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Tight-binding electronic structure of high $T_c$ superconductors

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Résumé. — Les nouveaux oxydes supraconducteurs ont des similarités importantes au niveau de leur structure cristallographique. Ce sont des perovskites, ou des composés de structure dérivée qui ont en commun une nature alternée : les premiers voisins des atomes d’oxygène sont des atomes métalliques et réciproquement. Nous montrons que cette particularité structurale a des conséquences très importantes sur la structure électronique. Dans ce but, nous présentons d’abord un formalisme général permettant de décrire simplement la structure électronique proche du niveau de Fermi, dès que l’on a un réseau alterné. Dans la seconde partie, nous illustrons la méthode pour différents oxydes en lien avec les supraconducteurs à haute température critique à base de cuivre ou de bismuth. Enfin, nous montrons les résultats obtenus par la méthode du réseau alterné pour le modèle à deux bandes du plan CuO$_2$, entité de base des nouveaux supraconducteurs à base de cuivre.

Abstract. — New superconducting oxides have important crystallographic similarities. They are bulk perovskites or structure derived compounds such as the K$_2$NiF$_4$ one, with an alternating nature: the oxygen atoms nearest-neighbours are metallic atoms and vice-versa. We show that this structural property has important consequences on the electronic structure. We first present a general formalism allowing us to describe in a simple way the electronic structure as soon as one has an alternating lattice. In a second part, we illustrate this method for different oxides related with the high $T_c$ superconductors. Lastly, we show the results we obtain with the alternating lattice method in the two-band model of the CuO$_2$ plane which is characteristic of the copper-based new superconductors.

1. Introduction.

Since the discovery of the high $T_c$ superconductivity by Bednorz and Müller in BaLaCuO systems [1], and in other copper compounds [2] and more recently in the copper free (BaK)BiO$_3$ alloys [3], a lot of attention has been focused on the possible origins of superconductivity. All these compounds have in common typical phase diagrams: the insulating oxide becomes superconducting when it is doped. In copper based systems, the pure compound is antiferromagnetic and in BaBiO$_3$ there is a charge density wave. Many

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mechanisms have been invoked [4], but the understanding of their electronic structure is crucial.

These materials have a peculiar crystal structure: perovskite, $\text{K}_2\text{NiF}_4$ type or derived one, in which oxygen-octahedron with a metallic atom at the centre play an important role. By eliminating one or two oxygen atoms, the octahedron is reduced to a pyramid or a square respectively. In all cases these compounds present a crystal structure having an alternating nature: one kind of atom, like bismuth (oxygen) in $\text{BaBiO}_3$ has first nearest neighbours of the other kind, i.e. oxygen (bismuth) (Fig. 1). This alternating nature of the crystal structure will have important consequences on the electronic structure.

![Fig. 1. — Figure showing the alternating nature of the A-B lattice in the perovskite structure. For example in $\text{BaBiO}_3$: A = Bi, B = O, and in $\text{SrTiO}_3$: A = Ti, B = O.](image)

The aim of this paper is to discuss the electronic structure of many perovskite type compounds. Although the effect of the correlations is considered by many people to be important, we do not discuss it here specifically. We just point out that, if the interaction parameter $U$ between electrons is not too important as compared with the bandwidth $W$, the one-electron band structure gives a good starting point to the study of electronic properties. We shall show that in these materials the main features of the electronic structure near the Fermi level involve a small number of orbitals of metal and oxygen atoms and then can be described in a simple way due to their crystal alternating nature. Particularly, the shape of the local densities of states can be analysed in a simple way, and it is possible to scale the difference of the atomic energy levels of the pure elements and thus to study the effects of the covalency. Our results will confirm some of the analysis of Friedel who stressed the importance of the shape of the density of states near the Fermi level. More precisely, he points out that the quasi-two dimensional character of these layered structures leads to a strong density of states near the Fermi level which favors superconductivity [5].

