	-5.971906
H	-1.994006	-5.532239	-5.034754
H	-0.967630	-3.012776	-7.616221
H	-1.919252	-2.425964	-6.517817
H	-4.151632	-2.599803	-3.135332
H	-4.146515	-3.992564	-3.853037
H	0.996186	-4.351057	-3.518888
H	-0.125193	-5.249416	-4.270919
H	0.556795	2.665063	-1.475681
H	-0.637665	2.338854	-0.485082
H	0.355298	-0.949237	-1.517885
H	0.205402	0.609124	-1.545546
H	-0.937364	-3.607158	-3.323923
H	-2.267268	-3.039718	-3.962731
O	1.846716	-2.843089	-3.150332
H	2.735915	-2.419948	-3.206609
H	1.592765	-2.808770	-2.212383

$CaCl_2(H_2O)_1$

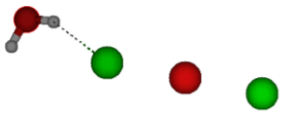

Figure S_{177} : $CaCl_2$ optimized structure with 1 water molecule.

E =-143.430478

H =-143.429533

Ca	0.066588	0.079024	1.238550
Cl	-1.150668	-0.227917	3.349551
Cl	1.276405	0.399202	-0.898737
H	3.382248	0.054478	-2.260574
O	3.852591	-0.165547	-3.073140
H	3.160233	-0.139240	-3.740407

$CaCl_2(H_2O)_2$

Figure S_{178} : $CaCl_2$ optimized structure with 2 water molecules.

E =-219.800604

H =-219.799659

O	4.023858	0.082345	-3.956245
Cl	1.793906	0.119836	-1.353902
Ca	0.658182	-0.208703	0.811998
Cl	-0.458513	-0.548781	2.985340
H	3.701114	-0.055657	-3.058656
H	3.275626	0.496134	-4.397080
H	-2.025271	-0.156654	4.988087
O	-2.308939	-0.422128	5.870000
H	-1.738459	-1.171067	6.067528

$CaCl_2(H_2O)_3$

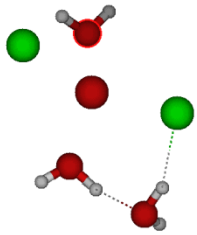

Figure S_{179} : $CaCl_2$ optimized structure with 3 water molecules.

E =-296.268756

H =-296.267812

O	1.782651	-0.842107	-1.269360
Cl	2.751873	1.948464	-0.324826
Ca	1.186440	0.226217	0.737735
Cl	0.918260	-1.560139	2.578187
O	-1.852576	-0.201952	3.081209
H	2.407781	-0.167797	-1.591500
H	2.136079	-1.710311	-1.488581
H	-1.023994	-0.714267	3.205300
H	-2.516182	-0.864447	2.858313
O	-0.881545	1.131422	1.091057
H	-1.194524	2.034592	0.984215
H	-1.387037	0.698254	1.848476

$CaCl_2(H_2O)_4$

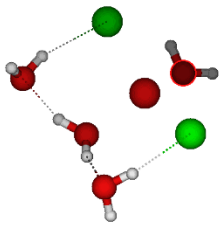

Figure S_{180} : $CaCl_2$ optimized structure with 4 water molecules.

E =-372.656692

H =-372.655748

O	0.902326	-0.997714	-1.839380
Ca	1.197805	-0.343001	0.401205
O	0.178880	1.325570	1.503652

Cl	3.055701	1.066927	-0.767557
Cl	0.677014	-2.229880	2.055905
O	-0.506726	0.187483	3.801725
H	1.601392	-0.513378	-2.306673
H	0.719474	-1.808765	-2.324189
H	-0.131067	-0.671744	3.524548
H	-1.450458	0.018392	3.896667
H	0.651329	2.196459	1.496074
H	-0.135135	1.095253	2.416472
O	1.812435	3.394595	1.090633
H	2.289768	2.926613	0.379112
H	2.480556	3.544400	1.768431

$CaCl_2(H_2O)_5$

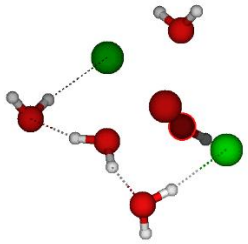

Figure S_{181} : $CaCl_2$ optimized structure with 5 water molecules.

E =-449.055188

H =-449.054244

O	0.997390	-0.875837	-1.239851
Ca	1.593808	-0.375567	0.976597
O	0.567230	1.350435	1.975339
Cl	0.315420	-2.186227	2.326473
Cl	3.046485	1.335799	-0.612964
O	-1.307139	0.294363	3.532973
O	1.231296	3.616219	0.744894
H	1.542939	-0.292565	-1.791301
H	0.622588	-1.574983	-1.782766
H	-0.881099	-0.576960	3.399899
H	-2.165193	0.199847	3.105212
H	0.644694	2.284797	1.665060

H	-0.194551	1.195285	2.586653
H	1.797659	3.094555	0.142541
H	1.854583	4.148534	1.251135
O	3.846648	-0.843774	1.441818
H	4.413627	-1.303438	2.067404
H	4.372809	-0.209318	0.931191

$CaCl_2(H_2O)_6$

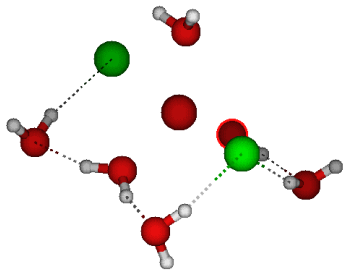

Figure S_{182} : $CaCl_2$ optimized structure with 6 water molecules.

E =-525.447577

H =-525.446633

O	1.397167	-1.627048	-0.650791
Ca	1.980241	-0.201377	1.064918
O	0.423089	1.345745	1.567626
O	4.155046	-0.380047	1.965438
Cl	0.871420	-1.897821	2.847133
O	-1.222887	0.449432	3.469784
O	1.179220	3.702110	0.582868
Cl	3.423409	1.608018	-0.272790
H	1.332944	-1.461514	-1.595314
H	0.851687	-2.432817	-0.418106
H	-0.665860	-0.350666	3.532837
H	-2.057176	0.129702	3.109306
H	0.517406	2.293411	1.300668
H	-0.272365	1.213439	2.255954
H	1.905029	3.236285	0.120080
H	1.632170	4.255306	1.228536
H	4.568532	-0.581993	2.809674

H	4.650119	0.329302	1.525671
H	0.091393	-3.206467	1.260748
O	0.024600	-3.604191	0.365948
H	0.522171	-4.426889	0.433220

$CaCl_2(H_2O)_7$

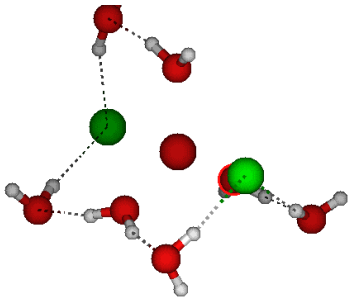

Figure S_{183} : $CaCl_2$ optimized structure with 7 water molecules.

E =-601.839712

H =-601.838768

O	1.208932	-1.488690	-0.726975
Ca	1.975374	0.004455	0.863109
O	0.407980	1.412689	1.671439
O	4.185519	0.021390	1.542313
O	0.159450	-3.556872	0.484722
O	0.407817	3.724096	0.334343
O	-0.885046	0.313557	3.733110
Cl	2.629564	1.856263	-1.001806
Cl	1.330685	-1.796687	2.781415
H	0.914747	-1.278625	-1.617745
H	0.758865	-2.325325	-0.416919
H	-0.236542	-0.416870	3.704824
H	-1.715326	-0.098081	3.469732
H	0.244877	2.317403	1.310748
H	-0.181842	1.196829	2.433136
H	1.043513	3.322098	-0.289855
H	0.920492	4.402420	0.787451
H	4.544681	-0.296387	2.375348
H	4.819336	0.675433	1.131194

H	0.375844	-3.155494	1.354333
H	0.714361	-4.343705	0.441287
H	4.686937	2.092325	-0.262315
O	5.511932	1.837744	0.204315

$CaCl_2(H_2O)_8$

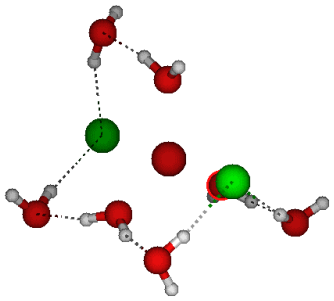

Figure S_{184} : $CaCl_2$ optimized structure with 8 water molecules.

E =-678.224604

H =-678.223660

O	1.512088	-1.790651	-0.257311
Ca	1.865005	0.049835	1.063921
O	0.377092	1.627166	1.719886
O	4.051247	0.533583	1.640508
O	1.304222	-4.279690	0.412416
O	5.074365	2.195606	-0.107515
O	0.293261	3.657283	-0.018165
O	-0.277946	1.301076	4.297642
Cl	2.261759	1.455399	-1.234939
Cl	1.521063	-1.201829	3.433593
H	1.469524	-1.690621	-1.213523
H	1.424313	-2.769216	-0.031614
H	0.304756	0.516902	4.311545
H	-1.165315	0.936564	4.386486
H	0.224118	2.462276	1.214867
H	0.037997	1.689536	2.644388
H	0.807041	3.103474	-0.638169
H	0.897829	4.369947	0.216057

H	4.413858	0.512431	2.530643
H	4.573021	1.175337	1.081398
H	1.016371	-4.299507	1.364208
H	2.154467	-4.731126	0.401904
H	4.232711	2.161731	-0.612480
H	5.719029	1.782294	-0.692677
H	0.980247	-3.309116	3.262203
O	0.655154	-4.194431	2.996515
H	-0.294706	-4.156556	3.151359

$CaCl_2(H_2O)_9$

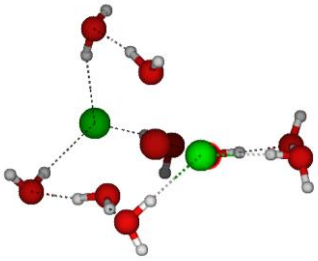

Figure S_{185} : $CaCl_2$ optimized structure with 9 water molecules.

E =-754.611027

H =-754.610083

O	1.407695	-1.300067	-0.470852
Ca	1.743209	0.300782	1.085522
O	0.159080	1.778762	1.779587
O	3.973039	0.432486	1.693863
O	1.700541	-3.880822	-0.035949
O	5.308586	2.200629	0.274160
O	1.339298	-4.169802	2.616873
O	0.274140	4.122130	0.465691
O	-0.648456	1.175597	4.262285
Cl	1.399582	-1.097453	3.366640
Cl	2.390532	2.151390	-0.902840
H	1.486839	-1.071011	-1.426974
H	1.499886	-2.287532	-0.359799
H	0.004543	0.448931	4.280070

H	-1.499096	0.723719	4.235335
H	0.067220	2.690707	1.414564
H	-0.236408	1.718476	2.682997
H	0.881033	3.712589	-0.179034
H	0.817238	4.773021	0.923554
H	4.289451	0.204679	2.573067
H	4.606629	1.066677	1.260898
H	1.544203	-4.033332	0.930421
H	2.605476	-4.169958	-0.189690
H	4.488447	2.425812	-0.210372
H	5.879575	1.801916	-0.391984
H	1.444521	-3.260129	2.961701
H	0.424518	-4.392614	2.820231
H	2.035453	0.611551	-2.536378
O	1.717059	-0.223517	-2.928011
H	0.870986	0.006657	-3.327298

$CaCl_2(H_2O)_{10}$

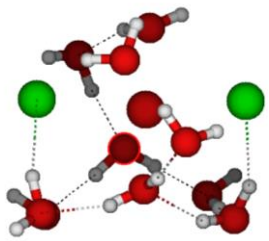

Figure S_{186} : $CaCl_2$ optimized structure with 10 water molecules.

E =-831.006833

H =-831.005889

O	2.638398	-0.699796	-0.361794
Ca	2.350489	0.064391	1.849107
O	-0.026507	0.178360	1.652928
O	4.677646	-0.012059	2.213190
O	5.133030	0.536649	-0.298321
O	1.884079	-3.179668	-0.358033
O	-0.182256	0.557561	4.259835

O	-0.259542	2.163866	-0.224692
O	-0.003821	-2.701845	1.466415
Cl	2.034973	-1.785560	3.741825
O	1.203153	0.721353	-2.123435
Cl	2.606017	2.637541	0.703492
H	2.099148	-0.219081	-1.047071
H	2.435382	-1.681079	-0.462023
H	0.529449	1.210070	4.355873
H	0.266914	-0.283216	4.462485
H	-0.368693	0.867586	1.047464
H	-0.304186	0.387441	2.587887
H	0.591628	2.556052	0.083191
H	-0.880196	2.891062	-0.340600
H	5.093437	-0.792635	2.593151
H	5.080955	0.166831	1.316012
H	1.121877	-3.093268	0.275707
H	2.472223	-3.835821	0.028863
H	4.812846	1.450907	-0.304500
H	4.341944	0.016241	-0.553674
H	0.501683	-2.685625	2.300275
H	-0.302546	-1.780611	1.379029
H	1.796794	1.403524	-2.456701
H	0.542633	1.210585	-1.594228
H	3.157339	1.749288	4.163236
O	2.362301	1.819484	3.620877
H	2.528467	2.531818	2.971345

$CaCl_2(H_2O)_{11}$

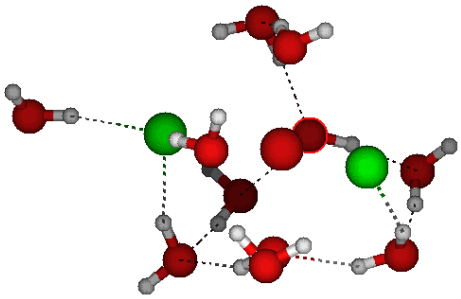

Figure S_{187} : $CaCl_2$ optimized structure with 11 water molecules.

E =-907.379743

H =-907.378798

O	2.652451	-0.719623	-0.299462
Ca	2.326829	-0.098536	1.951436
O	4.637866	-0.276682	2.358873
O	-0.041850	0.080497	1.694985
O	2.307292	1.499029	3.865844
O	1.828301	-3.164518	-0.513249
O	5.201151	0.349810	-0.111596
O	-0.302172	0.265945	4.313170
Cl	1.925886	-2.039018	3.730974
O	-0.054438	-2.790025	1.337864
O	1.279101	0.836989	-1.990088
O	-0.187473	2.209698	-0.038108
Cl	2.672602	2.530605	1.010185
H	2.138542	-0.179389	-0.960770
H	2.426067	-1.685617	-0.475307
H	0.407732	0.903043	4.488573
H	0.135790	-0.590740	4.469078
H	-0.361657	0.813160	1.130462
H	-0.351273	0.223697	2.632734
H	0.654651	2.564745	0.326311
H	-0.785969	2.957608	-0.140419
H	5.007802	-1.092709	2.711160
H	5.073345	-0.076429	1.481472

H	1.070651	-3.119516	0.129767
H	2.387987	-3.887724	-0.214374
H	4.973043	1.289648	-0.111287
H	4.376045	-0.091219	-0.408940
H	0.431789	-2.834163	2.181848
H	-0.342818	-1.862188	1.301887
H	1.870681	1.514209	-2.336083
H	0.629341	1.326701	-1.448233
H	3.059304	1.337038	4.448471
H	2.534819	2.273474	3.317823
H	3.069938	4.675188	0.088045
O	3.079497	5.624502	-0.097451
H	3.597390	5.988691	0.626882

$CaCl_2(H_2O)_{12}$

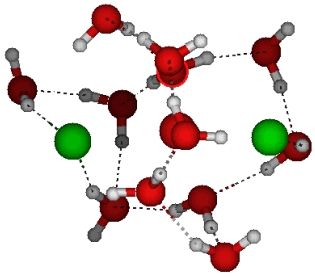

Figure S_{188} : $CaCl_2$ optimized structure with 12 water molecules.

E=-983.780540

H=-983.779595

O	2.626808	-0.297825	-0.218462
Ca	2.168426	-0.031643	2.069295
O	4.476277	-0.706470	2.510558
O	-0.172209	0.207486	1.767413
O	2.030580	1.029502	4.256405
O	1.726291	-2.648757	-0.897322
O	5.163299	0.605902	0.380948
O	-0.587188	-0.005367	4.358855
Cl	1.702063	-2.333747	3.418682
O	-0.275808	-2.523761	0.873331

O	1.447873	1.494660	-1.702053
O	-0.118308	2.586603	0.445569
Cl	2.804437	2.658005	1.595744
O	3.123054	3.667663	-1.464868
H	2.175366	0.374969	-0.824811
H	2.384223	-1.205977	-0.569491
H	0.217209	0.488427	4.604875
H	-0.308426	-0.930544	4.443283
H	-0.423983	1.047941	1.329054
H	-0.529114	0.197489	2.701016
H	0.740738	2.850071	0.838704
H	-0.681463	3.367631	0.462984
H	4.588565	-1.657320	2.389035
H	4.954487	-0.248695	1.752882
H	0.923878	-2.676007	-0.312570
H	2.218807	-3.453091	-0.708605
H	4.877962	1.487363	0.668257
H	4.368822	0.258647	-0.084137
H	0.156052	-2.773978	1.708247
H	-0.497719	-1.586542	1.012736
H	2.059501	2.259829	-1.782380
H	0.708936	1.845481	-1.176917
H	2.705442	0.524607	4.803111
H	2.333697	1.943208	4.167249
H	3.159398	3.595489	-0.494896
H	4.030965	3.541453	-1.760264
H	3.236828	-1.394488	5.150724
O	3.783070	-0.601622	5.288853
H	4.366690	-0.603315	4.510428

$CaCl_2(H_2O)_{13}$

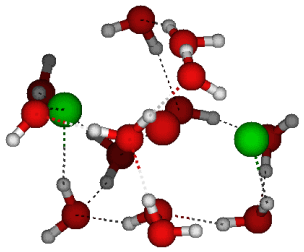

Figure S_{189} : $CaCl_2$ optimized structure with 13 water molecules.

E=-1060.166602

H=-1060.165658

O	2.661872	-0.341187	-0.225195
Ca	2.185529	0.105448	2.034898
O	-0.154545	0.229929	1.636873
O	1.893986	1.013450	4.240120
O	4.500943	-0.472316	2.524218
O	5.159702	0.702508	0.279366
O	3.602590	-0.682313	5.317790
O	1.883346	-2.783412	-0.711879
O	1.437010	1.252900	-1.902066
O	-0.704908	0.127509	4.200088
O	-0.330646	-2.520697	0.794043
Cl	1.865902	-2.340207	3.153069
O	-0.221206	2.488024	0.105454
O	3.123897	3.444087	-1.911921
Cl	2.686137	2.802928	1.253020
H	2.193864	0.244868	-0.900008
H	2.453179	-1.291220	-0.483162
H	0.178515	0.485691	4.438562
H	-0.645086	-0.812296	4.414157
H	-0.450991	1.018500	1.137345
H	-0.554969	0.237430	2.553535
H	0.618624	2.830566	0.475395
H	-0.815451	3.240594	0.017955
H	4.572562	-1.430175	2.420690

H	4.978463	-0.061180	1.746430
H	0.999732	-2.743989	-0.260002
H	2.373857	-3.455697	-0.226879
H	4.853998	1.597247	0.489752
H	4.371462	0.288923	-0.140759
H	0.104929	-2.765888	1.627980
H	-0.477357	-1.564865	0.906265
H	2.032091	2.018205	-2.058669
H	0.682526	1.633639	-1.422638
H	2.512236	0.470169	4.806739
H	2.104885	1.971466	4.392355
H	3.139380	3.511264	-0.942389
H	4.027711	3.223225	-2.161748
H	3.125920	-1.462731	4.981400
H	4.296175	-0.545647	4.653888
H	2.728425	3.627521	3.350209
O	2.558839	3.597417	4.310302
H	1.845347	4.226004	4.462568

$CaCl_2(H_2O)_{14}$

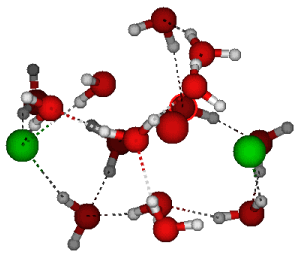

Figure S_{190} : $CaCl_2$ optimized structure with 14 water molecules.

E=-1136.556161

H=-1136.555217

O	2.861307	-0.509974	-0.085805
Ca	2.269568	-0.189419	2.162396
O	0.007707	0.202518	1.616504
O	1.906728	0.898597	4.302741
O	4.451452	-1.066716	2.789949

O	1.825359	-2.776208	-0.868337
O	1.846791	1.388235	-1.530390
O	5.449684	0.068865	0.683077
O	-0.737491	0.019712	4.132981
O	3.486791	-0.831514	5.510324
O	2.841565	3.446678	3.979647
O	-0.271623	-2.535088	0.773031
Cl	1.557375	-2.477983	3.432478
O	-0.346566	2.341983	0.029028
O	3.033889	3.855566	-1.675631
Cl	1.726106	4.262591	1.216931
H	2.501887	0.211613	-0.695364
H	2.553539	-1.386235	-0.465693
H	0.097864	0.420135	4.446305
H	-0.593639	-0.928427	4.266903
H	-0.281137	0.975113	1.076216
H	-0.458572	0.211024	2.500254
H	0.194806	3.059091	0.438734
H	-1.170665	2.750718	-0.255796
H	4.433888	-2.029687	2.723229
H	5.030342	-0.718286	2.041890
H	0.987040	-2.760476	-0.334923
H	2.264882	-3.601472	-0.642085
H	5.165918	0.954309	0.965497
H	4.680045	-0.220295	0.145442
H	0.097796	-2.823606	1.625418
H	-0.396125	-1.577918	0.904649
H	2.346415	2.222638	-1.674231
H	0.982435	1.668904	-1.183740
H	2.483277	0.361925	4.917317
H	2.150895	1.843664	4.392807
H	2.694468	4.236888	-0.844933
H	3.990531	3.946603	-1.623751
H	2.912940	-1.596689	5.334674

H	4.143068	-0.887264	4.795080
H	2.349048	3.901712	3.258643
H	3.168227	4.134269	4.568701
O	3.553904	1.875705	1.843477
H	3.034957	2.555647	1.351831
H	3.689821	2.336044	2.695255

$CaCl_2(H_2O)_{15}$

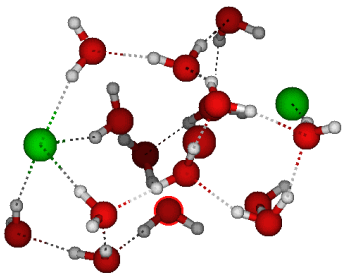

Figure S_{191} : $CaCl_2$ optimized structure with 15 water molecules.

E =-1953.123832

H =-1953.122888

O	3.141059	-0.116973	-0.381802
Ca	2.438098	-0.488039	1.913251
O	0.184249	0.086442	1.416851
O	1.888698	0.433524	4.123240
O	4.745452	-1.002385	2.515146
O	3.523791	1.757443	1.910579
O	1.916633	1.580841	-1.858678
O	5.666563	0.493760	0.605904
O	2.114691	-2.482873	0.462899
O	-0.798927	-0.237001	3.790085
O	3.893115	-0.829505	5.308145
O	-0.509474	-2.483323	0.547483
O	-0.225474	2.263504	-0.127062
Cl	2.287792	-2.903069	3.531861
O	2.453069	3.137861	4.021645
O	2.972938	4.099275	-1.778885
Cl	1.753568	4.175421	1.174854

H	2.683345	0.557061	-0.995323
H	2.917928	-1.003526	-0.705063
H	0.067817	-0.081029	4.212208
H	-0.921402	-1.207379	3.791411
H	-0.075685	0.879491	0.892479
H	-0.322359	0.075862	2.288919
H	0.293667	2.977174	0.320278
H	-1.084745	2.644318	-0.337291
H	4.961441	-1.941111	2.471156
H	5.290151	-0.517001	1.820331
H	1.118032	-2.592805	0.391873
H	2.385210	-3.187538	1.070372
H	5.237746	1.252474	1.040206
H	4.963212	0.222269	-0.019203
H	-0.740713	-2.837867	1.427553
H	-0.506901	-1.517663	0.692641
H	2.361218	2.457474	-1.933019
H	1.059471	1.777782	-1.439070
H	2.581875	0.032060	4.718780
H	1.952628	1.404607	4.229999
H	2.635236	4.366703	-0.903249
H	3.929457	4.184193	-1.711199
H	3.473864	-1.699768	5.182398
H	4.489582	-0.778061	4.542054
H	2.053970	3.638596	3.276229
H	2.686753	3.783734	4.695643
H	3.029881	2.443940	1.405203
H	3.521769	2.156548	2.802122
H	0.200494	-3.113345	3.487601
O	-0.763763	-2.996219	3.318791
H	-1.207817	-3.703791	3.797686

$CaCl_2(H_2O)_{16}$

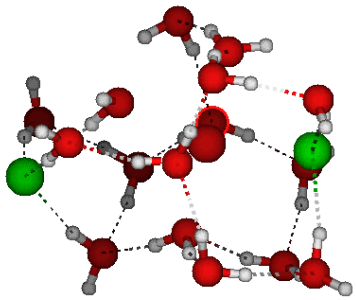

Figure S_{192} : $CaCl_2$ optimized structure with 16 water molecules.

