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M. Khan, S. Bouarab, A. Vega, L. Balbás. An ab-initio Study of Optical Properties of Perovskites : LaMO₃ and YMO₃ (M = Ti-Cu). Journal de Physique IV Proceedings, 1997, 07 (C1), pp.C1-717-C1-718. 10.1051/jp4:19971292 . jpa-00255009

HAL Id: jpa-00255009

<https://hal.science/jpa-00255009>

Submitted on 1 Jan 1997

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An ab-initio Study of Optical Properties of Perovskites: LaMO_3 and YMO_3 ($M = \text{Ti-Cu}$)

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Abstract. A self-consistent first principles energy band calculation is performed. The energies and eigen functions thus obtained are used to calculate interband transition elements in dipole approximation. The imaginary part of the dielectric constant as well as the optical conductivities of perovskites LaMO_3 and YMO_3 ($M = \text{Ti-Cu}$) are calculated. The origin of the structures can be explained on the basis of their respective energy bands. When compared with available experimental data one finds a good agreement with theoretical results.

1. INTRODUCTION

The discovery of easy metal insulator transitions and high temperature superconductivity in certain perovskites [1] have generated a considerable fundamental and technological interest in these materials. A number of these compounds are magnetic with antiferromagnetic (AF) phase with different kinds of alignments [2]. Thus for the same compound there are different possibilities of magnetic moments and physical properties. One of the important experimental results are the optical properties measured by Arima *et al.* [3]. In the optical properties, the interband transitions from occupied to empty states is the basic factor. So, from theoretical point of view it is important to know the eigenvalues and vectors of energy bands to calculate the transition matrix elements in dipole approximation [4]. Such a calculation has been performed for a number of compounds [5] and excellent agreement with experimental data, whenever available, is found. In this communication we give a short presentation of optical properties of LaMO_3 and YMO_3 based on one electron energy bands.

2. RESULTS AND DISCUSSION:

For energy band calculation we use Linear-Muffin-Tin-Orbital (LMTO) method in atomic sphere approximation (ASA) where combined correction is included [6]. Once energies $E_n(k)$ and functions $|n\vec{k}\rangle$ for n bands are obtained self-consistently, the imaginary part $\epsilon_2(\omega)$ of the dielectric constant, for a given photon energy ω is calculated [4,5]. The real part of the optical conductivity $\sigma_1(\omega)$ which is often measured by experimentalists is given by: $\sigma_1(\omega) = \omega\epsilon_2(\omega)/4\pi$. Three possibilities of antiferromagnetic (AF) phases are considered according to the inter and intraplane coupling in (001) plane: (i) interplane AF but intraplane ferromagnetic (F) (A-type), (ii) interplane as well intraplane AF (G-type) and (iii) interplane F but intraplane AF (C-type). For Ti, Co, Ni and Cu, the total energy difference calculated between paramagnetic (P) and AF or F phases is quite small. For these compounds, one obtains almost the same optical transitions in either phase.

In figure 1 we show the calculated optical conductivity along with the measured data of Arima *et al* [3] for LaMO_3 and YMO_3 ($M = \text{Ti, Co and Ni}$). In the case of LaMO_3 , it is clear that the overall agreement is quite good. The situation for $M = \text{Co}$ is somewhat unsatisfactory when we compare the relative intensities, but the main structures are reproduced in the theoretical curve. We have considered LaCoO_3 in cubic phase without any distortion whereas some experimental data [2] show that it is slightly distorted. This may be the origin of the disagreement.

For magnetic phases the agreement between experiment and theory are further enhanced when $\sigma_1(\omega)$ is calculated for the corresponding AF phase except in the case of $M = \text{Fe}$ for which a better agreement is found between P theoretical curve and experimental data [7].

For YMO_3 the experimental data is only available when $M = \text{Ti, Co and Ni}$ [3]. For these particular cases our results bring out the general trends of the measured spectra. For the rest of the compounds there is, to our knowledge, no experimental data nor theoretical calculation.

In summary, we present the first *ab-initio* calculation of the optical conductivities of perovskites $RM O_3$ ($R=\text{La, Y}$ and $M=\text{Ti, Ni and Co}$). We have actually performed the calculation for the whole series of $M=\text{Ti-Cu}$ in non-magnetic and magnetic phases [8], but due to the lack of the space only a few examples are given here. The available experimental data is quite well explained through the energy band scheme. For YMO_3 when $M= \text{V, Cr, Mn, Fe and Cu}$, our calculated values are the only available and they will have to be checked through experiments. But in the light of a good agreement between theory and experiments as shown in figure 1, we almost know what the experimental data for other YMO_3 would be.

Figure 1: The optical conductivity σ_1 as function of photon energy ω for $LaMO_3$ (upper row) and YMO_3 (lower row). $M=\text{Ti, Co and Ni}$ (from left to right); experimental (dotted line) [3] and theoretical (continuous line).

Acknowledgments

This work has been supported by DGICYT (Grant PB92-0645-CO3-O2) and Junta de Castilla y León (Grant VA58/93) from Spain. M.A. Khan and S. Bouarab would like to thank Ministerio de Educación y Ciencia (Spain) for Sabatical grant and financial support respectively.

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