In the first section, we present the formalism of the method. We show that the real tight-binding Hamiltonian can be transformed into an effective Hamiltonian acting in a reduced lattice retaining only one kind of orbitals. The density of states (DOS) can be deduced through a «universal» DOS calculated on this effective lattice. We apply this procedure to various cases. We first describe the results obtained for cubic perovskites involving s-orbitals ($\text{BaBiO}_3$) or d-orbitals ($\text{SrTiO}_3$) on the reduced lattice and we notice that the alternating lattice method results are in good agreement with results obtained by ab initio band structure calculations involving more orbitals. Then we apply the formalism to the case of $\text{K}_2\text{NiF}_4$ structure involving d-orbitals on the reduced lattice: $\text{Sr}_2\text{VO}_4$ and $\text{La}_2\text{CuO}_4$. We compare both compounds and illustrate the difference of states contributing to the Fermi level (mainly
t_{2g} orbitals in Sr_2VO_4 and e_g orbitals in La_2CuO_4). Finally we show the results of the
alternating lattice method in the case of the simplified Cu_2O plane.

2. The alternating lattice method.

The electronic structure near the Fermi level for numerous compounds can be interpreted in a
very simple way due to the alternating nature of the perovskite or K_2NiF_4 lattice for which we
make the approximation that an A-atom (respectively a B-atom) is just coupled to B-atoms
(resp. A-atoms). For example A and B in La_2CuO_4 are respectively the copper and oxygen
atoms for which we take into account respectively the d and p orbitals. As we have already
exposed the principle of this method elsewhere [6, 8], we only present the outlines of it. Let us
recall that this method is valid if the states contributing to the Fermi level are mainly made
with the A-orbitals strongly hybridized with the B-orbitals. It is in fact well known from band
structure calculations that the other orbitals contributions (like Ba in BaBiO_3, La in
La_2CuO_4 and Sr in SrTiO_3 or SrVO_4) are far enough from the Fermi level and that we can
neglect them in the tight-binding Hamiltonian.

We start from a Hamiltonian $H$:

$$H = H_0 + H_c$$  \hspace{1cm} (1)

where $H_0$ is the on-site energy respectively $\epsilon_A (\epsilon_B)$ on a AB)-atom and $H_c$ is the hopping
energy which just couples, in a first nearest neighbours approximation, the A-orbitals to the
B-orbitals. We neglect the direct A-A or B-B coupling as it generally involves parameters
which are much smaller.

An eigenstate $|\Psi\rangle$ with energy $E$ obeys the Schroedinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$ \hspace{1cm} (2)

and can be decomposed in its components $|\Psi_A\rangle, |\Psi_B\rangle$ on the A- or B-sublattice

$$|\Psi\rangle = |\Psi_A\rangle + |\Psi_B\rangle.$$ \hspace{1cm} (3)

By projecting the two members of the Schroedinger equation on each sublattice, one obtains

$$H_c|\Psi_A\rangle = (E - \epsilon_B)|\Psi_B\rangle$$ \hspace{1cm} (4a)

$$H_c|\Psi_B\rangle = (E - \epsilon_A)|\Psi_A\rangle.$$ \hspace{1cm} (4b)

By multiplying by $H_c$ one of these equations and inserting the other one, we obtain two formal
Schroedinger equations

$$H_c^2|\Psi_A\rangle = (E - \epsilon_A)(E - \epsilon_B)|\Psi_A\rangle$$ \hspace{1cm} (5a)

$$H_c^2|\Psi_B\rangle = (E - \epsilon_A)(E - \epsilon_B)|\Psi_B\rangle$$ \hspace{1cm} (5b)

which can be written as

$$\tilde{H}|\Psi_\epsilon\rangle = \tilde{E}|\Psi_\epsilon\rangle$$ \hspace{1cm} (6a)

with

$$\epsilon = A \text{ or } B$$

$$\tilde{H} = H_c^2$$ \hspace{1cm} (6b)

and

$$\tilde{E} = (E - \epsilon_A)(E - \epsilon_B).$$ \hspace{1cm} (6c)
$\tilde{H}$ is an effective Hamiltonian, homogeneous to the square of an energy, which only couples one kind of orbitals together. Thus, the alternating lattice has been reduced to a lattice with only one kind of orbitals (A or B). One checks easily that $\tilde{H} = H_c^2$ has diagonal as well as off-diagonal elements in the basis of atomic orbitals. The calculations have been made on the metal (Cu, Ti, Bi or V) sublattice which is the easiest one to treat: a simple cubic lattice in the case of the cubic perovskites or square lattice in the case of the K$_2$NiF$_4$-structure.