E=-1289.329702

H=-1289.328758

O	3.001454	-0.433324	-0.270491
Ca	2.470968	-0.277926	2.003940
O	0.223172	0.205838	1.502021
O	1.980566	0.461937	4.235210
O	3.500459	1.919542	1.835367
O	4.779104	-0.828009	2.590497
O	5.538304	0.437353	0.458266
O	-0.726141	-0.296681	3.861978
O	1.870884	1.427486	-1.686416
O	1.914355	-2.810247	-0.577155
O	4.120250	-0.446398	5.371274
O	-0.295204	2.319678	-0.053772
O	-0.591267	-2.220715	0.265910
O	2.488068	3.189481	4.031713
O	3.006999	3.926854	-1.650124
Cl	2.279796	-2.933195	2.784035
O	-0.789134	-2.980483	3.044044
Cl	1.645436	4.282122	1.236501
H	2.578029	0.261368	-0.869364
H	2.656284	-1.331346	-0.551930
H	0.136808	-0.158796	4.294233
H	-0.841885	-1.263058	3.770094
H	-0.084652	0.989483	0.985381

H	-0.292974	0.132103	2.361924
H	0.207957	3.062135	0.362160
H	-1.163919	2.667644	-0.280463
H	4.910982	-1.782566	2.530148
H	5.272897	-0.407114	1.819923
H	0.958446	-2.675103	-0.349862
H	2.253493	-3.331717	0.162254
H	5.138028	1.258369	0.790028
H	4.810048	0.053440	-0.075108
H	-0.823408	-2.670681	1.095787
H	-0.428772	-1.304938	0.557469
H	2.357999	2.276882	-1.772077
H	1.008155	1.677692	-1.313585
H	2.751947	0.116667	4.792757
H	1.996886	1.436208	4.330418
H	2.641813	4.274050	-0.815454
H	3.958628	4.052058	-1.581664
H	3.974156	-1.388704	5.624003
H	4.658911	-0.498774	4.564010
H	2.035738	3.690932	3.317629
H	2.755580	3.836551	4.692289
H	2.952973	2.600643	1.374937
H	3.553808	2.312462	2.729794
H	0.178571	-3.144491	3.035148
H	-1.194148	-3.763526	3.431107
H	3.169275	-3.218396	4.811140
O	3.570468	-3.092635	5.692310
H	2.863691	-3.285546	6.317038

$CaCl_2(H_2O)_{17}$

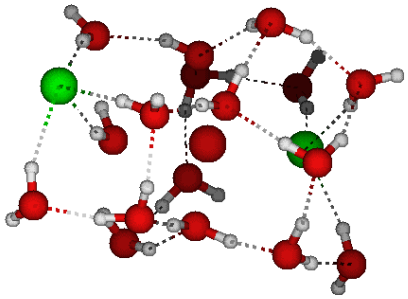

Figure S_{193} : $CaCl_2$ optimized structure with 17 water molecules.

E=-1365.710303

H=-1365.709359

O	3.036851	-0.447378	-0.181762
Ca	2.464778	-0.221948	2.060600
O	0.221508	0.243424	1.550308
O	1.930171	0.554984	4.275342
O	3.437116	1.994415	1.846535
O	4.773090	-0.666856	2.733930
O	4.086114	-0.208877	5.496343
O	-0.757892	-0.268668	3.898293
O	5.529374	0.482538	0.544852
O	1.966459	1.487045	-1.571799
O	1.948816	-2.660813	-0.882393
O	-0.306848	2.319357	-0.049640
O	-0.477730	-2.224002	0.319707
O	3.602296	-2.853240	5.955786
O	2.395826	3.279348	4.019144
O	3.022126	4.025175	-1.583707
Cl	2.364613	-2.859335	3.016316
O	-0.724075	-2.969057	3.119305
Cl	1.554022	4.358186	1.239879
H	2.652948	0.273966	-0.769297
H	2.682215	-1.335925	-0.536773
H	0.097173	-0.104886	4.336836
H	-0.845050	-1.238216	3.810477

H	-0.093194	1.010957	1.013644
H	-0.311021	0.167018	2.398703
H	0.160530	3.085058	0.365347
H	-1.175804	2.636716	-0.316520
H	4.932602	-1.618509	2.730316
H	5.264060	-0.275761	1.943658
H	1.034218	-2.605646	-0.519286
H	2.333534	-3.475210	-0.499346
H	5.129382	1.323493	0.820701
H	4.802109	0.066053	0.030227
H	-0.679309	-2.688174	1.148098
H	-0.357625	-1.302438	0.610091
H	2.429335	2.347898	-1.667388
H	1.078977	1.715283	-1.247872
H	2.700770	0.260095	4.859585
H	1.917597	1.532491	4.336095
H	2.617131	4.371341	-0.766917
H	3.966013	4.183809	-1.484570
H	3.974326	-1.142413	5.792434
H	4.632379	-0.274159	4.695348
H	1.945067	3.774682	3.298323
H	2.659619	3.931638	4.676036
H	2.885318	2.652037	1.361512
H	3.467539	2.408350	2.733107
H	0.240867	-3.129633	3.167078
H	-1.149339	-3.749953	3.488614
H	3.202637	-3.026768	5.082897
H	2.894143	-3.009643	6.589319
H	2.844726	-4.393106	1.397042
O	2.988435	-4.824480	0.537130
H	3.943948	-4.912640	0.458816

$CaCl_2(H_2O)_{18}$

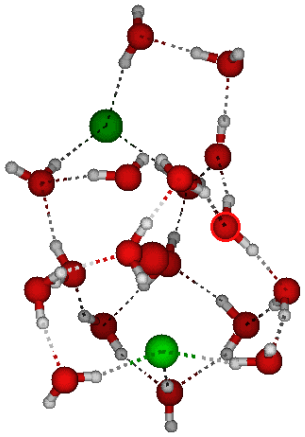

Figure S_{194} : $CaCl_2$ optimized structure with 18 water molecules.

E=-1442.103056

H=-1442.102112

O	2.992862	-0.455591	-0.114666
Ca	2.392821	-0.243498	2.135067
O	0.116905	0.146929	1.668619
O	1.881620	0.457750	4.371708
O	3.158430	2.008037	1.829794
O	4.725400	-0.562205	2.799447
O	1.905454	-2.588347	-0.993948
O	5.423437	0.625497	0.613111
O	4.060915	-0.255263	5.581410
O	-0.776759	-0.489406	4.021147
O	2.018559	1.873063	-0.805888
O	-0.599063	2.247021	0.161962
O	3.710045	-2.942599	5.923818
O	2.217676	3.204243	4.097264
O	-0.460473	-2.288425	0.353015
O	2.983237	3.943952	-2.170491
O	3.112950	-4.697824	0.366921
Cl	2.455634	-2.917755	2.986802
O	-0.617145	-3.154955	3.122106
Cl	0.880288	4.410876	1.655987

H	2.572925	0.346391	-0.535560
H	2.620705	-1.301727	-0.553056
H	0.074492	-0.284225	4.448208
H	-0.806571	-1.458957	3.901265
H	-0.257148	0.912580	1.169608
H	-0.389937	0.014779	2.524641
H	-0.287832	3.049956	0.646010
H	-1.462330	2.458908	-0.207597
H	4.928769	-1.504990	2.766551
H	5.188320	-0.130269	2.014383
H	1.005722	-2.574630	-0.584518
H	2.332885	-3.393098	-0.633519
H	5.009845	1.467162	0.855823
H	4.703508	0.176914	0.118244
H	-0.615166	-2.792514	1.168264
H	-0.383813	-1.371940	0.677194
H	2.363404	2.621992	-1.363212
H	1.057750	2.005959	-0.727036
H	2.663973	0.168180	4.943806
H	1.841875	1.435317	4.453189
H	3.023202	4.607497	-1.433692
H	3.894992	3.812536	-2.447686
H	3.999218	-1.206940	5.830266
H	4.613329	-0.251215	4.782417
H	1.635829	3.721679	3.487684
H	2.613984	3.840432	4.701781
H	2.602307	2.511462	1.202249
H	3.084712	2.491641	2.680169
H	0.354161	-3.278451	3.158120
H	-1.007872	-3.967869	3.459364
H	3.320940	-3.107145	5.044546
H	3.008689	-3.153736	6.549009
H	2.965307	-4.315631	1.249441
H	4.069223	-4.701999	0.254652

H	2.471287	5.391392	0.507343
O	3.092253	5.754266	-0.160458
H	2.674585	6.586846	-0.429865

$CaCl_2(H_2O)_{19}$

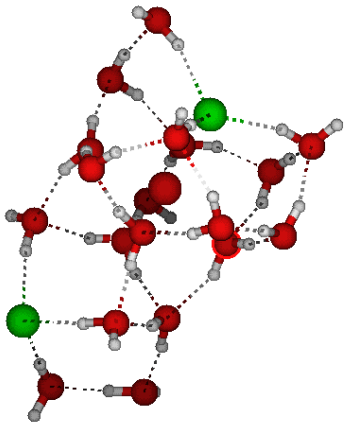

Figure S_{195} : $CaCl_2$ optimized structure with 19 water molecules.

E=-1518.494866

H=-1518.493922

O	2.866265	-0.713645	-0.152019
Ca	2.542840	-0.418267	2.171172
O	0.255657	0.081627	1.715258
O	3.263332	1.802181	1.633424
O	2.049193	0.435991	4.346131
O	4.850242	-0.777453	2.713363
O	1.462673	-2.730849	-0.882884
O	5.957644	1.537634	1.978724
O	4.157803	-0.560641	5.453519
O	-0.687040	-0.268586	4.108808
O	2.267792	1.897058	-0.778073
O	2.914201	4.067334	-2.112930
O	-0.286411	2.227959	0.179640
O	2.395189	5.987331	-0.329154
O	2.202577	3.162379	3.710987
O	3.345145	-3.114584	6.050846
O	-0.771655	-2.268123	0.558404

O	3.255409	-4.415290	0.562108
Cl	2.111780	-3.040463	3.083424
O	-0.945827	-2.974904	3.359554
Cl	0.474758	4.671111	1.749209
H	2.698956	0.121471	-0.639762
H	2.286160	-1.455925	-0.540826
H	0.193596	-0.152411	4.510513
H	-0.853194	-1.229454	4.054625
H	-0.035652	0.872145	1.201244
H	-0.237048	0.061114	2.592014
H	-0.135095	3.064354	0.701279
H	-1.133695	2.335040	-0.265452
H	5.096424	-1.467049	2.038826
H	5.404737	0.017594	2.497972
H	0.611094	-2.696061	-0.378630
H	1.970660	-3.477541	-0.520740
H	5.048707	1.818850	1.735610
H	6.449948	1.486922	1.152965
H	-0.987024	-2.727898	1.385893
H	-0.510425	-1.379336	0.868096
H	2.557684	2.662245	-1.353446
H	1.303336	2.011977	-0.643080
H	2.832232	0.118242	4.905680
H	2.037686	1.414528	4.351175
H	2.709313	4.803734	-1.477741
H	3.844110	4.175364	-2.334401
H	3.936791	-1.453496	5.802266
H	4.647699	-0.739451	4.629294
H	1.510638	3.680392	3.220686
H	2.733058	3.820723	4.173182
H	2.889579	2.017777	0.728078
H	2.925656	2.445141	2.302291
H	0.014949	-3.169907	3.334256
H	-1.361981	-3.715711	3.812170

H	3.007374	-3.271892	5.150522
H	2.560100	-3.112076	6.608623
H	2.886187	-4.180869	1.438721
H	3.412849	-5.364913	0.576507
H	1.842546	5.597746	0.385032
H	1.852252	6.702663	-0.677043
O	5.106381	-2.286388	0.548031
H	4.510320	-1.707601	0.037674
H	4.649814	-3.148648	0.541320

$CaCl_2(H_2O)_{20}$

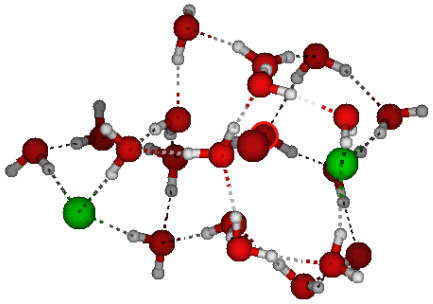

Figure S_{196} : $CaCl_2$ optimized structure with 20 water molecules.

E=-1594.878603

H=-1594.877659

O	2.871093	-0.682064	-0.062137
Ca	2.614278	-0.339534	2.249923
O	0.304661	0.210384	1.988341
O	2.324611	0.576785	4.444697
O	3.352297	1.858184	1.634704
O	4.939297	-0.713729	2.744447
O	1.909784	-2.791628	-1.122229
O	4.381773	-0.562592	5.494582
O	-0.424363	0.056103	4.479358
O	2.237566	1.926279	-0.722437
O	2.819567	4.076699	-2.122229
O	5.218301	-2.191693	0.577240
O	6.044172	1.594071	1.970354

O	2.429298	6.032103	-0.343089
O	-0.248320	2.318031	0.398581
O	-0.610453	-3.452672	-0.578005
O	2.485840	3.288851	3.753687
O	3.442724	-3.098391	5.986748
Cl	2.070644	-2.943195	3.081705
O	-0.894770	-2.673306	3.946884
O	3.453175	-4.362937	0.663099
Cl	0.638788	4.772991	1.881294
H	2.695480	0.139919	-0.566676
H	2.418176	-1.470202	-0.531440
H	0.497757	0.147256	4.785771
H	-0.642964	-0.893411	4.525362
H	0.019494	0.997133	1.464990
H	-0.093196	0.270401	2.911132
H	-0.047192	3.162549	0.889773
H	-1.126930	2.430412	0.020418
H	5.187541	-1.389197	2.054190
H	5.484177	0.088057	2.529194
H	0.955052	-3.006262	-0.947787
H	2.410128	-3.496202	-0.674166
H	5.136943	1.862845	1.707402
H	6.543833	1.507382	1.151963
H	-0.964154	-2.879707	0.154495
H	-1.207555	-3.308147	-1.318361
H	2.497163	2.683688	-1.321509
H	1.284686	2.050965	-0.529531
H	3.106033	0.213085	4.980088
H	2.363669	1.554323	4.438321
H	2.661280	4.825467	-1.488323
H	3.736229	4.169304	-2.399101
H	4.110174	-1.456177	5.803022
H	4.836723	-0.731106	4.647811
H	1.762384	3.803239	3.308090

H	3.067674	3.952003	4.141106
H	2.941996	2.066133	0.743708
H	3.068240	2.522970	2.306967
H	0.012125	-2.922084	3.668301
H	-1.243906	-3.424617	4.436951
H	3.064797	-3.216619	5.096047
H	2.681557	-3.095486	6.576510
H	2.961586	-4.098963	1.467653
H	3.599876	-5.311684	0.732348
H	1.923869	5.657284	0.412736
H	1.866832	6.743819	-0.666469
H	4.585787	-1.637917	0.084865
H	4.789551	-3.068554	0.604415
O	-1.536358	-1.835366	1.310839
H	-1.542550	-2.243004	2.194541
H	-0.896526	-1.104576	1.412394

$CaCl_2(H_2O)_{21}$

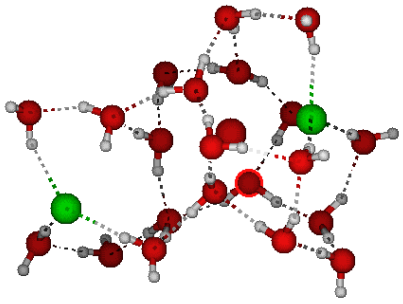

Figure S_{197} : $CaCl_2$ optimized structure with 21 water molecules.

E=-1671.261094

H=-1671.260150

O	2.936837	-0.641595	0.011814
Ca	2.574024	-0.305538	2.310649
O	2.163662	0.556500	4.506952
O	4.883169	-0.602189	2.880936
O	-1.491296	-1.895439	1.168044
O	3.217611	1.935182	1.746835
O	0.262181	0.199498	1.935788

O	4.214025	-0.536186	5.619168
O	2.256313	1.922720	-0.701238
O	2.789663	3.944207	-2.303944
O	-0.568352	0.011632	4.389889
O	2.089801	-2.778116	-1.100931
O	5.313420	-2.061562	0.724485
O	-0.306581	2.274370	0.284617
O	5.900406	1.774169	2.234640
O	1.889238	6.052545	-0.925012
O	2.031683	3.219098	3.768771
O	3.335518	-3.113137	6.021275
O	-0.967541	-2.719688	3.830977
O	3.614375	-4.288576	0.754175
O	-0.432781	-3.515434	-0.654906
Cl	2.034863	-2.930055	3.087785
Cl	0.390860	4.910161	1.595100
H	2.756056	0.178085	-0.497042
H	2.530731	-1.439620	-0.480206
H	0.339970	0.103948	4.737546
H	-0.782324	-0.939939	4.418552
H	-0.027574	0.972220	1.397676
H	-0.180656	0.240653	2.839411
H	-0.162478	3.159150	0.713051
H	-1.168121	2.321589	-0.143391
H	5.194280	-1.257353	2.196768
H	5.397307	0.229868	2.703555
H	1.137979	-3.025394	-0.960329
H	2.598411	-3.464629	-0.634691
H	4.996609	2.033919	1.952587
H	6.437577	1.769932	1.435883
H	-0.835255	-2.941559	0.050307
H	-0.995617	-3.395081	-1.425819
H	2.510589	2.636416	-1.353083
H	1.291650	2.015448	-0.565076

H	2.932779	0.209898	5.070345
H	2.169569	1.536385	4.510777
H	2.447179	4.742078	-1.823210
H	3.722319	4.124122	-2.456963
H	3.964425	-1.447541	5.890897
H	4.712079	-0.661073	4.789651
H	1.195308	3.463190	3.333511
H	2.413606	4.110817	3.967044
H	2.873290	2.128011	0.830044
H	2.814138	2.561135	2.402860
H	-0.042663	-2.948091	3.596760
H	-1.322365	-3.477866	4.306155
H	2.978264	-3.216547	5.120240
H	2.562000	-3.134843	6.594348
H	3.072120	-4.037536	1.529737
H	3.790675	-5.230950	0.839317
H	1.474423	5.727617	-0.097415
H	1.186550	6.543393	-1.363656
H	4.676623	-1.529396	0.213766
H	4.911821	-2.951353	0.741348
H	-1.533669	-2.305087	2.049943
H	-0.867514	-1.156289	1.301589
H	1.992390	5.844208	2.985805
O	2.586317	5.832731	3.760464
H	2.112743	6.335849	4.432003

$CaCl_2(H_2O)_{22}$

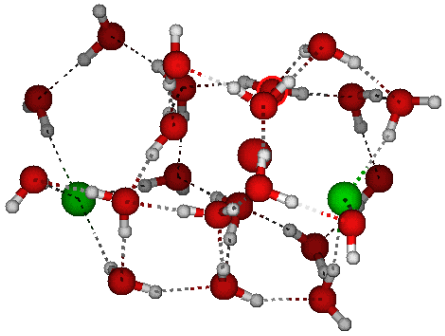

Figure S_{198} : $CaCl_2$ optimized structure with 22 water molecules.

E=-1747.649344

H=-1747.648399

O	3.106147	-0.634417	-0.023970
Ca	2.696136	-0.349412	2.277620
O	2.345405	0.463333	4.511656
O	0.401170	0.166419	1.789294
O	4.985708	-0.697974	2.850893
O	3.231547	1.925423	1.842532
O	2.121266	-2.734170	-1.110573
O	4.294190	-0.825184	5.587619
O	-0.401171	0.382142	4.296680
O	2.498000	1.951410	-0.701258
O	2.995925	4.078416	-2.186115
O	5.402435	-2.159926	0.698722
O	5.910586	1.742900	2.342740
O	-0.401505	-3.491646	-0.636918
O	-1.475290	-1.845833	1.168694
O	2.221875	3.094157	3.959706
O	2.375311	5.716749	3.397739
O	1.557085	6.049303	-1.070719
O	-0.161705	2.078376	-0.011466
O	3.420534	-3.417755	5.862318
Cl	1.939049	-2.915518	3.072305
O	3.573775	-4.290518	0.763087

O	-1.000839	-2.317651	3.952515
Cl	0.040424	4.731261	1.361679
H	2.974238	0.205855	-0.515702
H	2.647655	-1.397539	-0.519036
H	0.521954	0.347211	4.632162
H	-0.761314	-0.522744	4.390677
H	0.147138	0.883132	1.157593
H	-0.018607	0.360820	2.671235
H	-0.151860	2.976977	0.421604
H	-0.976524	2.031505	-0.522782
H	5.304706	-1.334181	2.151855
H	5.483382	0.150730	2.705777
H	1.168404	-2.964384	-0.958345
H	2.616781	-3.432510	-0.647701
H	4.998923	2.017856	2.099274
H	6.441542	1.846763	1.546814
H	-0.822519	-2.938987	0.071469
H	-0.972985	-3.392243	-1.404413
H	2.763039	2.706907	-1.297737
H	1.520532	1.977396	-0.666810
H	3.055830	-0.006062	5.066202
H	2.498696	1.434260	4.563369
H	2.448979	4.808571	-1.797061
H	3.898859	4.410186	-2.169059
H	4.043959	-1.751394	5.802375
H	4.807063	-0.894876	4.760958
H	1.232414	3.141102	4.065414
H	2.490657	4.043093	3.944986
H	2.941031	2.151486	0.918656
H	2.774881	2.499572	2.524458
H	-0.098928	-2.621226	3.711467
H	-1.364209	-2.996457	4.530664
H	2.966622	-3.425776	4.999423
H	2.715032	-3.492047	6.513340

H	3.007863	-4.035680	1.519652
H	3.710619	-5.240586	0.835500
H	1.118686	5.718724	-0.259001
H	0.833386	6.375441	-1.615458
H	4.799282	-1.599076	0.177734
H	4.945289	-3.021818	0.734929
H	-1.567802	-2.186642	2.073757
H	-0.791995	-1.155312	1.271629
H	1.711147	5.548192	2.701477
H	1.914084	6.274102	4.033821
O	-0.426406	3.231823	4.244593
H	-0.757321	2.318223	4.246677
H	-0.671003	3.632876	3.394185

$CaCl_2(H_2O)_{23}$

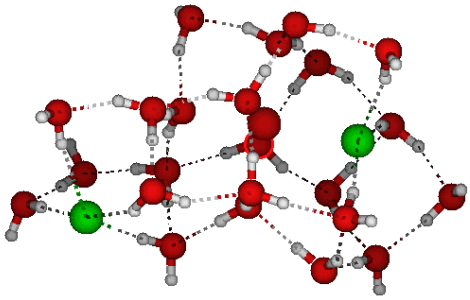

Figure S_{199} : $CaCl_2$ optimized structure with 23 water molecules.