The effective density of states $\tilde{N}$, associated with $\tilde{H}$, is calculated by recursion on the reduced lattice. $\tilde{N}$ does not depend on $\varepsilon_A$ and $\varepsilon_B$ but it just depends on the crystal structure and the kind of orbitals. Thus, $\tilde{N}$, in reduced units, is a universal density of states, characteristic of the structure and the involved orbitals. Some simple relations permit to obtain the total $N(E)$ and projected $N_\alpha(E)$ densities of states from the effective ones $\tilde{N}$ and $\tilde{N}_\alpha$, which are respectively the total density and the local density on an orbital $\alpha$ in the reduced lattice and for the Hamiltonian $\tilde{H}$:

\begin{align}
N(E) &= 2 |E - (\varepsilon_A + \varepsilon_B)/2| \tilde{N}(\tilde{E}) \quad (7) \\
N_A(E) &= |E - \varepsilon_B| \tilde{N}(\tilde{E}) \quad (8a) \\
N_B(E) &= |E - \varepsilon_A| \tilde{N}(\tilde{E}) . \quad (8b)
\end{align}

We note the following points. First, because $\tilde{H} = H_c^2$ is positive, the energy $\tilde{E}$ must be positive

$$(E - \varepsilon_A)(E - \varepsilon_B) > 0 .$$

Thus, one has a gap for $\tilde{E} < 0$ i.e. for $E$ between $\varepsilon_A$ and $\varepsilon_B$. Second, if the sublattices A and B contain $N_A$ and $N_B$ orbitals and if $N_A > N_B$ (resp. $N_A < N_B$), there is a delta contribution containing $|N_A - N_B|$ states in the total real density of states which occurs at the energy $\varepsilon_A$ (resp. $\varepsilon_B$). If one takes into account the direct interaction, this delta-pike gives rise to a narrow band which can partially or completely fill the gap. Finally, one has

$$N(E) \, dE = \tilde{N}(\tilde{E}) \, d\tilde{E} . \quad (9)$$

This relation is interesting to find the position of the Fermi level and its variation with doping. If there are $n$ electrons in the lowest non completely filled band, then one imagines that these $n$ electrons are put in the effective DOS $\tilde{N}(\tilde{E})$. This gives an effective Fermi level $\tilde{E}_f$ and the true Fermi level $\varepsilon_f$ is such that

$$(\varepsilon_f - \varepsilon_A)(\varepsilon_f - \varepsilon_B) = \tilde{E}_f . \quad (10)$$

3. Applications.

We now present applications of the method. We recall this important result: when two compounds have the same crystal structure, and the same types of orbitals, one obtains the same effective density of states (in reduced units) for each case. The particularity of the compound is just represented by the on-site levels, used to compute the real DOS from the effective one (Eqs. (7) and (8)) and of course, also by the filling of the band. The possibility of varying the on-site levels allows us to study easily the covalency which can change because of the doping. This second aspect has been already studied elsewhere [6] for La$_2$CuO$_4$ compound and will not be discussed here.
In this section, we show the differences of singularities for cubic perovskites when there are
s (case of BaBiO$_3$) or d (case of SrTiO$_3$) type of orbitals. Then, for the K$_2$NiF$_4$ structure and
in case of d-orbitals, we present the similarities of Sr$_2$VO$_4$ with La$_2$CuO$_4$.

### 3.1 Cubic perovskites.

**BaBiO$_3$.** — As a first example of application of the method discussed above, it is interesting
to study the case of BaBiO$_3$. Its interest is obvious: by substituting the Ba-atom by a K-atom
with concentration $x$, the alloy has been found to be superconducting with a $T_c$ around 30 K
for $x = 0.4$ [3]. *Ab initio* APW band structure calculations [7] show that the states near the
Fermi level are mainly due to the hybridization of the Bi-s orbitals with the O-p ones, with the
Slater Koster Parameter $sp\sigma$. Thus, in a first approach, these are the orbitals, we will retain
for the application of the alternating lattice method. In a forthcoming paper, we will show
how to take into account more orbitals. Because the Bi-atoms are located on a cubic site, the
reduced lattice is a simple cubic lattice on which the Bi-s are coupled by the effective
Hamiltonian $\hat{H}$. The effective density of states $\tilde{N}(\tilde{E})$ is the well-known simple cubic density
states (Fig. 2). The real density of states, projected on an s-Bi orbital is shown in figure 3a.
The insert is the exact result we obtained by an APW calculation [7] and shows the good
agreement. One has to point out that the local s-Bi DOS is a very small part of the total DOS
but is the main component at the Fermi level (Fig. 3b).