E=-1824.035926

H=-1824.034982

O	3.053074	-0.550164	0.026440
Ca	2.643829	-0.290494	2.330125
O	3.223909	1.964967	1.873562
O	4.918086	-0.758709	2.859241
O	0.338173	0.206565	1.815807
O	2.349192	0.595512	4.543752
O	2.026226	-2.644788	-1.029998
O	4.262474	-0.744336	5.614305
O	2.287370	3.223878	3.967976

O	5.299088	-2.234322	0.700866
O	-0.393992	0.587815	4.326817
O	2.507293	2.026421	-0.672898
O	3.016061	4.120470	-2.194097
O	5.908232	1.649180	2.319628
O	-0.354796	3.429696	4.260939
O	-0.372998	-3.746004	-0.163123
O	-1.444680	-1.920506	1.370259
O	1.573799	6.112389	-1.121556
O	-0.159167	2.129227	-0.000543
O	2.477592	5.822297	3.305665
O	3.328727	-3.295609	5.986235
O	-1.101176	-2.099427	4.190460
Cl	1.767828	-2.787943	3.233835
O	3.327694	-4.238424	0.812614
Cl	0.088987	4.800672	1.332346
H	2.952345	0.297618	-0.461657
H	2.561469	-1.285180	-0.469669
H	0.531132	0.537025	4.656589
H	-0.794547	-0.288073	4.496885
H	0.107607	0.918776	1.170006
H	-0.054923	0.453029	2.697806
H	-0.135975	3.030997	0.425816
H	-0.957825	2.104869	-0.538269
H	5.208397	-1.417960	2.170098
H	5.444937	0.068458	2.693191
H	1.106601	-2.912281	-0.827158
H	2.561212	-3.274957	-0.497216
H	5.005540	1.967454	2.097993
H	6.427557	1.737274	1.514138
H	-0.798036	-3.097375	0.474156
H	-1.035216	-3.933744	-0.835972
H	2.775997	2.772582	-1.280378
H	1.529672	2.051208	-0.641769

H	3.050270	0.107598	5.095902
H	2.533093	1.561248	4.584088
H	2.470673	4.860860	-1.822667
H	3.920482	4.448436	-2.181555
H	3.985273	-1.652638	5.870398
H	4.763473	-0.868294	4.787067
H	1.299772	3.296585	4.080641
H	2.576204	4.165263	3.916507
H	2.948044	2.205174	0.948873
H	2.803397	2.571316	2.551817
H	-0.195052	-2.420632	3.984357
H	-1.465710	-2.713377	4.836505
H	2.863589	-3.316841	5.129786
H	2.631407	-3.343929	6.648261
H	2.953822	-3.820299	1.608089
H	2.734261	-5.019754	0.699763
H	1.139800	5.789035	-0.304704
H	0.846852	6.423905	-1.670507
H	4.709216	-1.658231	0.184159
H	4.872509	-3.109931	0.673765
H	-1.573248	-2.135858	2.310283
H	-0.795104	-1.188289	1.402947
H	1.803210	5.638940	2.623641
H	2.032391	6.409839	3.925823
H	-0.698030	2.520494	4.275332
H	-0.589352	3.816881	3.400682
H	0.972838	-5.968154	1.686706
O	1.172641	-5.865238	0.750258
H	0.558788	-5.163511	0.441776

$CaCl_2(H_2O)_{24}$

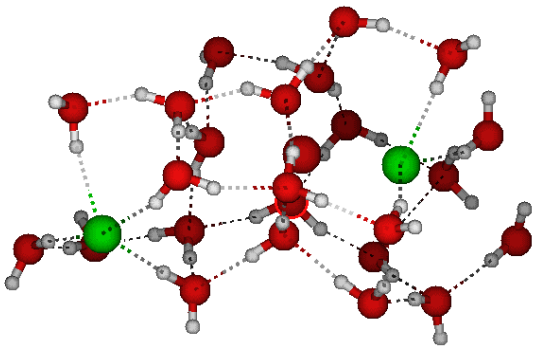

Figure S_{200} : $CaCl_2$ optimized structure with 24 water molecules.

E=-1900.414595

H=-1900.413651

O	2.964758	-0.487199	0.059364
Ca	2.508416	-0.229748	2.342616
O	3.119669	2.011022	1.878444
O	4.797405	-0.763822	2.765294
O	2.300238	0.685578	4.564867
O	0.216467	0.293273	1.795516
O	2.045846	-2.718002	-0.712987
O	4.243230	-0.813763	5.511614
O	2.308248	3.310366	3.998064
O	5.341616	-2.008393	0.511125
O	-0.482153	0.799977	4.308531
O	2.396565	2.064948	-0.673372
O	2.999305	4.119105	-2.216292
O	5.792567	1.660332	2.336877
O	-0.318908	3.624070	4.287827
O	1.689167	6.185875	-1.116982
O	2.591939	5.888707	3.283672
O	-0.256630	2.257564	0.003834
O	3.367758	-3.506609	5.622468
O	3.873408	-4.410272	0.503518
O	1.713740	-6.087848	0.665305
O	-0.212583	-3.937377	0.257434

O	-1.521029	-1.932414	1.404337
O	-1.603156	-1.735018	4.294617
Cl	1.292892	-2.435307	3.575342
Cl	0.164906	4.917191	1.333909
H	2.811897	0.334465	-0.458596
H	2.497265	-1.285467	-0.359771
H	0.422902	0.659826	4.659839
H	-0.999828	-0.004427	4.516451
H	-0.008774	1.006777	1.151035
H	-0.162858	0.558958	2.676271
H	-0.181136	3.152918	0.435266
H	-1.060677	2.278702	-0.525779
H	5.113222	-1.365328	2.031259
H	5.309103	0.082692	2.643387
H	1.180179	-3.073942	-0.416692
H	2.709321	-3.306459	-0.289205
H	4.897401	1.991355	2.102421
H	6.325198	1.744086	1.539422
H	-0.700340	-3.246234	0.787369
H	-0.811398	-4.175926	-0.458050
H	2.695311	2.793049	-1.288232
H	1.420277	2.123815	-0.646859
H	2.973536	0.158800	5.090071
H	2.525966	1.641853	4.613711
H	2.505700	4.890729	-1.836019
H	3.921727	4.392534	-2.222210
H	4.020371	-1.736304	5.736996
H	4.698583	-0.892309	4.651610
H	1.325253	3.426490	4.123414
H	2.635384	4.237459	3.925993
H	2.843055	2.253094	0.954829
H	2.736528	2.637326	2.560723
H	-0.712340	-2.139370	4.216211
H	-2.078114	-2.243697	4.960166

H	2.589080	-3.154145	5.144733
H	3.026809	-3.858143	6.452194
H	3.781557	-4.487231	1.476777
H	3.307133	-5.159073	0.217463
H	1.246184	5.872590	-0.300915
H	0.973022	6.535679	-1.657078
H	4.667810	-1.458762	0.072519
H	5.047196	-2.926645	0.366734
H	-1.790302	-2.010801	2.334497
H	-0.894034	-1.182340	1.420701
H	1.910305	5.715556	2.606114
H	2.166453	6.499823	3.894827
H	-0.673010	2.717754	4.288560
H	-0.525913	4.012795	3.420871
H	1.957493	-6.123123	1.601206
H	1.008161	-5.417301	0.620303
H	2.349393	-4.276646	3.103031
O	3.039230	-4.964194	3.062584
H	3.508082	-4.840070	3.902261

$CaCl_2(H_2O)_{25}$

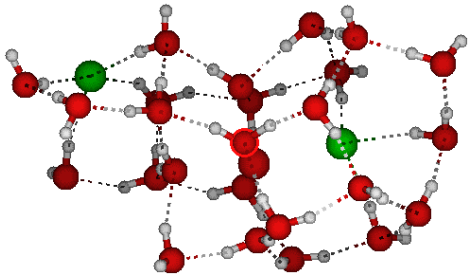

Figure S_{201} : $CaCl_2$ optimized structure with 25 water molecules.

E=-1976.808116

H=-1976.807172

O	3.030366	-0.541216	0.127641
Ca	2.544733	-0.165487	2.388395
O	3.093616	2.084463	1.855796

O	4.838578	-0.458908	2.957129
O	2.206085	0.740013	4.598452
O	0.251884	0.396362	1.820449
O	2.237666	-2.854417	-0.626041
O	2.207279	3.350460	3.974363
O	4.120140	-0.721481	5.627652
O	5.502527	-1.779773	0.820454
O	2.393674	1.981957	-0.709466
O	3.026546	4.003271	-2.289381
O	5.751567	1.997480	2.486178
O	-0.542168	0.871786	4.303208
O	-0.423874	3.697142	4.220505
O	1.765476	6.115855	-1.217068
O	2.542282	5.927201	3.273405
O	-0.251144	2.279952	-0.039723
O	-0.395663	-3.602485	-0.060459
O	-1.543196	-1.709405	1.342376
O	-1.433969	-1.742428	4.213601
O	4.249249	-4.201479	0.716611
O	0.053005	-6.183501	0.790446
O	3.945633	-5.332486	3.015200
Cl	1.405891	-2.509961	3.327201
O	3.582405	-3.488761	5.292845
Cl	0.183321	4.950599	1.252966
H	2.846261	0.244242	-0.432479
H	2.644940	-1.390388	-0.274089
H	0.363327	0.760361	4.667060
H	-1.015705	0.032767	4.477852
H	0.027130	1.094035	1.158252
H	-0.152213	0.667173	2.689836
H	-0.162172	3.185747	0.367408
H	-1.077605	2.284677	-0.533871
H	5.220186	-1.058941	2.245412
H	5.311758	0.409314	2.847274

H	1.331600	-3.121697	-0.369929
H	2.855329	-3.441829	-0.138324
H	4.854383	2.235842	2.165295
H	6.332868	2.058394	1.721355
H	-0.833716	-2.922541	0.534595
H	-0.851060	-3.539096	-0.906588
H	2.705139	2.691530	-1.338490
H	1.418707	2.055852	-0.695599
H	2.863529	0.224013	5.157377
H	2.425559	1.699290	4.631627
H	2.549815	4.788991	-1.916831
H	3.953607	4.260030	-2.305732
H	3.946412	-1.675503	5.735733
H	4.649681	-0.685893	4.806754
H	1.225156	3.480553	4.084917
H	2.549197	4.273081	3.915773
H	2.814544	2.276257	0.922499
H	2.662156	2.700373	2.515474
H	-0.518851	-2.075433	4.072154
H	-1.822148	-2.304786	4.892299
H	2.808849	-3.220066	4.753135
H	3.225075	-4.047662	5.992183
H	4.122138	-4.619660	1.632856
H	4.690847	-4.872036	0.185217
H	1.310225	5.834263	-0.396306
H	1.062972	6.480577	-1.765115
H	4.826996	-1.296582	0.311902
H	5.177299	-2.709266	0.811800
H	-1.756756	-1.895697	2.272680
H	-0.879883	-0.991218	1.412701
H	1.883223	5.755024	2.573611
H	2.097736	6.538975	3.870166
H	-0.778609	2.791396	4.234480
H	-0.611228	4.067540	3.341692

H	-0.805150	-6.584932	0.957695
H	-0.142373	-5.270992	0.484712
H	2.994841	-5.610912	3.074332
H	4.071942	-4.739683	3.774972
H	1.107542	-4.804689	3.237662
O	1.289319	-5.755652	3.189296
H	0.902476	-6.014817	2.320572

$CaCl_2(H_2O)_{26}$

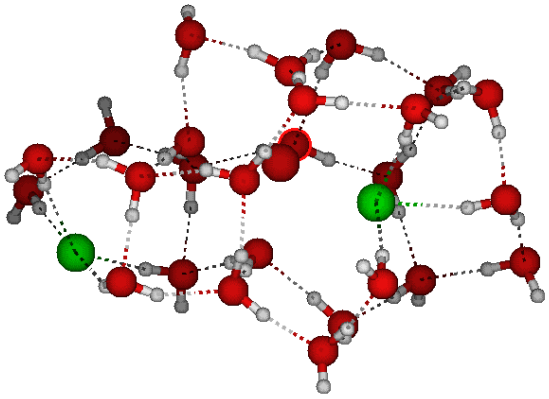

Figure S_{202} : $CaCl_2$ optimized structure with 26 water molecules.

E=-2053.189937

H=-2053.188993

O	3.034818	-0.511062	0.083123
Ca	2.569679	-0.138741	2.349782
O	4.878799	-0.379317	2.887269
O	3.107165	2.118048	1.814900
O	0.296830	0.421224	1.759835
O	2.158117	0.739715	4.567381
O	2.209375	-2.825044	-0.637925
O	5.541142	-1.653913	0.721579
O	2.218036	3.359440	3.956547
O	4.144274	-0.710281	5.537131
O	-0.395755	3.831163	4.128356
O	5.769837	2.086076	2.428618
O	2.436756	2.006602	-0.762666

O	3.119333	3.993267	-2.366531
O	-0.210073	2.295302	-0.125152
O	1.901381	6.137709	-1.307623
O	-0.610646	1.034646	4.157566
O	2.677246	5.905065	3.201468
Cl	1.582939	-2.534264	3.298286
O	4.383808	-4.116178	0.493575
O	4.268444	-5.334982	2.758734
O	1.652112	-5.782189	3.140798
O	0.086808	-6.250806	0.957618
O	-0.352125	-3.652545	0.158399
O	-1.500859	-1.712761	1.489902
O	3.930927	-3.525993	5.060716
O	-2.125816	-1.217981	4.256355
Cl	0.317006	4.966053	1.151935
O	-0.455079	-2.694992	5.645154
H	2.852836	0.275244	-0.477419
H	2.635904	-1.358778	-0.307663
H	0.245227	0.826263	4.583727
H	-1.226828	0.282416	4.319224
H	0.074028	1.085600	1.065316
H	-0.128759	0.735409	2.605049
H	-0.102947	3.197395	0.283450
H	-1.030556	2.319544	-0.628329
H	5.259563	-0.971387	2.168169
H	5.344358	0.493193	2.779024
H	1.342541	-3.113861	-0.286251
H	2.889986	-3.399562	-0.224248
H	4.866295	2.309083	2.114768
H	6.342790	2.152425	1.657921
H	-0.787317	-2.977946	0.760972
H	-0.848677	-3.612478	-0.666011
H	2.765439	2.703215	-1.397135
H	1.462085	2.084246	-0.768666

H	2.828206	0.227366	5.107279
H	2.380714	1.699030	4.599932
H	2.661781	4.793743	-2.001446
H	4.052469	4.226760	-2.385466
H	4.055015	-1.676855	5.624351
H	4.672440	-0.619940	4.718782
H	1.241553	3.542121	4.048736
H	2.607170	4.262221	3.895419
H	2.831178	2.308575	0.880825
H	2.665388	2.726046	2.472535
H	-1.595547	-1.818797	4.849329
H	-3.034426	-1.236804	4.573350
H	3.156585	-3.276379	4.512490
H	3.593977	-4.172549	5.691749
H	4.331119	-4.584549	1.393362
H	4.830117	-4.733115	-0.095610
H	1.443128	5.855025	-0.488740
H	1.201050	6.505343	-1.856567
H	4.833134	-1.185851	0.242113
H	5.260574	-2.596281	0.672186
H	-1.789921	-1.753152	2.419274
H	-0.824296	-1.005512	1.496869
H	2.027697	5.737388	2.492062
H	2.244704	6.553023	3.768027
H	-0.747012	2.922411	4.113950
H	-0.526807	4.199280	3.237849
H	-0.750958	-6.586956	1.290978
H	-0.099146	-5.326903	0.679521
H	3.324786	-5.622025	2.879769
H	4.435751	-4.740973	3.509224
H	1.430984	-4.839817	3.195546
H	1.158905	-6.078214	2.340289
H	0.226967	-2.716114	4.939549
H	-0.035425	-2.236730	6.381505

$CaCl_2(H_2O)_{27}$

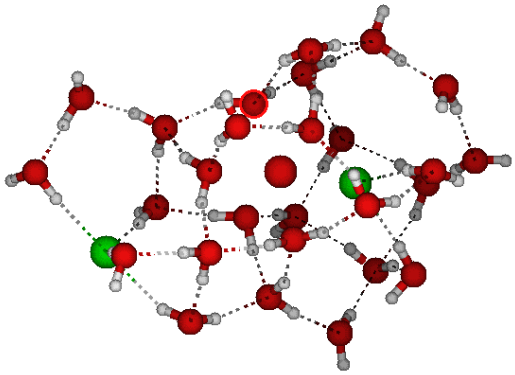

Figure S_{203} : $CaCl_2$ optimized structure with 27 water molecules.

E=-2129.572890

H=-2129.571946

O	3.115505	-0.409381	-0.093691
Ca	2.574145	-0.063302	2.166918
O	4.837279	-0.389345	2.853322
O	3.125577	2.208679	1.738380
O	0.209710	0.415750	1.616880
O	2.137005	0.722552	4.410615
O	2.530212	-2.760691	-0.988798
O	5.630161	-1.531480	0.648234
O	2.245132	3.373519	3.915881
O	3.882475	-0.944910	5.416497
O	-0.386510	3.743476	4.127370
O	5.757624	2.096319	2.519510
O	2.447950	2.141144	-0.842702
O	3.058193	4.187729	-2.405749
O	-0.215439	2.412221	-0.164970
O	1.886694	6.294267	-1.224744
O	-0.574799	0.948621	4.054299
O	2.613642	5.973286	3.287258
Cl	1.586331	-2.465995	2.706898
O	4.619944	-4.052026	0.296148
O	4.351753	-5.304514	2.548245

O	1.971457	-5.986964	3.694913
O	-0.237499	-5.525631	2.235718
O	0.111113	-3.885203	-0.086992
O	-1.222913	-1.817011	1.069209
O	3.528299	-3.699882	4.733374
O	-2.006958	-1.099205	5.085583
Cl	0.292038	5.037222	1.187494
O	0.038843	-3.117645	5.467175
H	2.927562	0.378223	-0.647375
H	2.803866	-1.268340	-0.532903
H	0.322831	0.801441	4.428456
H	-1.166048	0.268353	4.455417
H	-0.009686	1.143892	0.988736
H	-0.196394	0.646477	2.504532
H	-0.085127	3.295666	0.280901
H	-0.991385	2.515593	-0.725564
H	5.254964	-0.931465	2.118241
H	5.310910	0.483224	2.828000
H	1.694862	-3.140470	-0.649357
H	3.234536	-3.296388	-0.562726
H	4.883730	2.339636	2.145539
H	6.384390	2.162622	1.791855
H	-0.374955	-3.113933	0.287968
H	-0.421402	-4.206793	-0.822231
H	2.746901	2.862350	-1.463599
H	1.473065	2.205943	-0.819783
H	2.728392	0.123968	4.961941
H	2.405891	1.661549	4.520288
H	2.617250	4.975020	-1.994865
H	3.991187	4.419077	-2.447791
H	3.689638	-1.899212	5.472679
H	4.472868	-0.869070	4.641507
H	1.264703	3.520684	4.021315
H	2.604883	4.289710	3.894482

H	2.861446	2.434290	0.810293
H	2.689629	2.796759	2.419985
H	-2.153693	-1.850518	4.455043
H	-2.797629	-1.026282	5.628490
H	2.995213	-3.318053	4.004356
H	3.005638	-4.486699	4.957212
H	4.456890	-4.529509	1.172768
H	5.173048	-4.644200	-0.223362
H	1.430090	5.980456	-0.416481
H	1.190836	6.709193	-1.744827
H	4.931488	-1.069930	0.150616
H	5.388419	-2.481269	0.562344
H	-2.050753	-1.469292	0.722521
H	-0.636600	-1.034973	1.238847
H	1.970052	5.816465	2.570486
H	2.153914	6.566919	3.890768
H	-0.708165	2.823062	4.085244
H	-0.543414	4.141177	3.254853
H	-0.879806	-4.950141	2.682251
H	0.012290	-5.024676	1.435139
H	3.464488	-5.672323	2.761150
H	4.476667	-4.691626	3.294947
H	1.849944	-6.900187	3.972423
H	1.150486	-5.761670	3.180042
H	0.787446	-2.853634	4.908034
H	-0.398975	-2.287033	5.710893
H	-1.048014	-3.363649	4.102843
O	-1.797040	-3.246113	3.467645
H	-1.433265	-2.773412	2.692984

$CaCl_2(H_2O)_{28}$

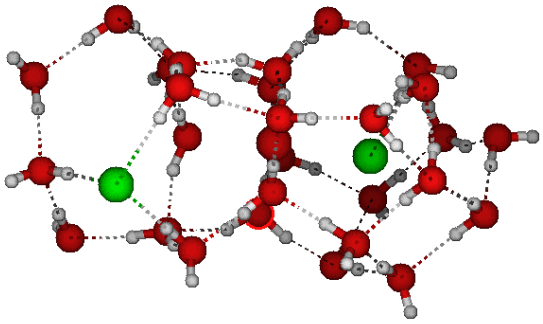

Figure S_{204} : $CaCl_2$ optimized structure with 28 water molecules.

E=-2205.964785

H=-2205.963841

O	2.920413	-0.306477	-0.134228
Ca	2.242884	0.022698	2.098459
O	2.596867	2.313391	1.552951
O	4.507905	0.070592	2.914856
O	1.593053	0.758182	4.282717
O	-0.135183	0.223591	1.475244
O	2.681509	-2.743397	-0.938628
O	5.509489	-1.034421	0.790580
O	3.510176	-0.601335	5.466231
O	-1.086226	0.890889	3.822390
O	1.659210	3.314545	3.722296
Cl	1.662925	-2.506256	2.605699
O	-0.930137	3.778566	3.883047
O	1.987968	2.141131	-1.015560
O	2.574897	4.519957	-2.075609
O	5.037706	2.765570	2.559330
O	1.492006	6.142771	-0.128597
O	3.697503	4.941017	3.937901
O	-2.296468	-1.320621	4.863850
O	-1.724676	-3.552709	3.425678
O	-1.266464	-2.178813	0.990697
O	-0.699328	1.947208	-0.538022
O	0.064695	-2.939080	5.368418

O	0.348778	-4.088787	-0.095082
O	4.865042	-3.674837	0.507875
O	4.683560	-4.940617	2.764082
O	2.344162	-5.855796	3.843274
O	0.142607	-5.656092	2.312271
O	3.581531	-3.375225	4.844051
Cl	-0.934540	4.599376	0.769989
H	2.679877	0.425455	-0.736956
H	2.744393	-1.217267	-0.548196
H	-0.199207	0.786850	4.235278
H	-1.644025	0.178598	4.208419
H	-0.402412	0.841175	0.752203
H	-0.604353	0.514857	2.315145
H	-0.828249	2.847571	-0.115196
H	-1.417988	1.855644	-1.172567
H	5.025066	-0.417960	2.201506
H	4.865017	0.985453	2.926612
H	1.874014	-3.200046	-0.626700
H	3.413207	-3.162586	-0.434751
H	4.206691	2.714328	2.025467
H	5.751201	2.961850	1.942941
H	-0.238877	-3.374534	0.243845
H	-0.129985	-4.511823	-0.815642
H	2.245395	2.959842	-1.513342
H	1.010426	2.083686	-1.054382
H	2.223124	0.281619	4.898776
H	1.742130	1.742985	4.313073
H	2.195945	5.133377	-1.405987
H	3.514015	4.727125	-2.109245
H	3.452970	-1.572202	5.544051
H	4.121800	-0.461909	4.719733
H	0.721663	3.637346	3.843108
H	2.335546	4.016619	3.948205
H	2.302435	2.458223	0.614856

H	2.087900	2.853264	2.233702
H	-2.316734	-2.132801	4.298165
H	-3.061126	-1.366222	5.445584
H	3.053154	-3.077056	4.074028
H	3.123708	-4.199889	5.075114
H	4.732337	-4.162161	1.384554
H	5.507958	-4.197012	0.017231
H	0.712985	5.623192	0.215004
H	1.091611	6.929644	-0.516786
H	4.780103	-0.701046	0.236898
H	5.400770	-2.012658	0.749483
H	-2.127401	-1.943876	0.629693
H	-0.789887	-1.324298	1.160602
H	4.366655	4.300133	3.643003
H	3.604590	5.570729	3.188677
H	-1.226245	2.850582	3.891993
H	-1.121499	4.100963	2.982453
H	-0.562350	-5.134188	2.730323
H	0.362265	-5.154541	1.503678
H	3.840026	-5.411629	2.947907
H	4.692830	-4.301688	3.500059
H	2.296997	-6.766688	4.149388
H	1.525295	-5.724969	3.293700
H	0.753231	-2.630988	4.755551
H	-0.493423	-2.164611	5.540215
H	-0.979527	-3.496184	4.073956
H	-1.426688	-3.080896	2.622338
H	3.049607	7.524462	2.299116
O	3.370802	6.729405	1.862037
H	2.681454	6.504371	1.203950

$CaCl_2(H_2O)_{29}$

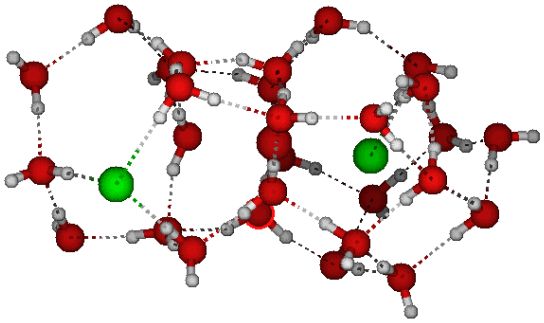

Figure S_{205} : $CaCl_2$ optimized structure with 29 water molecules.

E=-2282.362930

H=-2282.361986

O	2.881723	-0.253763	-0.120441
Ca	2.292867	0.065482	2.143544
O	2.663830	2.329772	1.555463
O	1.865469	0.940342	4.324779
O	4.617644	0.082523	2.777784
O	-0.074008	0.364025	1.527913
O	1.895807	3.508230	3.697031
O	2.616444	-2.693394	-0.885841
O	5.560650	-0.899485	0.568048
O	3.963716	5.161016	3.412639
O	-0.838703	1.072659	3.925728
O	3.817572	-0.449139	5.430909
O	-0.675129	3.938764	3.971926
Cl	1.442780	-2.335007	2.931181
O	1.998712	2.244645	-0.985924
O	2.789431	4.696706	-1.690861
O	5.171569	2.762957	2.349859
O	-1.279546	-1.950434	0.815921
O	-0.681005	2.138740	-0.445205
O	0.429179	-4.044301	0.223152
O	-2.222892	-1.017513	4.918451
O	-2.831132	-2.683956	3.041600

O	-1.402403	-4.750156	4.166063
O	4.957159	-3.548546	0.314449
O	4.995461	-4.584519	2.667405
O	2.903883	-5.802207	3.914666
O	0.653343	-5.750323	2.544927
O	1.092969	6.433451	-0.293458
O	3.565013	6.066778	0.743536
O	3.771173	-3.203401	4.767972
Cl	-1.103392	4.748379	0.891742
H	2.628940	0.481378	-0.713821
H	2.692978	-1.164074	-0.528401
H	0.054926	0.948984	4.315346
H	-1.412846	0.378552	4.332634
H	-0.340574	1.013000	0.833784
H	-0.487271	0.660225	2.396989
H	-0.847621	3.023732	-0.000831
H	-1.417161	2.025188	-1.055824
H	5.108052	-0.374545	2.025881
H	4.963625	1.002365	2.778925
H	1.866679	-3.166966	-0.469498
H	3.422404	-3.097240	-0.495926
H	4.295264	2.701372	1.891145
H	5.833880	2.867438	1.657998
H	-0.163194	-3.308178	0.498795
H	-0.055848	-4.536302	-0.447952
H	2.309778	3.102451	-1.382394
H	1.019087	2.253475	-1.002085
H	2.510037	0.456108	4.917941
H	2.032605	1.917201	4.341500
H	2.026046	5.278524	-1.518559
H	3.391359	4.969226	-0.977713
H	3.724301	-1.413336	5.537669
H	4.377619	-0.364094	4.637986
H	0.957121	3.823870	3.847295

H	2.559335	4.241646	3.775776
H	2.348306	2.478482	0.622351
H	2.217828	2.918856	2.240622
H	-2.521134	-1.627144	4.163741
H	-2.994211	-0.859973	5.472385
H	3.071135	-2.918287	4.143904
H	3.488401	-4.111585	4.971189
H	4.921249	-3.969055	1.238252
H	5.578626	-4.080474	-0.192739
H	0.375497	5.892761	0.135156
H	0.672153	7.271432	-0.512091
H	4.775708	-0.581498	0.085467
H	5.489985	-1.879121	0.497454
H	-1.832045	-1.658832	0.082881
H	-0.779317	-1.144193	1.113619
H	4.592992	4.437750	3.245104
H	3.795648	5.528365	2.523194
H	-0.958808	3.006258	4.003590
H	-0.956264	4.261328	3.094726
H	-0.071886	-5.411196	3.108933
H	0.696937	-5.122992	1.798924
H	4.262137	-5.190548	2.916112
H	4.897026	-3.903704	3.361001
H	2.981902	-6.720589	4.189770
H	2.047282	-5.748325	3.395368
H	-0.949324	-4.101754	4.790809
H	-1.834926	-5.409389	4.718281
H	-2.423286	-3.516534	3.367886
H	-2.311948	-2.446978	2.247101
H	4.075183	6.873651	0.614754
H	2.631361	6.313882	0.540666
H	0.409383	-2.638738	4.935001
O	-0.270047	-2.885266	5.589456
H	-0.925873	-2.159353	5.530400

$CaCl_2(H_2O)_{30}$

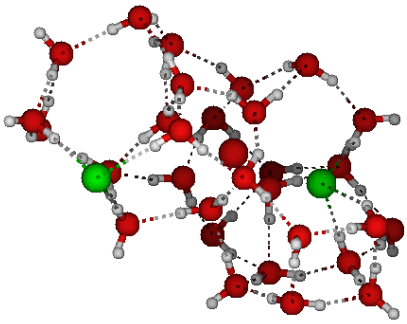

Figure S_{206} : $CaCl_2$ optimized structure with 30 water molecules.

E=-2358.755823

H=-2358.754879

O	2.971873	-0.210572	-0.223435
Ca	2.475103	-0.189688	2.173527
O	2.699306	2.129653	1.542294
O	2.107907	0.895270	4.294688
O	4.837605	0.067942	2.687461
O	0.088879	0.156223	1.641554
O	1.988331	3.443966	3.626964
O	2.936825	-2.651084	-1.377413
O	5.685806	-0.815031	0.387577
O	-0.635202	0.900498	4.027744
O	-0.574657	3.775385	4.055177
O	1.998038	2.239598	-0.999093
O	4.260110	-0.223552	5.417607
O	4.002726	5.143576	3.267688
Cl	1.193743	-2.234878	4.238282
O	5.200043	2.761428	2.169357
O	2.594118	4.741874	-1.707940
O	-2.495393	-0.933179	4.829979
O	-3.007067	-2.534914	2.851091
O	-1.258200	-1.942890	0.747925
O	-0.624609	1.959542	-0.281752
O	5.295974	-3.564791	0.216180

O	4.421429	-4.273065	2.728256
O	2.748020	-6.319304	3.148216
O	0.493746	-4.883039	2.800501
O	-1.902458	-4.749950	4.108501
O	-1.279170	-3.105180	6.030043
O	0.832741	-3.691757	0.347256
O	3.976182	-3.058752	5.196892
O	0.854673	6.361526	-0.216872
O	3.399755	6.134564	0.675031
Cl	-1.223840	4.555640	1.010061
H	2.708171	0.554303	-0.774149
H	2.870044	-1.062737	-0.729015
H	0.248495	0.738870	4.424381
H	-1.268707	0.249531	4.413853
H	-0.147599	0.847011	0.976865
H	-0.290619	0.454624	2.529615
H	-0.840726	2.837213	0.156709
H	-1.374692	1.785989	-0.860522
H	5.296928	-0.354850	1.900046
H	5.105626	1.012881	2.643914
H	2.192655	-3.142266	-0.988037
H	3.714311	-3.010753	-0.912674
H	4.295112	2.613540	1.785791
H	5.797917	2.863335	1.420679
H	0.061120	-3.086765	0.379237
H	0.662019	-4.311690	1.090313
H	2.238417	3.129100	-1.375433
H	1.020717	2.193334	-0.954322
H	2.799797	0.514807	4.899809
H	2.208817	1.880358	4.253584
H	1.802375	5.270258	-1.496892
H	3.210012	5.055493	-1.023604
H	4.187255	-1.183321	5.563872
H	4.738393	-0.167284	4.570363

H	1.049605	3.728299	3.826740
H	2.635679	4.194572	3.668741
H	2.385503	2.317755	0.616721
H	2.273828	2.738219	2.223239
H	-2.719320	-1.498347	4.021265
H	-3.324393	-0.546301	5.130511
H	3.038145	-2.868745	4.947894
H	3.922664	-3.631896	5.969872
H	5.078730	-3.854826	1.131289
H	6.028341	-4.115148	-0.078103
H	0.181020	5.779669	0.228241
H	0.381529	7.176226	-0.415454
H	4.843236	-0.530524	-0.015611
H	5.655326	-1.792736	0.326695
H	-1.740034	-1.633695	-0.026336
H	-0.764101	-1.153138	1.107947
H	4.628501	4.429724	3.051037
H	3.781586	5.531755	2.399139
H	-0.796327	2.826446	4.097592
H	-0.921128	4.080201	3.195213
H	-0.394013	-5.037510	3.197591
H	0.767177	-4.036312	3.226479
H	3.857248	-5.081136	2.854801
H	4.511651	-3.879887	3.621344
H	2.750812	-6.992961	2.460984
H	1.858736	-5.892189	3.087522
H	-1.659843	-4.175978	4.905952
H	-2.436328	-5.476288	4.445691
H	-2.719943	-3.403007	3.204392
H	-2.415197	-2.364285	2.090773
H	3.849387	6.976747	0.547540
H	2.441645	6.325313	0.535786
H	-0.368577	-2.862452	5.779168
H	-1.781043	-2.296661	5.787483

O	2.892490	-2.387366	1.542728
H	3.370390	-3.070529	2.065517
H	2.129769	-2.849793	1.120640

$CaCl_2(H_2O)_{31}$

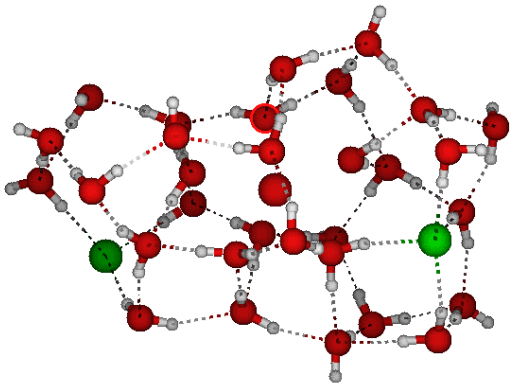

Figure S_{207} : $CaCl_2$ optimized structure with 31 water molecules.

E=-2435.142237

H=-2435.141293

O	2.903905	-0.162635	0.089340
Ca	2.287380	0.046175	2.435016
O	2.640226	-2.251046	2.109764
O	1.825234	1.600290	4.294386
O	2.683151	2.298346	1.556974
O	4.572587	0.213383	3.202325
O	-0.063772	0.392532	1.689348
O	1.863561	3.996917	3.338024
O	-0.816014	1.437038	3.972781
O	5.544967	-0.624442	0.917368
O	-0.732845	4.408243	3.570820
O	2.170420	2.211330	-1.024890
O	-1.403364	-1.813140	1.060509
O	5.127217	2.854717	2.468513
O	4.015433	5.481238	2.978736

O	2.909755	4.569670	-2.006253
O	3.428687	0.170708	5.842789
O	2.777027	-2.544226	-1.042578
O	4.272360	-4.446578	2.256898
O	2.649327	-6.580137	1.789731
O	0.465338	-5.287659	2.780275
O	0.737209	-3.561640	0.710559
O	-0.500348	2.006212	-0.456990
O	-1.462530	-1.047713	5.243315
O	-2.724241	-2.366385	3.436896
O	-1.928061	-4.922802	4.114086
O	-1.003286	-3.797164	6.283540
O	5.233623	-3.277585	0.140402
O	4.959717	-4.673368	4.824700
O	1.153115	6.372929	-0.773415
O	3.652491	6.176671	0.259539
Cl	-1.111843	4.769024	0.426032
Cl	1.908842	-4.076981	5.232087
H	2.733086	0.573977	-0.533471
H	2.800131	-1.037179	-0.390512
H	0.121622	1.520991	4.284769
H	-1.183556	0.686076	4.478047
H	-0.212302	1.004944	0.926414
H	-0.471680	0.826751	2.499498
H	-0.728248	2.934593	-0.148871
H	-1.184034	1.786384	-1.099125
H	5.073159	-0.237457	2.460054
H	4.880310	1.144245	3.154448
H	2.090281	-3.040034	-0.561428
H	3.631307	-2.898281	-0.720759
H	4.279478	2.697450	1.977203
H	5.831535	2.774305	1.815295
H	-0.062347	-2.998116	0.728908
H	0.589708	-4.247060	1.407458

H	2.467717	3.039396	-1.492181
H	1.191696	2.190284	-1.034978
H	2.408969	1.257047	5.021935
H	1.990603	2.567858	4.127610
H	2.132731	5.146479	-1.885761
H	3.513315	4.931794	-1.335211
H	2.805746	-0.557325	5.681183
H	4.110658	0.036889	5.161465
H	0.929621	4.327606	3.447142
H	2.553575	4.712168	3.344640
H	2.479026	2.399979	0.587453
H	2.240601	3.023488	2.085335
H	-1.996638	-1.536655	4.522525
H	-2.084387	-0.817120	5.943111
H	4.073359	-4.406187	5.144994
H	5.043251	-5.590215	5.108773
H	4.987172	-3.793192	0.959470
H	5.932400	-3.766711	-0.304190
H	0.428528	5.855631	-0.330494
H	0.720923	7.171258	-1.094409
H	4.714606	-0.366791	0.468599
H	5.610771	-1.579506	0.712850
H	-1.972091	-1.612534	0.309831
H	-0.919267	-0.970007	1.284697
H	4.597880	4.701645	2.933282
H	3.895296	5.750999	2.047123
H	-1.036922	3.504460	3.753073
H	-1.009499	4.589392	2.651215
H	-0.440126	-5.363034	3.151370
H	0.980073	-4.894711	3.524793
H	3.699668	-5.234153	2.082753
H	4.644507	-4.560712	3.170365
H	2.473819	-6.686023	0.849087
H	1.782861	-6.332381	2.177754

H	-1.577435	-4.570347	4.991130
H	-2.578756	-5.596635	4.337148
H	-2.557492	-3.320270	3.599513
H	-2.329569	-2.183914	2.558817
H	4.134545	6.990456	0.077638
H	2.708924	6.377520	0.054099
H	-0.041731	-3.981165	6.243160
H	-1.064494	-2.850819	6.065181
H	3.278186	-2.971507	2.311698
H	1.926183	-2.698267	1.596529
H	1.526942	-2.114126	4.471339
O	1.309980	-1.157646	4.391249
H	0.452989	-1.046304	4.836379

$CaCl_2(H_2O)_{32}$

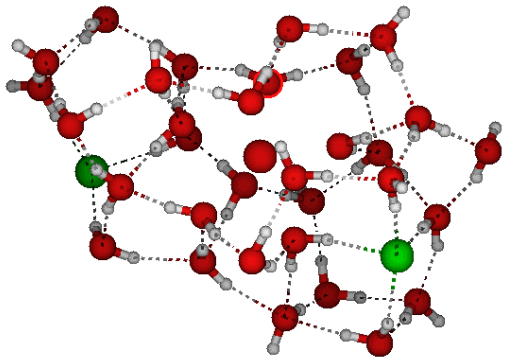

Figure S_{208} : $CaCl_2$ optimized structure with 32 water molecules.

E=-2511.530159

H=-2511.529214

O	2.946560	-0.213398	0.124000
Ca	2.614898	-0.062292	2.606226
O	2.631006	-2.347382	2.089176
O	5.122546	0.345291	2.561266
O	2.783946	2.256019	1.684837
O	2.011698	1.506243	4.396157

O	0.202127	0.284705	1.766922
O	1.145550	-1.188942	4.458024
O	1.995841	3.937933	3.500184
O	5.657092	-0.690580	0.239962
O	-0.643760	1.405621	3.989916
O	2.188348	2.197632	-0.892061
O	4.040567	5.534132	2.934838
O	-0.610240	4.323398	3.682196
O	2.614634	-2.557156	-1.091710
O	2.669744	0.100884	6.503517
O	-1.341060	-1.736572	1.035839
O	2.859639	4.557661	-1.942732
O	5.279878	3.064461	2.083037
O	0.677112	-3.586762	0.690862
O	0.385905	-5.331187	2.748527
O	-0.449311	1.923591	-0.354491
O	2.647476	-6.657274	1.974127
O	4.295636	-4.536949	2.210697
O	5.118635	-3.431090	-0.055940
O	4.671140	-3.784584	4.808323
O	-2.091649	-4.918581	3.912574
O	-1.294761	-3.821490	6.151212
O	-2.872085	-2.333750	3.245605
O	-1.644845	-1.084555	5.113905
O	1.018130	6.331759	-0.782844
O	3.513546	6.276637	0.254527
Cl	-1.120578	4.670463	0.544904
Cl	1.707966	-4.157222	5.292758
H	2.728943	0.551130	-0.449454
H	2.727669	-1.058842	-0.361083
H	0.292968	1.439935	4.317459
H	-1.083349	0.683164	4.474879
H	0.054265	0.894556	1.008126
H	-0.222324	0.732911	2.556177

H	-0.705098	2.837058	-0.027963
H	-1.121804	1.696976	-1.005347
H	5.469283	-0.089353	1.724413
H	5.378010	1.290199	2.516700
H	1.939979	-3.060572	-0.599704
H	3.469832	-2.951080	-0.830407
H	4.349202	2.815283	1.827521
H	5.752932	3.198752	1.254130
H	-0.105215	-2.998733	0.724402
H	0.525443	-4.277453	1.380162
H	2.473018	3.022122	-1.370664
H	1.208949	2.163854	-0.907213
H	2.303095	1.172464	5.291676
H	2.164431	2.480904	4.289813
H	2.052442	5.097917	-1.861248
H	3.430664	4.983835	-1.280530
H	1.994490	-0.496475	6.135028
H	3.465036	-0.252417	6.056219
H	1.053629	4.253112	3.585380
H	2.654301	4.677376	3.429879
H	2.511386	2.353664	0.733396
H	2.341285	2.956356	2.246818
H	-2.188751	-1.533322	4.373363
H	-2.266881	-0.799431	5.792715
H	3.736954	-3.979434	5.074392
H	5.221264	-4.106638	5.530488
H	4.920160	-3.886929	0.801486
H	5.726897	-3.998773	-0.538715
H	0.327120	5.796443	-0.307012
H	0.545941	7.105006	-1.108707
H	4.733089	-0.455292	0.008148
H	5.651975	-1.666253	0.186588
H	-1.813747	-1.437474	0.252157
H	-0.763500	-0.972227	1.326657

H	4.659847	4.794364	2.798537
H	3.836762	5.838558	2.029306
H	-0.880245	3.402131	3.835429
H	-0.899175	4.518161	2.769700
H	-0.541675	-5.399390	3.062292
H	0.852573	-4.929271	3.517864
H	3.717414	-5.342280	2.166190
H	4.623747	-4.445278	3.128725
H	2.523924	-6.869508	1.043328
H	1.758744	-6.383424	2.287948
H	-1.793778	-4.579586	4.812560
H	-2.764234	-5.584967	4.088552
H	-2.710776	-3.289890	3.395303
H	-2.408711	-2.126961	2.406084
H	3.955553	7.109039	0.056425
H	2.560768	6.426915	0.044776
H	-0.340547	-4.025824	6.200106
H	-1.321516	-2.873060	5.929905
H	3.248811	-3.097328	2.220689
H	1.888455	-2.728776	1.564633
H	1.396284	-2.129900	4.574743
H	0.202068	-1.147249	4.688671
O	4.210942	-1.024597	4.550684
H	4.445798	-1.970074	4.633628
H	4.900317	-0.586160	4.009231

$MgCl_2(H_2O)_1$

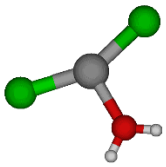

Figure S_{209} : $MgCl_2$ optimized structure with 1 water molecule.

E=-306.643332

H=-306.642388

Mg	0.380067	0.000793	1.466382
Cl	-0.025682	-0.008138	-0.725161
Cl	1.716323	0.006923	3.250231
O	-1.487347	0.002861	2.282154
H	-1.676895	0.000908	3.226866
H	-2.309815	-0.003347	1.780270

$MgCl_2(H_2O)_2$

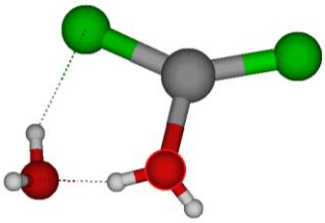

Figure S_{210} : $MgCl_2$ optimized structure with 2 water molecules.

E= -383.037758

H=-383.036814

O	-0.945864	0.210135	1.128151
Mg	0.759662	-0.050844	2.124780
Cl	0.515530	-0.059697	4.336585
Cl	2.248643	-0.300166	0.426716
H	-1.838614	0.085053	1.462012
H	-0.901206	0.072849	0.127563

H	0.532189	-0.400277	-1.123990
O	-0.398283	-0.194030	-1.341426
H	-0.355380	0.599235	-1.887974

$MgCl_2(H_2O)_3$

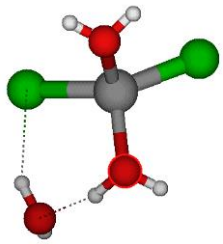

Figure S_{211} : $MgCl_2$ optimized structure with 3 water molecules.

E= -459.442301

H=-459.441357

O	-1.313914	-0.033059	1.157293
Mg	0.338875	0.577620	2.142613
Cl	1.851826	0.837017	0.410301
Cl	0.301264	-0.356340	4.213580
O	-0.464502	-0.563147	-1.234464
H	-1.924565	-0.645175	1.579997
H	-1.145731	-0.314268	0.206976
H	0.350045	-0.048863	-1.062711
H	-0.153331	-1.463866	-1.380767
O	0.203230	2.564517	2.735805
H	0.296330	2.630141	3.695966
H	0.857291	3.148386	2.331152

$MgCl_2(H_2O)_4$

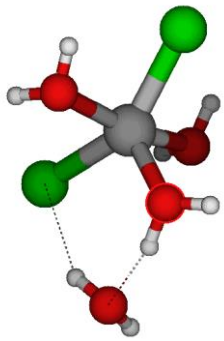

Figure S_{212} : $MgCl_2$ optimized structure with 4 water molecules.

E=-535.837080

H=-535.836135

O	-1.185045	-0.211265	1.284667
Mg	0.502492	0.398323	2.235877
O	0.029502	2.439445	2.518026
Cl	1.940196	1.046706	0.433024
Cl	0.506454	0.185958	4.584800
O	-0.432200	-0.265895	-1.205523
H	-1.764085	-0.903573	1.614848
H	-1.048316	-0.324902	0.297707
H	0.348457	0.285961	-0.993099
H	-0.058050	-1.100645	-1.509260
H	0.123355	2.588199	3.470424
H	0.676594	2.993550	2.061905
O	1.531063	-1.483217	2.255664
H	1.679443	-1.582689	3.210485
H	2.392024	-1.336594	1.840301

$MgCl_2(H_2O)_5$

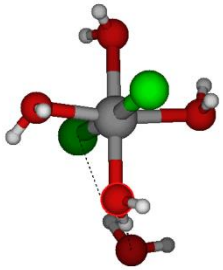

Figure S_{213} : $MgCl_2$ optimized structure with 5 water molecules.

E=-612.226069

H=-612.289213

O	-0.991970	0.173637	1.338373
Mg	0.914239	0.554708	2.070452
O	1.527679	-1.507722	2.011217
O	0.385345	2.562161	2.578893
Cl	1.788763	1.237923	-0.089857
Cl	0.226796	-0.011219	4.340995
O	-0.575664	-0.536300	-1.153303
H	-1.496767	-0.422924	1.902203
H	-0.988430	-0.179321	0.403666
H	0.184470	0.081628	-1.157282
H	-0.166742	-1.407306	-1.213521
H	-0.235442	2.439358	3.312417
H	-0.094495	2.982011	1.854255
H	1.315804	-1.668387	2.949499
H	2.491205	-1.523136	1.949457
O	2.924048	0.950959	2.744178
H	2.911329	1.434114	3.579681
H	3.253103	1.550001	2.057109

$MgCl_2(H_2O)_6$

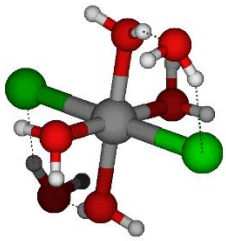

Figure S_{214} : $MgCl_2$ optimized structure with 6 water molecules.

E=-688.617799

H=-688.616854

O	-1.003968	-0.006347	0.858498
Mg	0.610550	0.155632	2.179667
O	2.227542	0.313001	3.498822
O	1.538526	-1.665987	1.493020
O	-0.315950	1.976299	2.865947
Cl	1.826866	1.695265	0.682252
Cl	-0.604684	-1.385751	3.676849
O	0.177090	0.107895	-1.482416
H	-1.532681	-0.788704	1.055031
H	-0.702456	-0.044079	-0.093747
H	0.789768	0.768694	-1.099695
H	0.729418	-0.672695	-1.607630
H	-1.238914	1.901978	2.589429
H	0.113028	2.543634	2.200021
H	1.106902	-2.233006	2.157581
H	2.459366	-1.588542	1.775962
H	1.930506	0.345596	4.452760
H	2.757429	1.094982	3.304240
H	0.443172	-0.473931	5.460462
O	1.060665	0.181058	5.845618
H	0.511140	0.960728	5.987376

$MgCl_2(H_2O)_7$

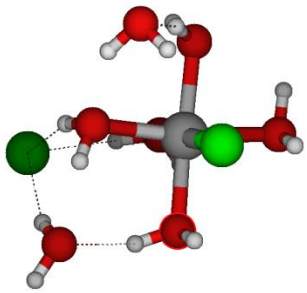

Figure S_{215} : $MgCl_2$ optimized structure with 7 water molecules.