Experimentally, it is well known that the BaBiO$_3$ compound is semiconducting with a
charge density wave (CDW) leading to formal Bi$^{3+}$ and Bi$^{5+}$. The explanation of this CDW
involves the electron-phonon coupling and is outside the scope of this paper. Let us mention
that the condition for the occurrence of this CDW has been studied recently by Nunez
Regueiro et al. [8] in a simplified model taking into account the s orbitals of Bi and the p$\sigma$ of
oxygen.

![Fig. 2. — Density of states of the simple cubic lattice with s-orbitals.](image)

**SrTiO$_3$.** — Another compound having a perovskite structure is the semiconducting SrTiO$_3$
which becomes superconducting when it is doped. Its electronic structure has been already
studied but we present it to illustrate the difference due to the orbital symmetry: in this case,
the hybridizations are mainly between the Ti-d orbitals and the O-p orbitals involving the
parameter $pd\pi$ (for hybridization between Ti-$t_{2g}$ orbitals with O-p$\pi$ orbitals, i.e. orbitals
having their lobes perpendicular to the bond Ti-O) and the parameter $p\sigma$ (for the hybridization between Ti-$e_g$ orbitals with O-$p\sigma$ orbitals, i.e. orbitals having their lobes parallel to the bond Ti-O). In a cubic structure, the bonds are perpendicular and the sets of orbitals Ti-$t_{2g}$-O-$p\pi$ and Ti-$e_g$-O-$p\sigma$ are not coupled, and for each set it is possible to apply the alternating lattice method. Let us recall that the only role of the Sr atom is to provide electrons to the system and in our calculation, we neglect its bands since they are higher than the Fermi level.

Let us focus first on the $t_{2g}$-orbitals. Despite the cubic nature of the perovskite, a $t_{2g}$-orbital ($xy$, $yz$ or $zx$) is only coupled with its neighbouring $p\pi$-orbitals in a plane ($xy$, $yz$ or $zx$). Thus, the effective DOS $\bar{N}(\bar{E})$ (Fig. 4) is the square-lattice DOS with a characteristic two-
dimensional Van Hove singularity. Due to the degeneracy of \( t_{2g} \) orbitals in this symmetry, we obtain the same features for \( xy \), \( yz \) or \( zx \)-orbitals.

The \( e_g \) orbitals are also degenerated. Because a \( 3z^2 - r^2 \) orbital is coupled with \( p\sigma \) orbitals in three directions, the effective DOS (Fig. 4) \( \hat{N}(\hat{E}) \) presents three dimensional Van Hove singularities, analogous to those pictured in figure 2. However, because of the mixing of the \( x^2 - y^2 \) and \( 3z^2 - r^2 \) orbitals, this effective DOS is more complicated than the simple cubic DOS of figure 2.

In figure 5, we have reconstructed the real DOS of \( \text{SrTiO}_3 \), in good agreement with the exact APW result obtained by Mattheiss [9], shown in the insert. The peak just below \( E_F \) in the exact result can be interpreted as the delta peak of the non-bonding \( p \)-oxygen states (three \( p\pi \) states at \( \varepsilon_{p\pi} \) and one \( p\sigma \) state at \( \varepsilon_{p\sigma} \)), widened by direct oxygen-oxygen interaction.

The same method would apply to any other cubic perovskite involving transitional metal, such as \( \text{SrVO}_3 \), \( \text{LaNiO}_3 \)... The main differences would be the values of the levels and the position of the Fermi level. It is also possible with this method to study the axial distorsion of this cubic lattice leading for example to a tetragonal or orthorhombic lattice. The main effect is to split the two-dimensional Van Hove singularity peak in two or three peaks respectively, as one lifts the degeneracy of the \( t_{2g} \) and \( e_g \) orbitals.

Fig. 5. — Total density of states of \( \text{SrTiO}_3 \) obtained by the alternating lattice method. Insert: exact result obtained by APW-calculation (after Ref. [9]).