E=-765.008725

H=-765.007781

O	-0.371799	-1.153458	0.579971
Mg	0.894798	-0.720946	2.207761
Cl	-1.028596	-1.239720	3.631739
O	2.232175	-0.358437	3.803006
O	1.462917	-2.766568	2.570425
O	0.440555	1.370548	2.130332
Cl	2.059688	2.227962	-0.253954
O	-0.832608	1.291986	-0.357627
O	0.569655	1.199927	5.050669
H	-1.181084	-1.440280	1.028510
H	-0.611213	-0.328718	0.084005
H	0.063994	1.665570	-0.554303
H	-1.417285	1.594617	-1.059735
H	-0.413619	1.488844	1.680677
H	1.068799	1.833749	1.509338
H	0.640602	-3.064389	2.994097
H	2.073680	-2.624400	3.308559
H	1.724333	0.246820	4.427652
H	3.046917	0.094161	3.557735
H	-0.146399	0.542176	5.091823
H	0.367060	1.682192	4.232252
O	2.512783	-0.484669	0.910324
H	2.503820	0.389699	0.425861

H	2.593576	-1.166938	0.234501

$MgCl_2(H_2O)_8$

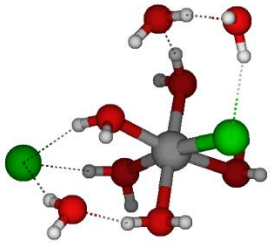

Figure S_{216} : $MgCl_2$ optimized structure with 8 water molecules.

E=-841.393912

H=-841.392967

O	-0.193025	-1.184029	0.288626
Mg	0.933052	-0.853141	2.046101
O	2.577753	-0.327621	0.856995
Cl	-1.051376	-1.741727	3.216713
O	2.198166	-0.608771	3.696459
O	1.647411	-2.884386	2.189143
O	0.296604	1.174935	2.195975
O	0.886688	1.054916	5.106164
O	-0.899055	1.292390	-0.353870
Cl	1.886918	2.448711	-0.017357
H	-0.987725	-1.621878	0.626693
H	-0.502707	-0.323996	-0.100085
H	-0.034219	1.766585	-0.454595
H	-1.460322	1.592564	-1.075934
H	-0.569258	1.273627	1.767620
H	0.883868	1.755330	1.635603
H	0.830346	-3.319461	2.482101
H	2.163544	-2.773231	3.002129
H	1.744302	0.017259	4.366921
H	3.031718	-0.191753	3.449089
H	0.167238	0.564802	5.578290
H	0.459104	1.455039	4.333941

H	2.499264	0.593344	0.477460
H	2.724006	-0.913997	0.106104
H	-1.154952	-1.060158	5.349647
O	-1.091429	-0.474430	6.128215
H	-1.949618	-0.039392	6.171037

$MgCl_2(H_2O)_9$

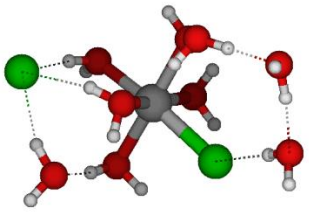

Figure S_{217} : $MgCl_2$ optimized structure with 9 water molecules.

E=-917.775003

H=-917.774059

O	0.192923	-1.166694	-0.144927
Mg	1.057504	-0.904100	1.768527
O	0.209151	1.031086	2.024723
O	2.772236	-0.112801	0.862928
Cl	-1.006611	-2.060913	2.518329
O	2.066027	-0.767688	3.589165
O	1.918966	-2.890137	1.827543
O	0.687330	0.859034	4.943982
O	-0.681519	1.290052	-0.650425
O	-1.008050	-0.094068	6.768995
Cl	1.907534	2.658681	0.143407
H	-0.593306	-1.684960	0.087120
H	-0.151524	-0.300642	-0.488511
H	0.136827	1.846479	-0.587320
H	-1.164154	1.605831	-1.421098
H	-0.610242	1.091789	1.507762
H	0.790707	1.718374	1.595962
H	1.106987	-3.415684	1.906521
H	2.249159	-2.828201	2.737320

H	1.527306	-0.162764	4.218513
H	2.920991	-0.337786	3.468294
H	0.064171	0.489234	5.625929
H	0.149537	1.190056	4.212023
H	2.641930	0.832301	0.565248
H	3.072463	-0.597610	0.085892
H	-1.634633	-0.686010	6.289544
H	-1.536746	0.641101	7.094126
H	-2.059916	-1.862208	4.442091
O	-2.559191	-1.677021	5.259491
H	-3.480065	-1.640800	4.987886

$MgCl_2(H_2O)_{10}$

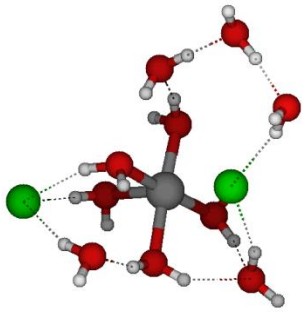

Figure S_{218} : $MgCl_2$ optimized structure with 10 water molecules.

E=-994.163935

H=-994.162991

O	0.190815	-1.133456	-0.038745
Mg	0.959797	-0.890014	1.899416
O	1.541752	-2.930297	1.768763
O	0.274167	1.105743	2.106932
O	2.745248	-0.186688	1.011805
Cl	-1.263814	-1.583375	2.901019
O	1.986630	-0.908840	3.696532
O	0.860578	0.941068	5.011010
O	-0.874183	0.175170	6.881932
O	-0.865849	1.262902	-0.482386
O	-2.783403	-1.321440	5.655753

Cl	1.869723	2.520347	-0.009398
H	-0.374750	-1.921927	-0.109429
H	-0.313889	-0.338983	-0.344702
H	-0.016316	1.771479	-0.528320
H	-1.407211	1.579641	-1.212200
H	-0.596444	1.172785	1.683016
H	0.838351	1.732915	1.575060
H	0.795669	-3.438087	1.382416
H	1.609068	-3.192539	2.696051
H	1.561205	-0.229326	4.334539
H	2.888444	-0.602024	3.544795
H	0.205091	0.673754	5.707615
H	0.358235	1.283909	4.258015
H	2.615730	0.723674	0.626823
H	2.992134	-0.742631	0.263661
H	-1.599714	-0.377018	6.506114
H	-1.302276	0.876753	7.380534
H	-2.273439	-1.596626	4.870062
H	-3.487196	-0.778343	5.284754
H	-1.297113	-3.121233	1.450059
O	-0.868418	-3.582545	0.692428
H	-1.410508	-4.344930	0.467510

$MgCl_2(H_2O)_{11}$

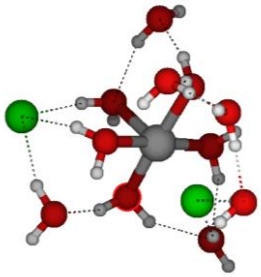

Figure S_{219} : $MgCl_2$ optimized structure with 11 water molecules.

E=-1070.546029

H=-1070.545085

O	0.016993	-1.128179	-0.120852
Mg	0.850932	-0.959375	1.824099
O	1.932145	-1.132641	3.543630
O	1.313641	-3.030138	1.607196
O	0.298391	1.066034	2.078134
O	2.586013	-0.348606	0.667897
O	0.986428	0.765250	4.998425
Cl	-1.399361	-1.534144	2.823121
O	-0.974147	1.320437	-0.431487
O	-0.776934	0.034623	6.886439
O	-2.849811	-1.199395	5.614599
O	-1.162382	-3.523654	0.590628
Cl	1.847592	2.430814	-0.129182
H	-0.583215	-1.893409	-0.175482
H	-0.481345	-0.309629	-0.368398
H	-0.110459	1.795981	-0.528329
H	-1.559596	1.684408	-1.102886
H	-0.583711	1.185160	1.689835
H	0.870277	1.677456	1.542710
H	0.527192	-3.492842	1.246648
H	1.386071	-3.278536	2.538956
H	1.611048	-0.457402	4.225246
H	2.901591	-1.001635	3.422650
H	0.332578	0.508655	5.696323

H	0.485885	1.172000	4.278331
H	2.471444	0.603783	0.367990
H	2.504479	-0.864565	-0.145342
H	-1.558458	-0.420245	6.495805
H	-1.127030	0.748189	7.427147
H	-2.373612	-1.502708	4.818696
H	-3.484169	-0.564561	5.264669
H	-1.548326	-3.050805	1.364637
H	-1.761755	-4.237806	0.352994
H	4.089143	-0.563272	1.825972
O	4.477653	-0.772602	2.694548
H	4.978842	-1.583992	2.564559

$MgCl_2(H_2O)_{12}$

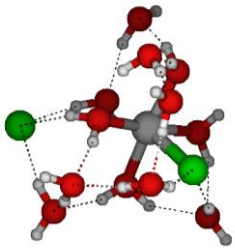

Figure S_{220} : $MgCl_2$ optimized structure with 12 water molecules.

E=-1146.937165

H=-1146.936221

O	-0.093823	-1.058988	0.125284
Mg	0.911634	-1.110538	2.014486
O	2.510562	-0.282676	0.750912
O	2.194944	-1.525934	3.564354
O	1.514708	-3.073160	1.378194
O	0.517811	0.862376	2.606202
Cl	-1.108010	-2.069969	3.091973
O	1.399793	0.204326	5.319480
O	-1.352121	1.364271	-0.146940
O	-1.005908	0.111649	6.531949
O	4.599493	-0.784228	2.549386

O	-1.019028	-3.607944	0.546324
O	-2.920196	0.108043	4.598262
Cl	1.413170	2.489811	0.201117
H	-0.627752	-1.868494	0.015988
H	-0.673012	-0.281594	-0.031907
H	-0.465455	1.826928	-0.135266
H	-1.774298	1.626408	-0.972556
H	-0.425340	1.135701	2.699968
H	0.899163	1.522435	1.975524
H	0.723786	-3.545364	1.040777
H	1.708269	-3.439369	2.252898
H	1.910580	-0.988735	4.369467
H	3.132093	-1.287461	3.375453
H	0.550693	0.075445	5.812105
H	1.161266	0.794619	4.590104
H	2.287459	0.657462	0.503635
H	2.381846	-0.783545	-0.065618
H	-1.731039	0.148956	5.862504
H	-1.157133	0.854378	7.123288
H	-2.634786	-0.734724	4.207300
H	-2.750456	0.745271	3.885028
H	-1.326527	-3.289540	1.430728
H	-1.598655	-4.325788	0.273465
H	4.111995	-0.513410	1.750685
H	5.173411	-1.505513	2.272594
O	-2.011491	1.840988	2.448192
H	-1.969881	2.796055	2.569449
H	-2.008853	1.693416	1.475290

$MgCl_2(H_2O)_{13}$

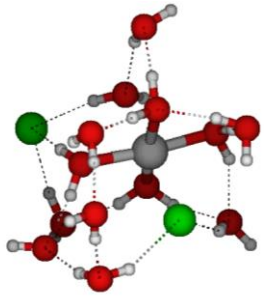

Figure S_{221} : $MgCl_2$ optimized structure with 13 water molecules.

E=-1223.330617

H=-1223.329673

O	-0.195554	-1.035185	0.199678
Mg	0.825910	-1.125280	2.068632
Cl	-1.206977	-2.015811	3.222934
O	2.057312	-1.332272	3.747669
O	1.361119	-3.076020	1.465086
O	0.452582	0.898951	2.535637
O	2.486574	-0.406632	0.825844
O	1.346666	0.612475	5.246417
O	-1.036275	0.494417	6.461640
O	4.494539	-0.949542	2.694513
O	-2.035452	1.967764	2.303899
O	-1.266912	-3.484504	0.582997
O	-1.323621	1.433714	-0.253379
O	-2.936023	0.343022	4.535851
Cl	1.504401	2.378806	0.105702
H	-0.769891	-1.819467	0.093092
H	-0.720853	-0.233378	-0.007193
H	-0.410889	1.842466	-0.245379
H	-1.707682	1.660815	-1.107333
H	-0.482677	1.207221	2.590593
H	0.870642	1.503437	1.871076
H	0.602893	-3.485169	1.009403
H	1.455813	-3.579529	2.324629
H	1.801321	-0.641078	4.453415

H	3.014053	-1.198362	3.528891
H	0.502318	0.512507	5.758693
H	1.086052	1.104672	4.452853
H	2.303451	0.520859	0.510538
H	2.381094	-0.962642	0.042464
H	-1.759496	0.482309	5.787321
H	-1.236970	1.226371	7.051631
H	-2.655742	-0.525360	4.199535
H	-2.782175	0.932961	3.779636
H	-1.521102	-3.196709	1.490143
H	-1.927429	-4.115092	0.280511
H	4.048249	-0.689453	1.867772
H	4.957615	-1.769530	2.493479
H	-1.961342	2.920968	2.424317
H	-2.011629	1.817457	1.331164
H	1.781848	-3.096195	4.170956
O	1.499491	-4.007468	3.940880
H	0.566767	-4.011064	4.195461

$MgCl_2(H_2O)_{14}$

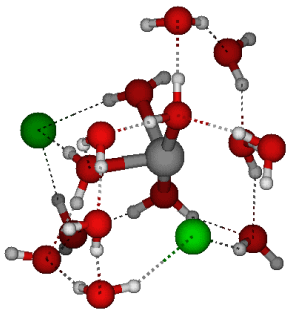

Figure S_{222} : $MgCl_2$ optimized structure with 14 water molecules.

E=-1299.718025

H=-1299.717081

O	-0.227149	-1.156335	0.250808
Mg	0.776044	-1.178757	2.114595
O	0.457493	0.860465	2.546520
O	1.912118	-1.519243	3.852340
O	1.160418	-3.277389	1.661258

O	2.500992	-0.469775	1.099424
Cl	-1.365531	-1.921807	3.254049
O	1.370034	0.563413	5.231397
O	1.016444	-4.054844	4.131669
O	-1.012957	0.652672	6.457463
O	4.458015	-1.538249	2.973178
O	-1.416091	-3.557446	0.723367
O	-2.925199	0.571532	4.537174
O	-1.974794	2.036206	2.224498
O	-1.298964	1.308522	-0.298476
Cl	1.507018	2.248821	0.051592
H	-0.844762	-1.905629	0.161146
H	-0.703281	-0.335889	-0.003279
H	-0.379828	1.710592	-0.299465
H	-1.677150	1.512180	-1.160919
H	-0.462975	1.212361	2.580562
H	0.903351	1.421970	1.861011
H	0.380840	-3.613255	1.173894
H	1.115994	-3.711431	2.577888
H	1.727153	-0.768762	4.518692
H	2.887259	-1.527592	3.661276
H	0.527385	0.544125	5.754976
H	1.127786	1.026505	4.413454
H	2.324911	0.330400	0.551159
H	2.930964	-1.155037	0.552723
H	-1.733801	0.669971	5.780782
H	-1.159439	1.420411	7.017234
H	-2.709665	-0.321850	4.220208
H	-2.749943	1.128755	3.760745
H	-1.694246	-3.190198	1.595431
H	-2.077871	-4.200332	0.450796
H	4.353071	-0.693498	2.514600
H	4.399160	-2.180693	2.242735
H	-1.826322	2.987377	2.269108

H	-1.960100	1.809862	1.266061
H	1.413410	-3.180258	4.347372
H	0.079269	-3.909425	4.327777
H	2.749200	-3.252723	0.909167
O	3.608183	-2.875129	0.611864
H	3.961760	-3.452517	-0.070743

$MgCl_2(H_2O)_{15}$

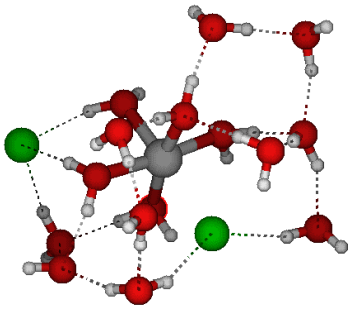

Figure S_{223} : $MgCl_2$ optimized structure with 2 water molecules.

E=-1376.099301

H=-1376.098356

O	-0.627061	-0.220849	0.009296
Mg	0.769591	-0.522783	1.635972
O	2.263734	0.575389	0.631861
O	0.262650	1.327649	2.534652
O	1.918007	-1.083592	3.256596
O	1.424420	-4.386429	1.800573
Cl	-1.321063	-1.861420	2.412886
O	1.491424	0.717389	5.038357
O	0.976292	-3.478028	4.238295
O	-0.853723	0.016130	6.154839
O	4.148168	-4.454727	1.898912
O	4.350506	-1.889268	2.721622
O	-2.886115	0.166318	4.368628
O	-2.284027	2.292078	2.501683
O	-1.593395	2.330613	-0.120804
O	-1.164743	-4.803238	1.106993

Cl	1.121920	3.396210	0.470070
H	-1.362453	-0.720800	0.403599
H	-0.977991	0.684670	-0.152967
H	-0.712727	2.799798	-0.021816
H	-2.005047	2.693012	-0.913036
H	-0.683151	1.571516	2.663836
H	0.624719	2.074510	1.991347
H	0.573016	-4.773154	1.491746
H	1.246569	-4.113629	2.749165
H	1.855307	-0.414621	4.021095
H	2.879080	-1.310111	3.079670
H	0.675451	0.440067	5.527510
H	1.151144	1.317506	4.356833
H	2.064657	1.526397	0.445502
H	2.528865	0.167994	-0.199218
H	-1.610850	0.115792	5.527617
H	-1.128334	0.442844	6.971111
H	-2.644353	-0.600201	3.821552
H	-2.852342	0.911576	3.746596
H	-1.407342	-3.929081	1.467796
H	-1.686681	-5.434356	1.613477
H	4.781196	-1.393016	2.019054
H	4.309817	-2.827503	2.404653
H	-2.257615	3.200955	2.820928
H	-2.260860	2.352403	1.519171
H	1.353631	-2.591051	4.041854
H	0.028671	-3.291030	4.276690
H	3.190511	-4.610174	1.752858
H	4.382174	-5.023339	2.639835
H	0.779938	-2.263691	-0.240892
O	1.414126	-2.134894	0.473999
H	1.458506	-3.011726	0.971018

$MgCl_2(H_2O)_{16}$

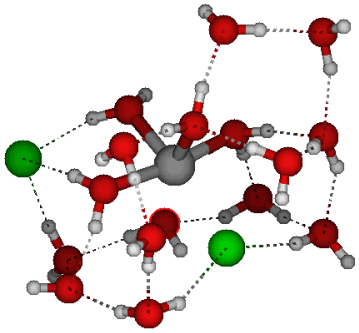

Figure S_{224} : $MgCl_2$ optimized structure with 16 water molecules.

E=-1452.487772

H=-1452.486828

O	-0.590684	-0.322150	0.017534
Mg	0.930224	-0.570705	1.630895
O	1.734879	-2.130519	0.573161
O	2.361921	0.609008	0.656991
O	0.296297	1.267883	2.481741
O	1.963822	-1.087258	3.342258
O	1.411549	0.741241	5.065153
Cl	-1.213295	-1.921956	2.414861
O	1.679633	-4.460386	1.918301
O	4.447292	-1.848550	3.017689
O	1.030407	-3.516772	4.294634
O	-0.953424	0.036035	6.140362
O	4.381952	-4.443516	2.274397
O	-2.929132	0.093567	4.280118
O	-0.847858	-4.468063	0.643268
O	-2.275783	2.176273	2.384426
O	-1.539004	2.207220	-0.227730
Cl	1.108547	3.374941	0.430767
H	-1.280190	-0.738542	0.569957
H	-0.924414	0.581081	-0.198951
H	-0.672554	2.701219	-0.108976
H	-1.940319	2.554514	-1.032021

H	-0.659533	1.480265	2.584087
H	0.645768	2.025414	1.945275
H	0.889936	-4.800431	1.461289
H	1.383579	-4.193506	2.836391
H	1.838900	-0.412990	4.092558
H	2.939169	-1.300631	3.240280
H	0.584728	0.467816	5.536904
H	1.089605	1.313933	4.352117
H	2.140250	1.544380	0.428156
H	2.751226	0.188717	-0.116705
H	-1.692020	0.103125	5.488435
H	-1.257642	0.486563	6.933022
H	-2.656012	-0.688301	3.772730
H	-2.872955	0.817913	3.635106
H	-1.105001	-3.745718	1.256558
H	-1.582651	-5.090691	0.643441
H	4.923829	-1.370408	2.332368
H	4.454249	-2.798825	2.735313
H	-2.259985	3.085045	2.705105
H	-2.237318	2.239098	1.402744
H	1.377753	-2.618839	4.092917
H	0.076486	-3.369016	4.327280
H	3.450929	-4.622844	2.024631
H	4.535219	-4.980890	3.058523
H	1.231752	-2.376637	-0.249088
H	1.814098	-2.974272	1.088325
O	0.066874	-2.739352	-1.407510
H	-0.402911	-1.907608	-1.236319
H	-0.401125	-3.416080	-0.882166

$MgCl_2(H_2O)_{17}$

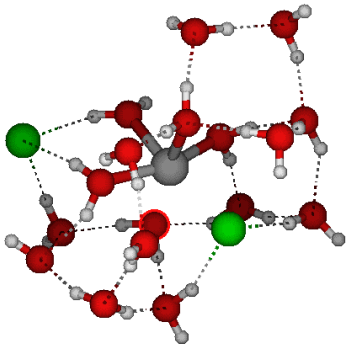

Figure S_{225} : $MgCl_2$ optimized structure with 2 water molecules.

E=-1528.868092

H=-1528.867148

O	-0.867915	-0.367714	0.386200
Mg	0.761996	-0.783532	1.795431
O	1.966719	-1.271648	3.417753
O	1.582144	-2.201689	0.532025
O	2.221789	0.362572	0.785502
O	0.308558	1.131805	2.688196
O	1.177497	0.349477	5.271994
O	4.510043	-1.500248	2.844534
Cl	-0.979533	-2.441386	2.771629
O	-0.376775	-2.766854	-1.170000
O	2.052091	-4.562330	1.734334
O	1.564449	-3.875622	4.236379
O	-1.404819	-0.094310	5.959590
O	4.735211	-3.991481	1.798567
O	-1.084322	2.249176	-0.287540
O	-1.830017	2.827991	2.299804
O	-3.083295	1.038638	4.123651
O	-0.615677	-4.791637	0.791728
Cl	1.478922	3.288102	0.807313
H	-1.740309	-0.450425	0.832440
H	-0.879093	0.538970	-0.003012
H	-0.198292	2.658847	-0.064396

H	-1.335381	2.602885	-1.147765
H	-0.590313	1.525039	2.702730
H	0.827189	1.832903	2.221751
H	1.271064	-4.991838	1.344067
H	1.831220	-4.397837	2.696769
H	1.743190	-0.698114	4.223117
H	2.955960	-1.266663	3.252728
H	0.278329	0.093727	5.597570
H	0.971547	1.001574	4.584477
H	2.175066	1.331563	0.606769
H	2.547319	-0.106039	0.009828
H	-1.998606	0.309279	5.283360
H	-1.666457	0.304589	6.794703
H	-3.302021	0.410729	3.413490
H	-2.780973	1.823313	3.638827
H	-0.814031	-4.123367	1.486175
H	-1.275375	-5.485193	0.898174
H	4.765518	-0.876358	2.157770
H	4.619894	-2.399554	2.444665
H	-1.319622	3.633917	2.446556
H	-1.816427	2.699553	1.327948
H	1.742957	-2.922865	4.061531
H	0.611771	-3.876205	4.396466
H	3.832733	-4.334647	1.634282
H	5.094559	-4.562581	2.485410
H	0.971035	-2.453781	-0.210487
H	1.829834	-3.050147	0.981263
H	-0.828727	-1.997163	-0.785032
H	-0.665717	-3.538537	-0.647409
H	-2.672373	-1.398009	2.320358
O	-3.202955	-0.690649	1.877912
H	-3.989616	-1.122732	1.527628

$MgCl_2(H_2O)_{18}$

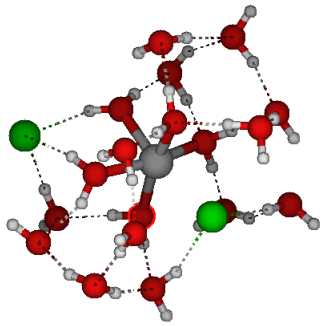

Figure S_{226} : $MgCl_2$ optimized structure with 18 water molecules.

E=-1605.256965

H=-1605.256021

O	-0.987037	-0.301738	0.450299
Mg	0.693607	-0.742047	1.762703
O	0.283232	1.136106	2.717138
O	1.883302	-1.308881	3.389769
O	1.270594	-2.214099	0.384496
O	2.290997	0.342925	0.864201
O	1.033901	0.209757	5.281361
Cl	-1.014210	-2.458085	2.793321
O	4.334656	-0.880385	2.567068
O	-0.843970	-2.835578	-1.032650
O	2.159929	-4.475595	1.473779
O	1.718235	-3.952532	3.998831
O	-1.536149	-0.074294	6.046915
O	-1.078331	2.312504	-0.224997
O	4.497659	-3.113850	0.829057
O	-3.135393	1.153233	4.215630
O	-1.812471	2.887641	2.367961
O	-3.247607	-0.636304	2.033695
O	-0.640637	-4.874162	0.895372
Cl	1.479309	3.302395	0.938607
H	-1.835393	-0.348553	0.945827
H	-0.979049	0.601600	0.050390
H	-0.182378	2.687897	0.020706

H	-1.291630	2.677840	-1.090618
H	-0.605150	1.553939	2.732999
H	0.822729	1.840754	2.272934
H	1.404445	-4.992891	1.146788
H	1.996950	-4.362904	2.460901
H	1.585923	-0.791092	4.215858
H	2.855096	-1.128804	3.227503
H	0.129388	-0.006727	5.623404
H	0.854480	0.897508	4.621240
H	2.232157	1.314372	0.723992
H	2.755979	-0.080632	0.088520
H	-2.107653	0.378069	5.381130
H	-1.727704	0.362095	6.882404
H	-3.349553	0.510799	3.516473
H	-2.797540	1.916780	3.720742
H	-0.801909	-4.203974	1.597903
H	-1.241434	-5.601751	1.089166
H	4.005477	-0.209106	1.948796
H	4.494656	-1.670287	2.013118
H	-1.264512	3.667560	2.522787
H	-1.810794	2.778128	1.393896
H	1.808181	-2.974931	3.890262
H	0.782567	-4.049975	4.216322
H	3.749013	-3.726859	0.991793
H	5.295908	-3.650440	0.859818
H	0.521399	-2.476567	-0.225767
H	1.613761	-3.052488	0.794842
H	-1.282448	-2.064685	-0.639050
H	-1.062082	-3.605974	-0.474254
H	-2.710008	-1.355451	2.447516
H	-4.046172	-1.057194	1.696942
O	3.411247	-1.162880	-0.996286
H	2.592311	-1.675783	-0.866219
H	4.060746	-1.725514	-0.539724

$MgCl_2(H_2O)_{19}$

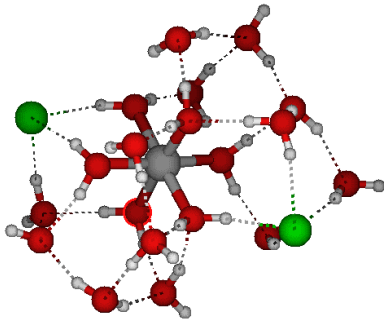

Figure S_{227} : $MgCl_2$ optimized structure with 19 water molecules.

E=-1681.667782

H=-1681.666837

O	-0.797149	0.317897	0.559709
Mg	0.635981	-0.425766	1.911391
O	2.285161	0.373119	0.880202
O	0.567643	1.469987	2.959451
O	1.875378	-1.208744	3.444073
O	0.736669	-2.153672	0.729884
O	1.164893	0.373520	5.454057
O	-1.507606	-3.514917	0.225231
O	4.265865	-0.887195	2.451351
Cl	-1.318541	-4.313959	3.280257
O	2.678183	-1.253970	-1.103304
O	2.232168	-4.249233	1.453134
O	1.834174	-3.958082	4.004988
O	-1.648787	-0.178302	5.312325
O	-0.835640	3.043370	0.228180
O	-3.344140	1.269861	3.951837
O	-1.612570	3.138202	2.783323
O	-3.169354	-0.448526	1.724737
O	4.301637	-2.905513	0.492870
O	0.045892	-5.823041	0.922706
Cl	1.970665	3.417751	1.098995
H	-1.728651	0.097675	0.765057

H	-0.787848	1.264804	0.304822
H	0.128948	3.262625	0.402894
H	-1.078069	3.504049	-0.582297
H	-0.277613	1.973456	2.998382
H	1.170412	2.106197	2.489341
H	1.643420	-4.974148	1.155015
H	2.160238	-4.229871	2.459522
H	1.708732	-0.697360	4.286802
H	2.846951	-1.110825	3.195127
H	0.233035	0.174003	5.654080
H	1.090708	1.076210	4.784854
H	2.316078	1.347255	0.740007
H	2.486192	-0.106422	0.018514
H	-2.327769	0.438008	4.893749
H	-2.126287	-0.741323	5.931273
H	-3.541060	0.718839	3.170637
H	-2.882457	2.047770	3.585775
H	-0.388274	-5.525682	1.755319
H	-0.035640	-6.782658	0.916265
H	3.898602	-0.203335	1.864182
H	4.430750	-1.639083	1.847128
H	-1.343644	3.982308	3.163070
H	-1.507454	3.234057	1.804998
H	1.847603	-2.978584	3.980442
H	0.887575	-4.179968	4.063976
H	3.621421	-3.551670	0.812848
H	5.090785	-3.409691	0.272542
H	-0.131682	-2.563993	0.463312
H	1.292464	-2.914060	1.053606
H	-1.731028	-3.700034	1.159395
H	-1.119304	-4.362848	-0.046319
H	-2.484189	-0.945612	2.235520
H	-3.743435	-1.106561	1.317412
H	1.856530	-1.691530	-0.816127

H	3.377905	-1.828399	-0.732460
H	-0.984817	-2.286855	3.111093
O	-0.998246	-1.297544	3.024606
H	-1.178024	-0.950400	3.945261

$MgCl_2(H_2O)_{20}$

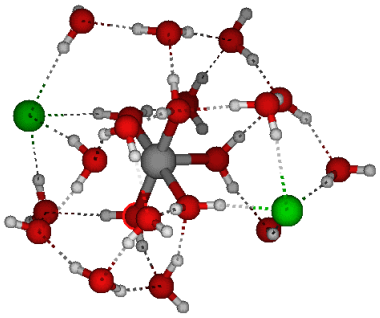

Figure S_{228} : $MgCl_2$ optimized structure with 20 water molecules.

E=-1758.049059

H=-1758.048115

O	-1.304093	0.236844	0.582903
Mg	0.369305	-0.421794	1.692558
O	-1.045181	-1.306126	3.066199
O	1.630961	0.427460	0.331080
O	0.390419	1.509180	2.725265
O	1.882186	-1.029092	3.028489
O	0.425375	-2.184449	0.561157
O	2.080312	-1.277039	-1.584024
O	4.230018	-0.722097	2.030529
O	-1.379526	-0.134987	5.406045
O	-3.251439	1.307393	4.277850
O	1.387059	0.531857	5.148148
O	-3.421604	-0.508187	2.155528
O	-1.717027	-3.769660	0.346569
O	2.202686	-4.101075	1.159149
O	2.078595	-3.731042	3.723864
O	4.018525	-2.615629	-0.088974
O	0.100646	-5.871986	1.002823

O	-1.184446	2.993731	0.143003
O	-1.779284	3.192718	2.758046
Cl	1.732711	3.496154	0.795151
Cl	-1.129076	-4.321199	3.415935
H	-2.195175	0.066814	0.947657
H	-1.281052	1.164628	0.277288
H	-0.216948	3.209005	0.229036
H	-1.487595	3.443984	-0.652904
H	-0.435784	2.029781	2.844364
H	0.968826	2.127810	2.215593
H	1.656092	-4.889115	0.962148
H	2.245787	-4.044415	2.166434
H	1.800874	-0.528520	3.885783
H	2.824342	-0.874346	2.668285
H	0.509571	0.281157	5.486892
H	1.166216	1.200306	4.477383
H	1.794942	1.380668	0.224174
H	1.869730	-0.080039	-0.495759
H	-2.102983	0.484398	5.082011
H	-1.766008	-0.680103	6.099801
H	-3.559393	0.717244	3.563084
H	-2.874480	2.074535	3.809966
H	-0.253053	-5.547741	1.862987
H	0.077681	-6.833067	1.059479
H	4.357278	0.193751	1.699615
H	4.256484	-1.309539	1.251927
H	-1.470419	4.044096	3.087818
H	-1.755923	3.256615	1.773901
H	2.034978	-2.754400	3.641354
H	1.159900	-3.997266	3.905540
H	3.435703	-3.290059	0.344829
H	4.816998	-3.076843	-0.363365
H	-0.423486	-2.683303	0.409048
H	1.085829	-2.874692	0.838712

H	-1.853280	-3.891032	1.306578
H	-1.263505	-4.597834	0.115963
H	-2.644440	-0.989163	2.536075
H	-4.059204	-1.176808	1.882887
H	1.337929	-1.753631	-1.172372
H	2.866221	-1.747404	-1.238326
H	-0.975737	-2.293118	3.166386
H	-1.087928	-0.941628	3.995204
H	3.793756	2.453237	1.211528
O	4.588780	1.895808	1.157997
H	4.878200	1.993338	0.245130

$MgSO_4(H_2O)_1$

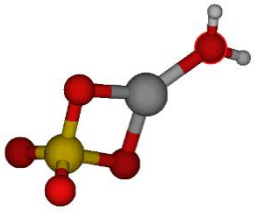

Figure S_{229} : $MgSO_4$ optimized structure with 1 water molecule.

E=-388.010361

H=-388.009417

O	1.278845	0.110362	2.396060
S	-0.375569	0.545612	2.523843
O	-0.551438	2.018593	2.152637
O	-0.953251	0.008848	3.833940
O	-0.881654	-0.444917	1.216724
Mg	0.887731	-1.018073	0.943228
O	1.882003	-2.257066	-0.299575
H	1.490947	-2.783335	-1.008590
H	2.832416	-2.427983	-0.292996

$MgSO_4(H_2O)_2$

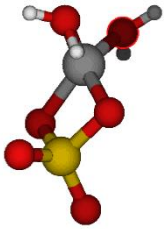

Figure S_{230} : $MgSO_4$ optimized structure with 2 water molecules.

E=-464.433134

H=-464.432189

O	1.571394	-2.691154	-0.299401
Mg	1.510263	-0.965297	0.764394
O	-0.116917	0.020825	0.681747
S	-0.100003	0.315469	2.350421

O	-1.370141	-0.218401	3.008326
O	1.232615	-0.702486	2.670787
O	0.352339	1.762489	2.606860
H	0.722049	-3.022269	-0.621764
H	2.131929	-3.455947	-0.122074
O	3.221057	0.059873	1.178489
H	3.412403	0.951978	0.864001
H	2.825114	0.157444	2.086473

$MgSO_4(H_2O)_3$

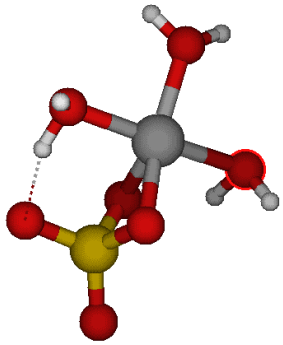

Figure S_{231} : $MgSO_4$ optimized structure with 3 water molecules.

E=-540.852187

H=-540.851242

O	1.038256	-2.953252	0.096074
Mg	2.074905	-1.410878	1.112305
O	3.115933	0.228383	1.802449
O	0.603461	-0.377502	0.193691
S	0.010357	0.052175	1.696607
O	0.835905	1.345691	2.103655
O	0.676439	-1.214836	2.524003
O	-1.506221	0.135831	1.772115
H	0.442108	-2.202296	-0.160397
H	0.493243	-3.508026	0.669379
H	2.285473	0.848165	1.901884
H	3.473348	0.198489	2.697834
O	3.816454	-2.077152	0.258453
H	4.487558	-1.404222	0.089758

H	3.799413	-2.688580	-0.487168

$MgSO_4(H_2O)_4$

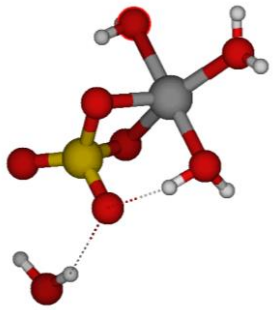

Figure S_{232} : $MgSO_4$ optimized structure with 4 water molecules.

E=-617.227665

H=-617.226721

O	1.511705	-3.023113	-0.336212
Mg	1.989324	-1.473210	1.025130
O	3.969126	-1.839133	0.657457
O	2.533592	0.189076	2.120620
O	0.636572	-0.541046	-0.152048
S	-0.371960	-0.400901	1.161412
O	-1.856806	-0.532349	0.839019
O	0.266060	-1.647410	2.027350
O	0.077975	0.947331	1.877947
H	0.880488	-2.361977	-0.712493
H	0.945227	-3.713936	0.032470
H	1.635112	0.686384	2.046459
H	2.649758	0.088379	3.073201
H	4.596517	-1.111256	0.744127
H	4.249243	-2.402354	-0.073540
H	-2.771297	0.499168	2.787338
O	-2.388127	0.990245	3.523609
H	-1.538348	1.265976	3.153320

$MgSO_4(H_2O)_5$

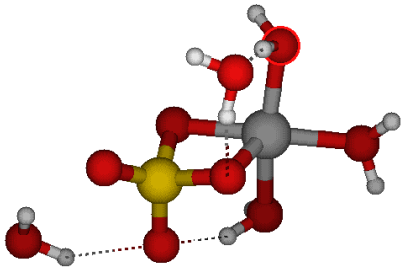

Figure S_{233} : $MgSO_4$ optimized structure with 5 water molecules.

E=-693.629263

H=-693.628319

O	0.951103	-3.390454	0.226750
Mg	1.472045	-1.559843	0.986601
O	-0.052122	-1.420288	2.315038
S	-0.630575	-0.095532	1.555166
O	0.083470	1.174318	2.172985
O	3.310419	-1.737988	0.078826
O	2.429010	0.012580	2.011474
O	0.134711	-0.351831	0.090919
O	-2.152268	-0.038327	1.415213
O	-2.174709	1.569739	4.070063
H	0.151552	-3.149313	-0.371104
H	0.603018	-4.014217	0.874953
H	1.640048	0.649640	2.088611
H	2.682095	-0.139479	2.929971
H	3.827166	-0.923786	0.042426
H	3.475676	-2.251529	-0.719358
H	-2.673463	1.125989	3.373716
H	-1.333129	1.742996	3.627015
H	-1.846403	-2.567474	-0.920711
O	-0.933604	-2.405270	-1.185393
H	-0.727297	-1.491601	-0.848706

$MgSO_4(H_2O)_6$

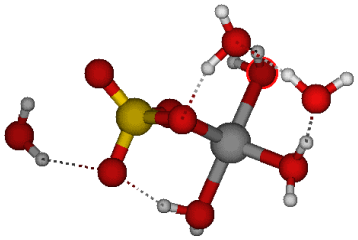

Figure S_{234} : $MgSO_4$ optimized structure with 6 water molecules.

E=-770.025690

H=-770.024746

O	1.372663	-3.339872	1.013201
Mg	1.906926	-1.364796	1.449704
O	0.570691	-0.418457	0.259277
S	-0.496837	-0.231970	1.536744
O	-1.954649	-0.386248	1.105915
O	0.092864	-1.439218	2.462356
O	3.652917	-1.444786	0.453869
O	2.401646	0.299548	2.579740
O	-0.078587	1.134959	2.207015
O	0.462543	-2.407563	-1.345737
O	-2.695814	1.289835	3.618162
H	0.993214	-3.290505	0.101897
H	0.587844	-3.362539	1.588813
H	1.536957	0.819750	2.491567
H	2.535736	0.222037	3.531372
H	4.147964	-0.619684	0.399259
H	3.548343	-1.796758	-0.489713
H	-3.000347	0.773196	2.862808
H	-1.810117	1.551928	3.333065
H	-0.321213	-2.581233	-1.877327
H	0.300528	-1.551959	-0.831056
O	3.110639	-2.289409	-1.919103
H	2.125197	-2.316405	-1.927525
H	3.403800	-3.178776	-2.143084

$MgSO_4(H_2O)_7$

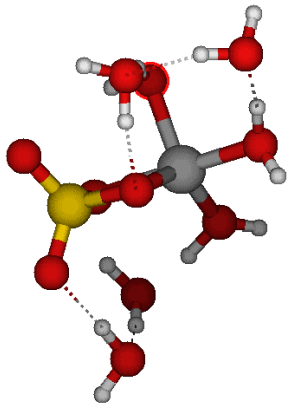

Figure S_{235} : $MgSO_4$ optimized structure with 7 water molecules.

E=-846.440896

H=-846.439952

O	1.259332	-3.376592	0.554712
Mg	1.458711	-1.568995	1.562951
O	2.030866	-1.276947	3.425673
O	0.329425	-0.420425	0.327659
S	-1.140162	-0.908167	0.960014
O	-1.907792	0.304304	1.547950
O	-0.514029	-1.843570	2.158747
O	3.243144	-1.067260	0.674058
O	-1.875995	-1.750107	-0.098122
O	0.686437	-2.038060	-1.696655
O	3.354722	-1.724151	-1.843528
O	-0.696557	1.577207	3.622034
H	1.026468	-3.102584	-0.372397
H	0.428070	-3.715202	0.921966
H	2.877246	-1.187777	3.866708
H	1.227254	-1.044726	4.069031
H	3.447982	-0.125447	0.685600
H	3.361044	-1.350879	-0.285420
H	-1.421591	2.049425	4.044005
H	-1.091575	1.195517	2.801898
H	-0.145568	-2.244657	-2.139334

H	0.456335	-1.287964	-1.067981
H	2.402462	-1.822567	-2.066534
H	3.760713	-2.574567	-2.041119
H	-0.569816	-1.287502	3.995274
O	-0.055466	-0.788410	4.662272
H	-0.283495	0.153714	4.433971

$MgSO_4(H_2O)_8$

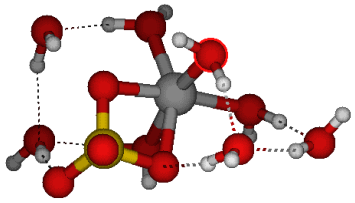

Figure S_{236} : $MgSO_4$ optimized structure with 8 water molecules.

E=-922.844093

H=-922.843148

O	1.378986	-3.196905	0.721751
Mg	1.513854	-1.203794	1.457779
O	3.313645	-0.980473	0.486424
O	2.048454	-1.593807	3.383433
O	0.200925	-0.506250	-0.108261
S	-1.180522	-0.781210	0.776356
O	-2.130886	-1.698609	0.000425
O	-0.466230	-1.505791	2.051874
O	-1.760343	0.597440	1.248011
O	-0.074648	-0.949418	4.679632
O	3.324271	-1.987019	-1.932992
O	0.657435	-2.424708	-1.757392
O	-0.438801	1.467432	3.354978
H	1.081739	-3.148625	-0.219304
H	0.609062	-3.522655	1.209349
H	2.901051	-1.468574	3.805913
H	1.304608	-1.341116	4.028595
H	3.584057	-0.057488	0.428739

H	3.398808	-1.371794	-0.433074
H	-0.776090	2.335374	3.598699
H	-1.033702	1.126698	2.621454
H	-0.092633	-2.752630	-2.264432
H	0.333526	-1.608325	-1.261935
H	2.367820	-2.147664	-2.098442
H	3.739912	-2.854675	-1.974787
H	-0.591352	-1.343424	3.949213
H	-0.199351	0.002996	4.494581
H	1.081901	1.105911	0.874854
O	1.599465	0.941175	1.683057
H	1.013329	1.281255	2.402472

$MgSO_4(H_2O)_9$

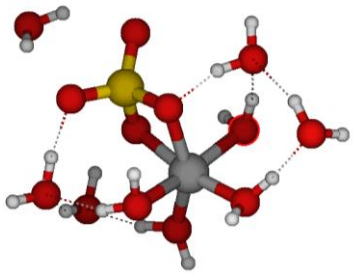

Figure S_{237} : $MgSO_4$ optimized structure with 9 water molecules.

E=-999.220021

H=-999.219077

O	1.603531	-3.206239	0.640826
Mg	1.524093	-1.214367	1.384610
O	1.427871	0.917506	1.648654
O	3.390537	-0.869460	0.599549
O	1.856523	-1.611270	3.349345
O	0.342540	-0.594275	-0.320496
S	-1.093961	-0.951928	0.414278
O	-1.806948	0.397580	0.803701
O	-0.495056	-1.638936	1.755391

O	-1.917889	-1.907027	-0.467309
O	-0.410937	-1.135960	4.455265
O	1.093678	-2.488781	-1.908676
O	3.728574	-1.857186	-1.799398
O	-0.806582	1.262193	3.105510
H	1.399088	-3.186197	-0.325044
H	0.830367	-3.614852	1.054110
H	2.650532	-1.479002	3.871826
H	1.033488	-1.423882	3.917294
H	3.622929	0.064976	0.571447
H	3.598154	-1.253357	-0.304041
H	-1.233212	2.087480	3.357741
H	-1.295284	0.920633	2.302321
H	0.435954	-2.859919	-2.506103
H	0.663658	-1.697125	-1.463587
H	2.810946	-2.089793	-2.065737
H	4.217220	-2.686917	-1.807443
H	-0.870585	-1.597406	3.731011
H	-0.592810	-0.202085	4.224046
H	0.994589	1.091383	0.795375
H	0.752394	1.200069	2.311846
H	-3.888978	-1.761174	0.514707
O	-4.342529	-1.180033	1.138906
H	-3.842071	-0.361325	1.028292

$MgSO_4(H_2O)_{10}$

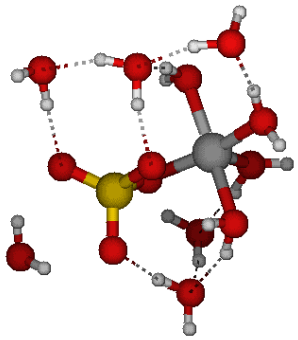

Figure S_{238} : $MgSO_4$ optimized structure with 10 water molecules

E=-1075.609916

H=-1075.608971

O	1.648846	-3.138675	0.602528
Mg	1.481749	-1.181422	1.344572
O	-0.530865	-1.610975	1.817700
S	-1.191966	-0.884700	0.536786
O	-2.159643	-1.798535	-0.264509
O	1.372118	0.948426	1.632168
O	3.288269	-0.790236	0.450993
O	1.907810	-1.567696	3.295117
O	0.175277	-0.561653	-0.299393
O	-1.859263	0.470003	0.978886
O	-0.303197	-1.138679	4.530049
O	1.030196	-2.541588	-1.887002
O	3.656351	-1.936959	-1.869777
O	-0.752395	1.284668	3.250131
O	-4.436380	-0.957504	1.509010
H	1.411125	-3.108465	-0.367823
H	0.978439	-3.687766	1.026971
H	2.726161	-1.423399	3.775257
H	1.114399	-1.401107	3.908012
H	3.507550	0.143291	0.366209
H	3.505455	-1.232347	-0.424821
H	-1.159425	2.106557	3.542749

H	-1.284166	0.963419	2.467680
H	0.234686	-3.030575	-2.227970
H	0.638089	-1.715154	-1.512350
H	2.739371	-2.198709	-2.115630
H	4.146945	-2.763010	-1.803216
H	-0.801087	-1.594818	3.828961
H	-0.500443	-0.202284	4.322848
H	0.890291	1.152829	0.813468
H	0.748005	1.224866	2.345618
H	-4.047845	-1.598340	0.900704
H	-3.890160	-0.180677	1.331839
H	-1.702983	-2.984205	-1.507923
O	-1.380143	-3.532009	-2.257057
H	-1.881316	-3.221715	-3.018337

$MgSO_4(H_2O)_{11}$

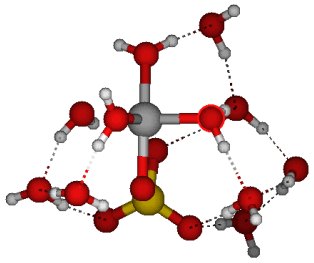

Figure S_{239} : $MgSO_4$ optimized structure with 11 water molecules.