3.2 COMPOUNDS WITH \( \text{K}_2\text{NiF}_4 \) STRUCTURE. — In this section we present two cases: \( \text{Sr}_2\text{VO}_4 \) and the widely studied \( \text{La}_2\text{CuO}_4 \). \( \text{Sr}_2\text{VO}_4 \) is a new insulating compound studied in Grenoble [10]. For both compounds the orbitals taken into account are the \( d \)-orbitals of the transition metal (Vanadium or Copper) which are strongly hybridized with the \( p \)-orbitals of oxygen. As mentioned above, we neglect the La or Sr orbitals which are mainly above the Fermi level. In this tetragonal symmetry, there is also no mixing between the sets \( t_{2g} - \text{Op}\pi \) and \( e_g - \text{Op}\sigma \), as in the previous case but only \( yz \) and \( zx \)-orbitals are degenerated, all other degeneracies are lifted. In this structure, the reduced lattice of \( d \)-orbitals is a square plane. For both compounds, the parameters that we use are listed in table I and have been deduced from \textit{ab initio} calculations [11, 12].
Sr$_2$VO$_4$. — We have calculated the DOS of Sr$_2$VO$_4$ by taking the VO$_6$ octahedron distortion predicted by Pickett et al. [11] and experimentally observed by Lambert [10] (the distance V-O in plane is equal to 1.92 Å, as the distance V-O out of plane is 1.99 Å). For Sr$_2$VO$_4$ the states contributing near the Fermi level are mainly V-t$_{2g}$ orbitals hybridized with O$p\tau$ orbitals. The xy-orbital is coupled in the xy plane, via the effective Hamiltonian $\hat{H}$ with its four surrounding $xy$-orbitals. Thus the effective DOS is still the well-known square lattice DOS shown as in cubic perovskite of figure 4. The yz (or zx) orbital is just coupled along a chain with its two neighbouring yz (zx) orbitals in the direction y (x). Thus, one obtains the effective DOS which is that of a chain (Fig. 6) with one dimension singularities, the role of the out of plane oxygens is to give a contribution to the effective on-site energy of yz and zx orbitals. This explains the fact that the effective DOS yz (zx) is displaced towards higher energies than the effective DOS of $xy$. By adding all contributions (including also the $e_g$.O$p\sigma$ states) and coming back to the real density of states (Fig. 7) one obtains a good agreement in the region of the Fermi level with an APW result [11] pictured in the insert. We stress that the Fermi level is very close to a one dimension Van Hove singularity.

Table I. — Slater-Koster parameters used for the K$_2$NiF$_4$-type compounds.

<table>
<thead>
<tr>
<th></th>
<th>Sr$_2$VO$_4$</th>
<th>La$_2$CuO$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>t$_{2g}$ on-site</td>
<td>8.3</td>
<td>4.9</td>
</tr>
<tr>
<td>e$_g$ on-site</td>
<td>10.7</td>
<td>6.25</td>
</tr>
<tr>
<td>Oxygen p on-site</td>
<td>5.9</td>
<td>4.5</td>
</tr>
<tr>
<td>pd$\sigma$</td>
<td>-2.4</td>
<td>-1.4</td>
</tr>
<tr>
<td>pd$\pi$</td>
<td>1.3</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Fig. 6. — Effective densities of states for Sr$_2$VO$_4$-like compounds. Full line: $xy$-band; dashed line: $yz$ or $zx$-band.

Fig. 7. — Total density of states of Sr$_2$VO$_4$ obtained by the alternating lattice method. Insert: exact result obtained by APW-calculation (after Ref. [11]).
La$_2$CuO$_4$. — Doped La$_2$CuO$_4$ was the first high $T_c$ material [1] and it has been intensively studied. Some features of its electronic structure have been described elsewhere [6] and we present it here to illustrate the similarity with Sr$_2$VO$_4$ as can be seen by comparing the total densities of states in figures 7 (Sr$_2$VO$_4$) and 8 (La$_2$CuO$_4$). Let us point out the importance of the Jahn-Teller distortion of the octahedron (the distance Cu-O in plane is equal to 1.89 Å, whereas the distance Cu-O out of plane is 2.43 Å). The differences between the two compounds are due to the Jahn-Teller distortion and the separation of atomic levels $\varepsilon_p$ and $\varepsilon_d$. Of course, the filling is different: for La$_2$CuO$_4$ the states contributing to the Fermi level are $e_g$-orbitals hybridized with $p\sigma$ ones (instead of $t_{2g}$ and $p\pi$-orbitals in Sr$_2$VO$_4$). By projecting the $e_g$-DOS on $x^2-y^2$ and $3z^2-r^2$, one sees that the $3z^2-r^2$ band is lower in energy than the $x^2-y^2$ one (Figs. 9 and 10). This is due to the Jahn-Teller distortion as can be seen in figure 11, where we present $x^2-y^2$ and $3z^2-r^2$ DOS for a "pseudo" La$_2$CuO$_4$ without octahedron distortion.