E=-1152.011698

H=-1152.010754

O	0.904223	-3.059874	0.946856
Mg	1.371582	-1.138385	1.526743
O	2.138230	-1.305811	3.408083
O	-0.496219	-0.860920	2.443695
S	-1.268471	-0.204823	1.188734
O	-1.632399	1.282636	1.487631
O	1.822246	1.005173	1.399064
O	3.075622	-1.227860	0.375661
O	-2.515043	-1.089194	0.815012

O	-0.112611	-0.321339	0.056077
O	0.439920	-0.024795	4.878766
O	2.927524	-2.394297	-1.945364
O	0.294464	-2.542729	-1.595298
O	-1.957532	-3.841556	-1.690157
O	0.201814	2.202563	3.204955
O	-3.395558	-1.529229	-1.748584
H	0.764845	-3.028309	-0.037285
H	0.031033	-3.375175	1.267639
H	3.057353	-1.358006	3.678529
H	1.600201	-0.804554	4.100802
H	3.440157	-0.347848	0.229952
H	3.093828	-1.708985	-0.508571
H	0.089310	3.150977	3.324752
H	-0.564783	1.894912	2.646948
H	-0.531930	-3.093995	-1.773246
H	-0.032256	-1.675076	-1.286059
H	1.946192	-2.487211	-2.030444
H	3.272134	-3.293013	-1.969009
H	-0.258693	-0.422258	4.326651
H	0.439450	0.892225	4.541298
H	1.230518	1.157896	0.642046
H	1.427976	1.554316	2.116964
H	-3.091088	-1.197462	-0.878653
H	-4.356004	-1.531972	-1.693589
H	-2.018383	-4.036997	-0.738269
H	-2.584114	-3.091993	-1.821631
H	-2.207897	-4.077516	1.929071
O	-1.781069	-3.665271	1.171377
H	-2.101476	-2.729431	1.151630

$MgSO_4(H_2O)_{12}$

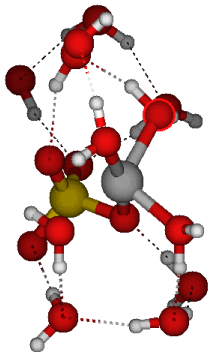

Figure S_{240} : $MgSO_4$ optimized structure with 12 water molecules.

E=-1228.397868

H=-1228.396923

O	0.952548	-3.058081	0.763973
Mg	1.387025	-1.154882	1.424248
O	3.087526	-1.189080	0.260891
O	2.149298	-1.359474	3.282265
O	-0.506414	-0.920682	2.280569
S	-1.289418	-0.259080	1.030407
O	-0.131364	-0.309630	-0.091640
O	-1.704360	1.201161	1.390104
O	-2.509312	-1.176532	0.644695
O	1.776137	0.989435	1.320597
O	0.934875	0.056083	5.021902
O	2.986407	-2.296298	-2.094050
O	0.351344	-2.502276	-1.771954
O	-1.864390	-3.860370	-1.919996
O	0.124217	2.066574	3.172053
O	-1.713987	-3.746036	0.948387
O	-3.362125	-1.584124	-1.936381
H	0.821232	-3.002852	-0.220156
H	0.089989	-3.414237	1.068797
H	3.060675	-1.550532	3.514216
H	1.715578	-0.812250	4.031437
H	3.446925	-0.302415	0.146594

H	3.122474	-1.644530	-0.635457
H	0.009935	3.014892	3.291590
H	-0.635976	1.759445	2.610033
H	-0.458648	-3.070164	-1.969749
H	0.001086	-1.647837	-1.453567
H	2.008396	-2.405047	-2.191911
H	3.347735	-3.187812	-2.134917
H	0.090803	-0.440644	5.148188
H	0.663654	0.842939	4.512456
H	1.190627	1.153475	0.561478
H	1.361051	1.501135	2.054470
H	-3.079036	-1.266197	-1.054551
H	-4.323229	-1.604201	-1.900969
H	-1.928817	-4.082736	-0.974497
H	-2.510831	-3.126086	-2.039141
H	-2.136595	-4.181033	1.695824
H	-2.053716	-2.817763	0.940439
H	-1.252930	-1.224401	3.844547
O	-1.422647	-1.279569	4.810456
H	-2.184967	-0.711408	4.962480

$MgSO_4(H_2O)_{13}$

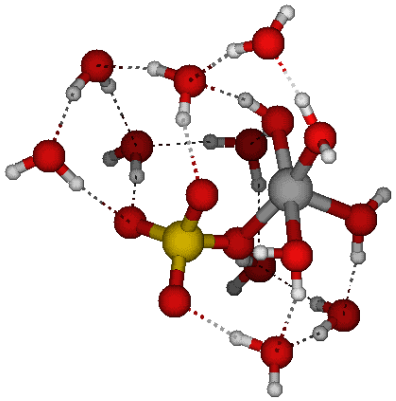

Figure S_{241} : $MgSO_4$ optimized structure with 13 water molecules.

E=-1304.787691

H=-1304.786747

O	1.347282	-2.816203	1.097778
Mg	1.531362	-0.794638	1.305062
O	-0.413647	-0.604509	2.178513
S	-1.191405	-0.069548	0.864496
O	-2.445140	-0.969663	0.549516
O	3.106248	-0.804585	-0.006122
O	2.411175	-0.810671	3.144101
O	-0.028515	-0.259068	-0.230288
O	-1.564064	1.430811	1.075319
O	1.717572	1.352802	1.201609
O	0.861843	0.210554	4.936004
O	2.917093	-2.333826	-2.101231
O	0.383228	-2.742710	-1.411198
O	-1.925222	-3.913927	-1.798240
O	0.015168	2.249005	3.127279
O	-2.453556	-3.623870	1.001103
O	-1.075085	-1.756244	4.407207
O	-3.128735	-1.467341	-2.090105
H	0.987856	-3.017108	0.199319
H	0.768880	-3.296699	1.756518
H	2.872318	-1.591830	3.461756
H	1.871338	-0.423140	3.910442

H	3.459590	0.055286	-0.252755
H	3.108055	-1.391045	-0.824585
H	-0.144293	3.180014	3.313384
H	-0.687957	1.961988	2.490796
H	-0.433256	-3.270493	-1.665785
H	0.059115	-1.840086	-1.219742
H	1.953800	-2.559703	-2.042967
H	3.378329	-3.169962	-1.976540
H	0.146845	-0.455435	4.976125
H	0.485643	0.957729	4.431204
H	1.132269	1.549300	0.453951
H	1.296736	1.810422	1.965524
H	-2.898253	-1.126538	-1.202947
H	-4.074185	-1.319456	-2.184731
H	-2.152241	-4.043413	-0.859452
H	-2.452209	-3.124728	-2.054762
H	-3.353457	-3.815726	1.284587
H	-2.407913	-2.641214	0.899487
H	-1.042588	-1.305386	3.523522
H	-1.978926	-1.675445	4.728401
O	-0.325956	-4.006814	2.784643
H	-1.118755	-4.023834	2.212907
H	-0.551342	-3.375805	3.492053

$MgSO_4(H_2O)_{14}$

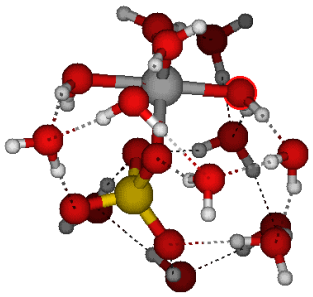

Figure S_{242} : $MgSO_4$ optimized structure with 14 water molecules.

E=-1381.172071

H=-1381.171127

O	1.273153	-2.711311	1.030052
Mg	1.477515	-0.712235	1.353602
O	1.636574	1.434428	1.398606
O	-0.375444	-0.573859	2.388339
S	-1.308462	0.005528	1.209428
O	-1.650099	1.500024	1.505051
O	2.927062	-0.613002	-0.081052
O	2.493237	-0.853268	3.115761
O	-2.571904	-0.892151	0.997085
O	-0.262324	-0.091329	-0.029031
O	1.067519	0.009272	5.086636
O	-0.898244	-1.933767	4.552315
O	2.625286	-1.995891	-2.245612
O	-0.271554	-4.051574	2.715948
O	0.168067	-2.517928	-1.398105
O	-2.136962	-3.600389	-1.777381
O	-2.511756	-3.609888	1.087495
O	0.082639	2.184270	3.500176
O	-3.378745	-1.187363	-1.775532
H	0.872650	-2.875102	0.140619
H	0.743983	-3.248824	1.687876
H	2.971236	-1.657451	3.337159
H	2.005463	-0.533906	3.945561

H	3.303055	0.248828	-0.281737
H	2.888847	-1.150501	-0.934843
H	-0.057686	3.095944	3.776295
H	-0.671056	1.947585	2.904886
H	-0.669866	-3.030677	-1.651600
H	-0.163357	-1.648363	-1.106597
H	1.673148	-2.250750	-2.131158
H	3.112070	-2.826724	-2.234806
H	0.360706	-0.664454	5.135458
H	0.649760	0.788098	4.671490
H	1.011253	1.709664	0.712838
H	1.271349	1.825269	2.226558
H	-3.309867	-1.006191	-0.824409
H	-2.825298	-0.479188	-2.165024
H	-2.330392	-3.840954	-0.854173
H	-2.660863	-2.770886	-1.916576
H	-3.402220	-3.845203	1.369080
H	-2.485194	-2.624836	1.090333
H	-0.920708	-1.414083	3.709463
H	-1.782476	-1.889347	4.930703
H	-1.102350	-4.060815	2.200662
H	-0.461220	-3.481357	3.482861
H	-2.100906	1.722343	-1.955963
O	-1.638273	0.935699	-2.263888
H	-1.054301	0.685703	-1.522958

$MgSO_4(H_2O)_{15}$

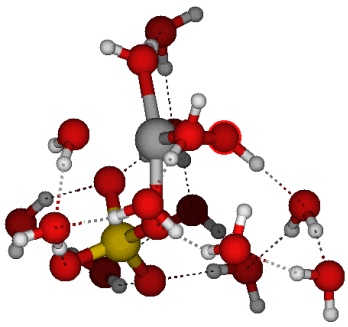

Figure S_{243} : $MgSO_4$ optimized structure with 15 water molecules.

E=-1457.548980

H=-1457.548036

O	1.102232	-2.684859	1.060022
Mg	1.424898	-0.705405	1.334424
O	2.307151	-0.683732	3.199974
O	1.756335	1.444662	1.047547
O	-0.377384	-0.308250	2.351749
S	-1.297026	0.069768	1.087260
O	-0.203618	-0.141831	-0.106418
O	3.041730	-0.813417	0.080118
O	-1.695109	1.583859	1.154162
O	-2.532316	-0.871792	0.946993
O	1.319923	1.106488	4.741243
O	2.777503	-2.292100	-2.018188
O	-1.221467	-3.831436	4.963741
O	-0.433259	-4.328691	2.363443
O	0.200731	-2.512647	-1.475924
O	-2.164822	-3.378818	-2.032482
O	-3.421763	-0.958579	-1.827106
O	0.119464	2.705946	2.801848
O	-2.642369	-3.593387	0.788467
O	-1.836162	1.361575	-1.929464
H	0.773685	-2.854693	0.144601
H	0.569388	-3.298347	1.655822
H	3.249689	-0.841584	3.311305

H	2.028693	0.088701	3.805603
H	3.411056	0.029536	-0.201552
H	3.018993	-1.422822	-0.728074
H	-0.026031	3.656352	2.850171
H	-0.653104	2.318646	2.312356
H	-0.653584	-2.951467	-1.797870
H	-0.092930	-1.628782	-1.183762
H	1.793134	-2.428618	-2.009055
H	3.155593	-3.173676	-1.932733
H	0.648889	0.497288	5.101256
H	0.823054	1.728726	4.170725
H	1.188353	1.564747	0.271737
H	1.336997	2.021123	1.729058
H	-3.366113	-0.891685	-0.861196
H	-2.945251	-0.153556	-2.112895
H	-2.414183	-3.682423	-1.141356
H	-2.649056	-2.521573	-2.124496
H	-3.549563	-3.772417	1.057399
H	-2.523687	-2.623580	0.898147
H	-0.959716	-2.895600	5.084877
H	-2.170726	-3.857146	5.116172
H	-1.257152	-4.246618	1.847985
H	-0.694000	-4.204219	3.301858
H	-2.188102	1.842761	-1.168142
H	-1.075875	0.895983	-1.543363
H	-0.543618	-0.972030	3.975385
O	-0.182582	-1.276140	4.838116
H	0.689710	-1.611002	4.580793

$MgSO_4(H_2O)_{16}$

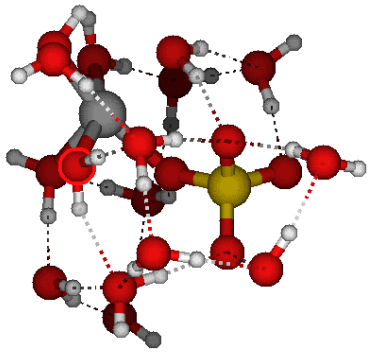

Figure S_{244} : $MgSO_4$ optimized structure with 16 water molecules.

E=-1533.938554

H=-1533.937610

O	0.952259	-2.712718	0.373659
Mg	1.642110	-1.252816	1.706131
O	3.404625	-1.405065	0.549925
O	2.813738	-0.363265	3.208484
O	-0.344192	-0.784419	2.160160
S	-1.439224	-0.089823	1.202511
O	-2.611897	-1.122293	0.990647
O	-0.739426	0.247853	-0.207167
O	-1.910484	1.235538	1.882323
O	1.679110	0.728944	0.796088
O	1.458537	1.124936	4.803909
O	3.017389	-2.057298	-1.990111
O	-0.526650	-4.315788	3.217818
O	0.308329	-1.700311	-1.947851
O	-1.865806	-3.064480	-2.212417
O	-0.275522	-1.054436	4.836156
O	0.380731	2.405192	2.599097
O	-1.793213	-3.620122	0.791926
O	-3.675741	-1.174772	-1.673146
O	-1.964391	-3.191692	5.211980
O	-2.583551	1.344153	-1.993077
H	0.744019	-2.396926	-0.553834

H	0.168990	-3.221816	0.632234
H	3.634019	0.079748	2.974099
H	2.342555	0.234359	3.885142
H	3.643036	-0.488338	0.360600
H	3.288868	-1.798035	-0.361016
H	0.313150	3.355730	2.462076
H	-0.516822	2.028032	2.382715
H	-0.497010	-2.253761	-2.214575
H	-0.084205	-0.916925	-1.516888
H	2.069368	-1.873397	-2.172549
H	3.153603	-2.970251	-2.262975
H	0.768998	0.486442	5.078764
H	1.014283	1.714028	4.159530
H	0.888474	0.712615	0.206299
H	1.424174	1.411171	1.455647
H	-3.496016	-1.103026	-0.719526
H	-3.390879	-0.295203	-2.001779
H	-1.841144	-3.459442	-1.327998
H	-2.584995	-2.376036	-2.138587
H	-2.577976	-4.178916	0.762756
H	-2.113735	-2.681201	0.920315
H	-1.462529	-2.348321	5.257369
H	-2.871330	-2.937853	5.013500
H	-1.026193	-4.136766	2.397539
H	-1.111131	-4.010293	3.956941
H	-3.150313	1.960684	-1.517591
H	-1.890401	1.097789	-1.349392
H	-0.582079	-0.809535	3.933883
H	0.457269	-1.655922	4.600192
O	1.411667	-2.693578	3.246405
H	0.669947	-3.411252	3.209601
H	2.211700	-3.095045	3.600863

$MgSO_4(H_2O)_{17}$

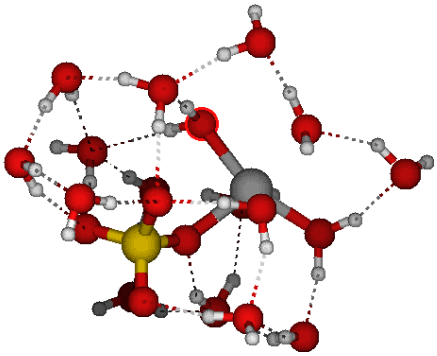

Figure S_{245} : $MgSO_4$ optimized structure with 17 water molecules.

E=-1610.320701

H=-1610.319756

O	0.929951	-2.738880	0.319981
Mg	1.581106	-1.278217	1.659661
O	1.352608	-2.760298	3.171655
O	3.314045	-1.205537	0.289572
O	2.855168	-0.498343	3.058860
O	-0.398023	-0.834135	2.130154
S	-1.520368	-0.124572	1.217100
O	-1.965435	1.193216	1.924233
O	-2.695202	-1.157467	1.022532
O	-0.862316	0.227888	-0.212968
O	1.558824	0.711975	0.709036
O	-0.609487	-4.350295	3.219672
O	1.629037	1.115727	4.706348
O	0.185230	-1.710754	-1.959814
O	-1.972358	-3.091101	-2.204781
O	-1.849654	-3.649833	0.777562
O	2.881422	-1.986856	-2.189228
O	0.371729	2.385769	2.547138
O	-3.790268	-1.223015	-1.630169
O	-0.196357	-1.034689	4.815841
O	-1.965866	-3.108368	5.198341
O	-2.741890	1.309759	-1.969562

H	0.683472	-2.413734	-0.596406
H	0.159157	-3.254940	0.602034
H	3.786145	-0.287614	2.824735
H	2.504832	0.160607	3.729827
H	3.159114	-0.258991	0.117716
H	3.218276	-1.628800	-0.613932
H	0.296629	3.335964	2.411875
H	-0.533096	2.008430	2.381094
H	-0.620254	-2.271715	-2.218075
H	-0.210429	-0.933511	-1.519318
H	1.917730	-1.829455	-2.312147
H	3.016571	-2.910067	-2.425985
H	0.944453	0.490241	5.013898
H	1.160608	1.702199	4.080879
H	0.726746	0.696953	0.173104
H	1.372990	1.410970	1.375499
H	-3.597868	-1.147598	-0.679264
H	-3.524920	-0.339111	-1.963741
H	-1.930683	-3.487309	-1.321127
H	-2.697711	-2.409975	-2.117997
H	-2.631107	-4.214151	0.760114
H	-2.177560	-2.716039	0.920428
H	-1.418660	-2.293113	5.243611
H	-2.855812	-2.804318	4.993103
H	-1.103357	-4.167082	2.397043
H	-1.172940	-3.995186	3.953728
H	-3.309224	1.922381	-1.489765
H	-2.038332	1.072721	-1.333821
H	-0.538354	-0.776704	3.931868
H	0.501590	-1.660224	4.540297
H	0.603184	-3.470019	3.173494
H	2.145538	-3.139483	3.562993
H	4.914580	-0.840083	1.237419
O	5.330626	-0.357412	1.976185

H 5.954648 -0.972626 2.374391

$MgSO_4(H_2O)_{18}$

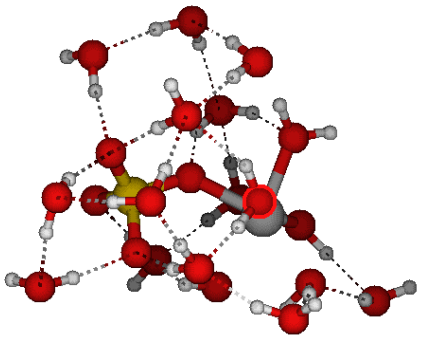

Figure S_{246} : $MgSO_4$ optimized structure with 18 water molecules.

E=-1686.708945

H=-1686.708001

O 1.072701 -2.725402 0.273613
Mg 1.682255 -1.272882 1.640690
O -0.327193 -0.900409 2.108935
S -1.469306 -0.217009 1.217306
O -0.859733 0.180728 -0.210561
O 1.491721 -2.765929 3.121950
O 2.929738 -0.440752 3.028829
O -1.992706 1.053777 1.957071
O -2.617009 -1.298297 1.009630
O 1.566145 0.730503 0.712537
O 3.399522 -1.117222 0.261209
O -0.408922 -4.394013 3.143828
O 0.274023 -1.711952 -1.994468
O -1.818766 -3.165380 -2.303548
O 1.671796 1.093116 4.721475
O 2.981987 -1.873490 -2.227445
O -1.674773 -3.793053 0.622010
O -3.702360 -1.371333 -1.670700
O 0.321684 2.344115 2.581118
O -0.070961 -1.090557 4.831449
O -1.978072 -3.203955 4.885102

O	5.400352	-0.224175	1.945706
O	-2.780737	1.217764	-1.952040
H	0.800010	-2.403642	-0.636231
H	0.343861	-3.298742	0.553894
H	3.854927	-0.203228	2.799357
H	2.564675	0.191082	3.718637
H	3.227083	-0.172254	0.102511
H	3.312903	-1.529523	-0.648308
H	0.214230	3.293093	2.459292
H	-0.571414	1.942428	2.430027
H	-0.509769	-2.300495	-2.266835
H	-0.150775	-0.948550	-1.561213
H	2.012350	-1.758181	-2.347628
H	3.160332	-2.784141	-2.483458
H	1.016723	0.426817	5.014492
H	1.173369	1.673199	4.115671
H	0.741509	0.700316	0.171379
H	1.356877	1.410445	1.390836
H	-3.507751	-1.311470	-0.720514
H	-3.481942	-0.468477	-1.984687
H	-1.779560	-3.602770	-1.438405
H	-2.569241	-2.516990	-2.201580
H	-2.427101	-4.391902	0.698086
H	-2.027498	-2.883277	0.803231
H	-1.418322	-2.448934	5.142156
H	-2.728882	-2.796217	4.398783
H	-0.876833	-4.284077	2.297386
H	-1.037540	-4.023592	3.837548
H	-3.378929	1.808256	-1.482293
H	-2.078489	1.005708	-1.307305
H	-0.449186	-0.847117	3.962780
H	0.613429	-1.722172	4.539444
H	0.744801	-3.494163	3.115330
H	2.287514	-3.134738	3.517061

H	4.999022	-0.722453	1.209540
H	6.048059	-0.814683	2.343300
H	-3.514257	-1.624797	2.551617
O	-3.920768	-1.952931	3.377645
H	-4.325326	-1.179876	3.783437

$MgSO_4(H_2O)_{19}$

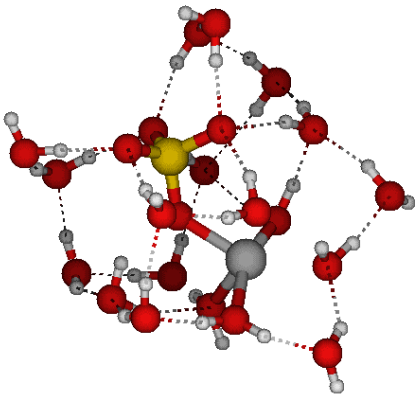

Figure S_{247} : $MgSO_4$ optimized structure with 19 water molecules.

E=-1763.093004

H=-1763.092059

O	1.063336	-2.719094	0.264556
Mg	1.700200	-1.272357	1.621658
O	2.941294	-0.429339	3.006285
O	-0.319523	-0.828122	2.060671
S	-1.431343	-0.187599	1.112418
O	-2.585162	-1.252730	0.905292
O	1.468547	-2.733957	3.112353
O	-0.789371	0.191686	-0.301688
O	-1.961844	1.129016	1.796173
O	3.442883	-1.191016	0.268734
O	1.638228	0.707194	0.646914
O	-0.425710	-4.347594	3.145024
O	1.688267	1.135251	4.665280
O	0.335851	-1.760067	-2.051473
O	-1.774815	-3.189974	-2.354244
O	-1.972052	-3.174451	4.875700

O	3.049197	-1.987422	-2.213561
O	-3.648880	-1.359429	-1.784993
O	-1.675728	-3.778310	0.583791
O	5.435157	-0.287540	1.963478
O	0.392478	2.376273	2.466873
O	-0.059944	-1.032601	4.817186
O	-3.857722	-1.890582	3.423578
O	-2.637964	1.187392	-2.142161
H	0.816958	-2.417772	-0.659162
H	0.330393	-3.289938	0.539076
H	3.874988	-0.215265	2.789489
H	2.578349	0.215526	3.686202
H	3.301576	-0.245857	0.084676
H	3.359899	-1.621497	-0.632174
H	0.314368	3.327505	2.339846
H	-0.505683	2.000028	2.301682
H	-0.454662	-2.342394	-2.317854
H	-0.078998	-0.973111	-1.654753
H	2.085623	-1.856436	-2.359735
H	3.218441	-2.903843	-2.454633
H	1.029811	0.475078	4.967070
H	1.196890	1.706532	4.046791
H	0.823112	0.684661	0.093018
H	1.432639	1.402335	1.310351
H	-3.466864	-1.282865	-0.833828
H	-3.400497	-0.470910	-2.117844
H	-1.756838	-3.620030	-1.484845
H	-2.521184	-2.534457	-2.275131
H	-2.430767	-4.371491	0.675968
H	-2.021027	-2.863410	0.741437
H	-1.421222	-2.430144	5.173602
H	-2.723854	-2.742642	4.396322
H	-0.891964	-4.251857	2.297136
H	-1.056203	-3.965583	3.840964

H	-3.219713	1.848099	-1.752804
H	-1.969526	0.998125	-1.456267
H	-0.492114	-0.783634	3.979591
H	0.601445	-1.668872	4.483146
H	0.713426	-3.464155	3.111034
H	2.254812	-3.092425	3.535303
H	5.042237	-0.806102	1.237348
H	6.070418	-0.869912	2.391965
H	-3.489295	-1.749122	2.536982
H	-4.010483	-0.972631	3.732965
H	-3.284107	0.980429	3.051354
O	-3.958304	0.846078	3.745543
H	-4.775780	1.185341	3.367089

$MgSO_4(H_2O)_{20}$

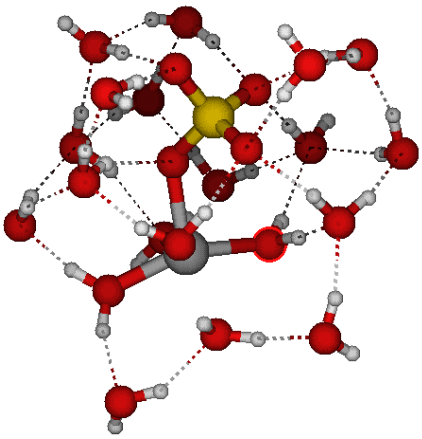

Figure S_{248} : $MgSO_4$ optimized structure with 20 water molecules.