Fig. 8. Total density of states of La$_2$CuO$_4$ decomposed in $t_{2g}$-$\pi$ band (full line) and $e_g$-$\pi\sigma$ band (dotted line).

Fig. 9. Effective density of states of the Jahn-Teller distorted La$_2$CuO$_4$ compound. Full line: $x^2-y^2$ band; dotted line: $3z^2-r^2$ band.

Fig. 10. Local density of states of the Jahn-Teller distorted La$_2$CuO$_4$. Full line: on a $x^2-y^2$ orbital; dotted line: on a $3z^2-r^2$ orbital.

Fig. 11. Local density of states of La$_2$CuO$_4$ without Jahn-Teller distorsion. Full line: on a $x^2-y^2$ orbital; dotted line: on a $3z^2-r^2$ orbital.
As a consequence of this energy lowering of $3z^2 - r^2$, the hole above the Fermi level is mainly located on $x^2 - y^2$ and pσ-orbitals. This allows a simple description of La$_2$CuO$_4$ by retaining only the $x^2 - y^2$ and pσ-orbitals in the CuO$_2$ plane.

Two bands model of CuO$_2$ plane. — This model, which takes into account Cu-d$x^2 - y^2$ and O-pσ orbitals, has been widely used as a starting point to study antiferromagnetism [13] and correlations [14] or superconductivity [15]. Some authors have treated the Cu-O hopping integral $t$ as a perturbation. This approach leads to two subbands, having a square lattice DOS. The upper band is the Copper band with an effective Cu-Cu hopping integral $t^2/\varepsilon_d - \varepsilon_p$. This perturbative approach does not give the right band edges and it is no longer valid if the Cu-O hopping is not small compared with $\varepsilon_d - \varepsilon_p$. Let us recall that band calculations [16] actually show that the covalency is important, i.e. $t/\varepsilon_d - \varepsilon_p$ is large, and thus the perturbative approach is not very good.

With no loss of simplicity, the alternating lattice method leads to an exact result whatever the parameter $t/\varepsilon_d - \varepsilon_p$. In figure 12, we show the densities of states obtained by the alternating lattice method and it appears that for realistic parameters, the oxygen partial DOS is not negligible in the upper band. Let us recall that in the limit of small $t/\varepsilon_d - \varepsilon_p$ (perturbative approach) the upper band would be purely made of copper states.

![Diagram](image-url)

Fig. 12. — (a) Effective density of states. (b) Total density of states of the Cu($x^2$-$y^2$)-O$_2$(pσ) plane. Insert: copper and oxygen projected densities of states.
Finally, the alternating lattice method allows us to show an important result concerning the position of the Fermi level using equations (9) and (10). For the stoechiometric compound (one electron in the copper band) the Fermi level is exactly in the Van Hove singularity for all values of \( t/\epsilon_d - \epsilon_p \). This confirms Friedel's proposition [15] that the Fermi level is close to the two dimensional Van Hove singularity for the doped superconducting phase, and could explain the high values of \( T_c \).

Conclusion.

Let us conclude with some general remarks. We have shown that a reliable description of the electronic structure, near the Fermi level, of various perovskite type compounds is achieved with a small set of orbitals of the metal and of oxygen. We have shown the importance of the alternating structure of the perovskite compounds. It allows a simple description of their electronic structure in term of a DOS which depends on the geometry and the type of the involved orbitals, but not on metal-oxygen covalency. We have applied this method to various oxides. Let us mention that this method is applicable to study various other physical properties such as the antiferromagnetism of the CuO\(_2\) plane and the phonon spectrum in alternating structures.

Acknowledgements.

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References