E=-1839.478676

H=-1839.477732

O	0.972921	-2.544843	0.226803
Mg	1.585249	-1.121016	1.581198
O	1.207873	-2.485024	3.087293
O	2.824981	-0.377854	3.022688
O	-0.434873	-0.466655	2.014680
S	-1.582841	-0.152273	0.949923

O	-2.472790	1.025210	1.512376
O	-2.488206	-1.437495	0.751617
O	-0.919970	0.313722	-0.423833
O	1.587945	0.828118	0.585305
O	3.395922	-1.088344	0.296359
O	-0.370279	-4.430543	3.108038
O	-2.037214	-3.345261	4.806745
O	1.712176	0.922058	4.983838
O	0.311297	-1.644616	-2.119447
O	-1.663630	-3.244370	-2.482720
O	3.039809	-1.857114	-2.206411
O	-3.693694	-1.620492	-1.860271
O	-1.533925	-3.924622	0.464820
O	-3.862137	-1.958536	3.309046
O	5.362872	-0.394982	2.111841
O	0.563948	2.113951	2.720459
O	-2.760173	0.485105	4.155849
O	-3.035969	1.056945	-2.139765
O	-0.445139	-0.892407	5.000663
H	0.740466	-2.263666	-0.708304
H	0.343171	-3.243223	0.458075
H	3.783076	-0.227274	2.862307
H	2.506574	0.136350	3.824691
H	3.287100	-0.141716	0.100712
H	3.324070	-1.519409	-0.603523
H	-0.063276	2.821298	2.430172
H	0.016090	1.307912	2.727725
H	-0.436723	-2.274153	-2.401359
H	-0.144275	-0.861974	-1.760837
H	2.080145	-1.729022	-2.372778
H	3.226093	-2.761480	-2.477936
H	0.952010	0.340317	5.199097
H	1.333948	1.633502	4.436424
H	0.770140	0.843865	0.044363

H	1.406580	1.470380	1.318902
H	-3.488371	-1.536152	-0.914365
H	-3.556710	-0.705145	-2.184098
H	-1.613204	-3.714442	-1.636132
H	-2.470389	-2.666940	-2.384687
H	-2.283340	-4.528718	0.521867
H	-1.892785	-3.013410	0.611810
H	-1.536195	-2.595744	5.171917
H	-2.761585	-2.923765	4.285418
H	-0.820799	-4.398029	2.247936
H	-1.046368	-4.112812	3.783639
H	-3.689586	1.508902	-1.595154
H	-2.267083	0.934792	-1.551642
H	-1.219271	-0.373225	4.699290
H	-0.086530	-1.304624	4.195340
H	0.609532	-3.331862	3.096206
H	1.919632	-2.582976	3.727535
H	4.956244	-0.832377	1.340309
H	5.908307	-1.064755	2.536612
H	-3.504426	-1.816477	2.417086
H	-3.741492	-1.091700	3.736043
H	-2.691265	0.783218	3.218505
H	-3.146122	1.211870	4.654979
H	-1.886258	2.731832	1.444200
O	-1.436058	3.570786	1.673600
H	-1.251501	4.009260	0.836873

$MgSO_4(H_2O)_{21}$

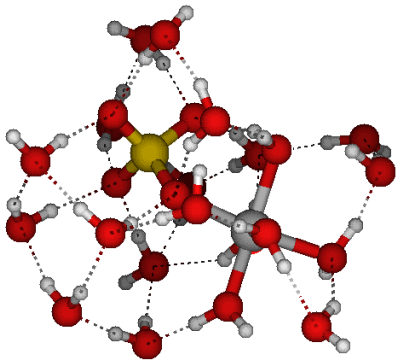

Figure S_{249} : $MgSO_4$ optimized structure with 21 water molecules.

E=-1915.874237

H=-1915.873293

O	1.120259	-2.503549	0.157858
Mg	1.765206	-1.201999	1.675914
O	-0.245579	-0.526592	2.155751
S	-1.460937	-0.254263	1.140087
O	-0.873291	0.206572	-0.265702
O	1.788378	-2.815043	2.902174
O	2.749985	-0.107019	3.101035
O	-2.333293	0.928828	1.708242
O	-2.344785	-1.557989	1.006316
O	1.748571	0.591420	0.481220
O	4.054386	-0.106135	-0.983099
O	-0.146300	-4.375963	3.373605
O	0.220758	-1.625085	-2.119651
O	-1.658719	-3.367904	-2.328577
O	1.520433	1.268075	4.955448
O	-1.759650	-3.042363	4.966839
O	2.641871	-0.860036	-3.164686
O	-3.687094	-1.793179	-1.556413
O	-1.278469	-4.005653	0.600615
O	0.768867	2.231219	2.400661
O	-1.311015	3.453127	1.195314
O	4.487551	-2.187124	3.426207

O	-3.313080	0.598055	4.217198
O	-3.846192	-2.068053	3.458865
O	-3.094141	0.900349	-1.869511
O	-0.781392	-0.315005	4.922083
H	0.820340	-2.202966	-0.752132
H	0.549028	-3.250390	0.396423
H	3.470274	-0.650182	3.475337
H	2.323050	0.395948	3.856644
H	3.394417	0.503872	-0.611127
H	3.637636	-0.410375	-1.827205
H	0.117304	2.856655	1.998667
H	0.240361	1.436059	2.577411
H	-0.486808	-2.316214	-2.352256
H	-0.277819	-0.900843	-1.701279
H	1.735124	-1.140741	-2.916314
H	2.960438	-1.516931	-3.790002
H	0.687428	0.781666	5.134158
H	1.273854	1.994774	4.360135
H	0.889323	0.587325	0.007579
H	1.635907	1.321944	1.144302
H	-3.431817	-1.709862	-0.623506
H	-3.585675	-0.875058	-1.883883
H	-1.516610	-3.818740	-1.481571
H	-2.478031	-2.825242	-2.172174
H	-1.971984	-4.664925	0.718573
H	-1.685793	-3.126224	0.787927
H	-1.341963	-2.194308	5.197408
H	-2.572201	-2.783045	4.475062
H	-0.590574	-4.377231	2.512879
H	-0.774055	-3.917364	4.008357
H	-3.739095	1.349984	-1.312908
H	-2.304413	0.797795	-1.306489
H	-1.662084	0.110810	4.922547
H	-0.631547	-0.517748	3.979547

H	1.047168	-3.470172	3.155499
H	2.570998	-2.949668	3.453403
H	4.517328	-2.135343	2.447979
H	5.393712	-2.250825	3.741240
H	-3.438865	-1.903616	2.592757
H	-3.935787	-1.177799	3.841470
H	-3.036149	0.797050	3.293937
H	-3.866500	1.329326	4.508740
H	-1.778473	2.594346	1.231645
H	-1.166139	3.629820	0.259950
O	3.681146	-1.811155	0.861079
H	3.945295	-1.163135	0.105436
H	3.392779	-2.619965	0.415975

$MgSO_4(H_2O)_{22}$

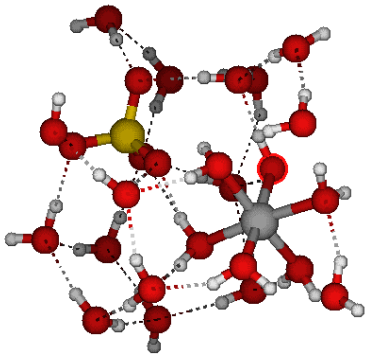

Figure S_{250} : $MgSO_4$ optimized structure with 22 water molecules.

E=-1992.257901

H=-1992.256957

O	1.258950	-2.369296	0.198659
Mg	2.249166	-1.552291	1.840643
O	4.070564	-2.022827	0.846040
O	-0.626593	0.131001	1.067295
S	-2.112659	0.183573	0.482987
O	-2.777976	-1.249225	0.752390
O	2.420711	-3.446550	2.660863
O	3.277455	-0.546230	3.346830

O	2.036535	0.369795	0.835758
O	-2.002692	0.485657	-1.053479
O	-2.919739	1.310160	1.243712
O	0.027259	-4.214081	3.368943
O	4.212881	-0.184828	-0.875148
O	0.177592	-1.102029	-1.872715
O	-1.364113	-3.154718	-2.289984
O	1.206284	0.614561	4.653255
O	-1.575904	-2.557566	4.983726
O	-3.831184	-2.338215	-1.687027
O	-1.255771	-3.504308	0.763493
O	2.610073	-0.596290	-2.984126
O	0.648491	2.098039	2.413352
O	-1.303144	3.659225	1.314075
O	-3.199352	0.958128	3.923414
O	5.040567	-2.582588	3.369490
O	-3.537072	-1.734370	3.441366
O	-4.244083	0.194230	-2.654928
O	-1.130747	0.111160	5.763828
H	0.887433	-1.830312	-0.555628
H	0.544515	-2.992146	0.417418
H	3.993523	-1.090534	3.724818
H	2.719442	-0.156034	4.054836
H	3.597129	0.391913	-0.391603
H	3.717359	-0.390530	-1.710788
H	0.200488	2.924539	2.131153
H	0.012753	1.434923	2.067160
H	-0.399520	-1.874073	-2.175493
H	-0.473814	-0.405699	-1.643365
H	1.682896	-0.735476	-2.682042
H	2.770605	-1.267514	-3.653318
H	0.394763	0.503965	5.225899
H	1.022563	1.369279	4.054942
H	1.159245	0.301460	0.408591

H	1.890155	1.138294	1.436524
H	-3.621558	-1.952201	-0.818232
H	-4.102354	-1.548613	-2.205113
H	-1.202756	-3.582898	-1.437931
H	-2.312050	-2.851551	-2.206327
H	-1.924285	-4.197967	0.732765
H	-1.753067	-2.646352	0.769459
H	-2.002196	-3.105054	5.652114
H	-2.310007	-2.306962	4.345884
H	-0.410008	-4.007037	2.525532
H	-0.390544	-3.580495	3.991700
H	-4.998493	0.606031	-2.221337
H	-3.473275	0.440963	-2.105062
H	-1.800297	0.523597	5.188805
H	-1.235938	-0.849792	5.604037
H	1.557150	-3.789640	3.051143
H	3.152666	-3.599812	3.272370
H	5.002162	-2.416863	2.404588
H	5.968972	-2.684326	3.599308
H	-3.334970	-1.633727	2.491281
H	-3.633658	-0.807879	3.739929
H	-3.057279	1.116976	2.957671
H	-3.887995	1.574882	4.191665
H	-1.927451	2.909134	1.243571
H	-1.190522	3.965010	0.408286
H	4.231512	-1.318234	0.101855
H	3.844986	-2.844343	0.390230
H	0.663753	-0.635472	3.626223
O	0.512165	-1.283648	2.891987
H	-0.156885	-0.870476	2.298592

$MgSO_4(H_2O)_{23}$

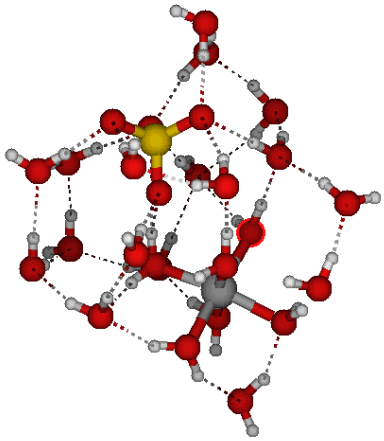

Figure S_{251} : $MgSO_4$ optimized structure with 23 water molecules.

E=-2068.644680

H=-2068.643736

O	1.203199	-2.322702	0.187825
Mg	2.176202	-1.413494	1.772522
O	0.503478	-1.315943	2.942338
O	4.012201	-1.852119	0.773279
O	2.465101	-3.345889	2.556515
O	3.217192	-0.463749	3.339760
O	2.074367	0.557956	0.914486
O	4.141117	-0.003342	-0.925943
O	-0.900174	0.159910	1.424494
S	-2.262136	0.097775	0.632961
O	-3.228313	1.210052	1.217983
O	-2.888181	-1.361920	0.797956
O	-1.972756	0.388853	-0.902973
O	0.112574	-4.253925	3.332852
O	0.015307	-1.298734	-1.911594
O	-1.520132	-3.368971	-2.242168
O	-3.948403	-2.386185	-1.675772
O	2.453317	-0.568546	-2.948556
O	1.128408	0.493111	4.831619
O	-1.276826	-0.044913	5.811586

O	5.064624	-2.414598	3.231327
O	0.550234	2.105520	2.691773
O	-3.394823	0.819039	3.940371
O	-1.300005	-3.600317	0.775987
O	-1.405810	3.392896	1.103534
O	-4.215350	0.216680	-2.537649
O	-3.600112	-1.905136	3.476465
O	-1.596077	-2.702362	4.977378
H	0.788207	-1.858245	-0.597269
H	0.558952	-3.005741	0.430910
H	3.972683	-1.008221	3.636866
H	2.673037	-0.189071	4.106724
H	3.577759	0.581838	-0.389633
H	3.581500	-0.215690	-1.717509
H	0.152230	2.965677	2.495119
H	-0.074857	1.483578	2.261090
H	-0.536955	-2.095397	-2.193684
H	-0.655364	-0.651076	-1.611602
H	1.533600	-0.769448	-2.667056
H	2.672478	-1.231647	-3.609040
H	0.297402	0.350119	5.363409
H	0.940981	1.267890	4.262058
H	1.385962	0.926786	0.281765
H	2.014127	1.202588	1.643855
H	-3.737391	-2.041245	-0.790917
H	-4.154413	-1.565021	-2.172609
H	-1.358026	-3.734329	-1.360244
H	-2.453131	-3.025024	-2.172644
H	-1.954975	-4.303341	0.854999
H	-1.809761	-2.753293	0.804610
H	-1.988890	-3.286828	5.634891
H	-2.346725	-2.468013	4.353998
H	-0.348541	-4.053926	2.501147
H	-0.319501	-3.643906	3.966918

H	-4.955774	0.616233	-2.069456
H	-3.434569	0.417640	-1.984292
H	-1.925234	0.371279	5.218168
H	-1.355800	-1.004232	5.626090
H	1.635242	-3.728545	2.969831
H	3.217614	-3.476557	3.148028
H	4.973973	-2.237856	2.269815
H	6.006068	-2.459684	3.422524
H	-3.409843	-1.800934	2.524214
H	-3.707501	-0.978926	3.772981
H	-3.311026	1.015510	2.976079
H	-4.149366	1.331652	4.247634
H	-2.111320	2.710998	1.140204
H	-1.789383	4.136003	0.627106
H	4.165458	-1.140305	0.031933
H	3.785230	-2.674716	0.320072
H	0.645328	-0.719811	3.719540
H	-0.238133	-0.917200	2.430549
H	-0.368139	1.408615	-0.911162
O	0.401906	1.931828	-0.623865
H	-0.018020	2.560660	-0.007955

$MgSO_4(H_2O)_{24}$

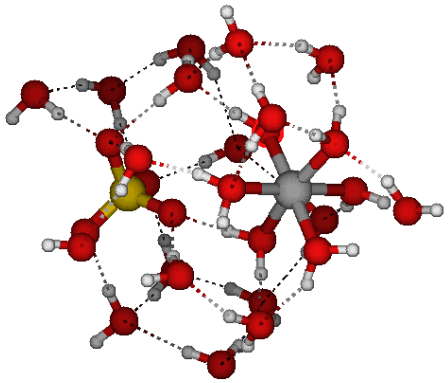

Figure S_{252} : $MgSO_4$ optimized structure with 24 water molecules.

E=-2145.036932

H=-2145.035988

O	1.218246	-2.396882	0.297149
Mg	2.276918	-1.413671	1.836436
O	2.057875	0.556494	0.966016
O	0.572131	-1.313478	2.979473
O	4.146765	-1.690407	0.891912
O	2.546038	-3.313123	2.655732
O	3.265053	-0.420884	3.417044
O	4.320896	0.394876	-0.681889
O	-0.880510	0.071797	1.398131
S	-2.235365	0.027620	0.594507
O	-1.916145	0.286814	-0.943455
O	-3.183514	1.171599	1.146370
O	-2.898346	-1.414241	0.772485
O	0.147153	-1.378862	-1.853986
O	-1.374644	-3.438416	-2.166727
O	0.190715	-4.239610	3.490382
O	0.423117	1.852865	-0.695934
O	-3.831467	-2.490288	-1.730407
O	5.101713	-2.389268	3.315612
O	1.107586	0.520494	4.860117
O	-1.311288	0.005655	5.823229
O	2.749214	-1.071796	-2.574431

O	0.481163	2.068965	2.678387
O	-1.260001	-3.607629	0.863480
O	-4.085280	0.085537	-2.666821
O	-3.395344	0.822605	3.877647
O	-3.583739	-1.912290	3.479281
O	-1.596352	-2.664802	5.033146
O	-1.371757	3.351829	1.001288
H	0.803636	-1.921378	-0.484673
H	0.521885	-3.000555	0.610597
H	4.018328	-0.963137	3.724716
H	2.711377	-0.152083	4.176847
H	3.621613	0.822732	-0.156039
H	3.835441	0.015079	-1.440547
H	0.088930	2.913740	2.410651
H	-0.130130	1.417842	2.270921
H	-0.406685	-2.185901	-2.123472
H	-0.527130	-0.715873	-1.598568
H	1.773492	-1.073014	-2.422163
H	2.870147	-0.960553	-3.522767
H	0.272194	0.383868	5.386217
H	0.919380	1.287633	4.282825
H	1.391227	0.874512	0.288768
H	1.896866	1.197721	1.686912
H	-3.667025	-2.126184	-0.843255
H	-4.027824	-1.682774	-2.253038
H	-1.250672	-3.800905	-1.277332
H	-2.315678	-3.105696	-2.142956
H	-1.871167	-4.343187	0.982633
H	-1.811899	-2.786207	0.858461
H	-1.998011	-3.238475	5.694806
H	-2.333509	-2.453597	4.387661
H	-0.262213	-4.060822	2.651787
H	-0.256569	-3.618922	4.101998
H	-4.851890	0.490658	-2.248198

H	-3.335872	0.299800	-2.076340
H	-1.945945	0.408697	5.206886
H	-1.384961	-0.957344	5.655305
H	1.743484	-3.696140	3.106924
H	3.341830	-3.458211	3.186023
H	5.022766	-2.184678	2.354116
H	6.037468	-2.502276	3.505775
H	-3.404057	-1.832007	2.523489
H	-3.692693	-0.979031	3.752500
H	-3.298395	1.002352	2.911905
H	-4.160845	1.331609	4.163186
H	-2.077064	2.668855	1.035157
H	-1.769067	4.117785	0.575287
H	4.389715	-0.880734	0.346932
H	4.048907	-2.408801	0.196063
H	0.685300	-0.703464	3.751992
H	-0.182384	-0.958045	2.460112
H	-0.360997	1.328376	-0.943420
H	0.021140	2.523502	-0.113640
O	3.519239	-3.330911	-1.060846
H	2.636273	-3.413170	-0.661338
H	3.373997	-2.658451	-1.756155

$MgSO_4(H_2O)_{25}$

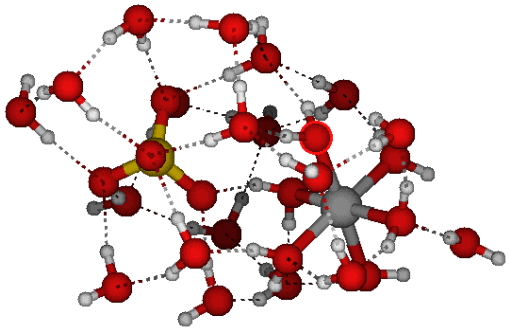

Figure S_{253} : $MgSO_4$ optimized structure with 25 water molecules.

E=-2221.421254

H=-2221.420310

O	1.271103	-2.416130	0.309531
Mg	2.326928	-1.429578	1.848100
O	3.312856	-0.431844	3.427209
O	2.099138	0.544063	0.988385
O	0.618448	-1.324440	2.982740
O	4.197825	-1.700204	0.906868
O	2.597213	-3.324401	2.673116
O	-0.913739	0.100435	1.499633
S	-2.204249	-0.013898	0.611126
O	-2.845660	-1.463354	0.788884
O	-1.833118	0.243536	-0.906390
O	-3.223793	1.107008	1.116579
O	0.221388	-1.414434	-1.853533
O	-1.313042	-3.448757	-2.199718
O	4.363668	0.382749	-0.668705
O	3.585826	-3.349560	-1.041882
O	0.246618	-4.256369	3.510450
O	0.454494	1.844163	-0.637500
O	-3.754834	-2.518496	-1.742839
O	1.157490	0.507877	4.864157
O	-1.254368	-0.010435	5.839670
O	5.152153	-2.396118	3.332143

O	2.821239	-1.099228	-2.569194
O	0.529520	2.095257	2.703460
O	-1.189910	-3.662164	0.872372
O	-4.128234	0.002599	-2.652558
O	-3.348977	0.804883	3.889428
O	-3.529108	-1.939032	3.503271
O	-1.538575	-2.685642	5.066556
O	-1.394887	3.335032	1.005337
H	0.863716	-1.955184	-0.485516
H	0.581541	-3.031074	0.616125
H	4.068427	-0.971348	3.734548
H	2.759881	-0.163052	4.187552
H	3.659321	0.808134	-0.148051
H	3.886636	-0.000174	-1.431172
H	0.151570	2.954291	2.468138
H	-0.103835	1.466544	2.297808
H	-0.340552	-2.216100	-2.131717
H	-0.447749	-0.749461	-1.594196
H	1.844538	-1.105148	-2.423699
H	2.949130	-0.995301	-3.517503
H	0.325749	0.369307	5.395427
H	0.969267	1.281137	4.295404
H	1.428670	0.881424	0.322198
H	1.966456	1.183949	1.714265
H	-3.581328	-2.167890	-0.853431
H	-3.975389	-1.696159	-2.247368
H	-1.190515	-3.844691	-1.325481
H	-2.256836	-3.114257	-2.166500
H	-1.788949	-4.411569	0.962824
H	-1.755102	-2.852481	0.866918
H	-1.930037	-3.260583	5.733223
H	-2.280586	-2.481641	4.426180
H	-0.210824	-4.087414	2.672137
H	-0.201524	-3.635871	4.121170

H	-4.780187	0.349082	-2.008303
H	-3.282346	0.247252	-2.244959
H	-1.885626	0.387742	5.217310
H	-1.326312	-0.974703	5.678280
H	1.795745	-3.710190	3.124018
H	3.393949	-3.468163	3.202426
H	5.076388	-2.192635	2.370324
H	6.087177	-2.509652	3.525724
H	-3.323614	-1.865845	2.552350
H	-3.635813	-1.004484	3.771819
H	-3.264123	0.988335	2.926149
H	-4.094031	1.333086	4.194016
H	-2.097753	2.653567	1.030888
H	-1.776917	4.080282	0.530443
H	4.437847	-0.890231	0.360898
H	4.105961	-2.420941	0.212622
H	0.735136	-0.714981	3.755377
H	-0.139624	-0.965814	2.472049
H	-0.321554	1.309146	-0.889220
H	0.040035	2.511172	-0.059795
H	2.701624	-3.435791	-0.646638
H	3.441485	-2.680124	-1.740472
H	-4.798018	0.962926	0.158071
O	-5.582062	0.812766	-0.404443
H	-5.961418	-0.009284	-0.075864