



SDI Review Form 1.6

Journal Name:	Journal of Materials Science Research and Reviews
Manuscript Number:	Ms_JMSRR_43380
Title of the Manuscript:	Analysis of electronic structure and X-ray Absorption and Emission spectra in MgO within the FP-LAPW method
Type of the Article	Original Research Article

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

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PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
<u>Compulsory</u> REVISION comments	The authors report on an Ab initio calculations in order to analyse the electronic properties, DOS, XANES and XES spectra for the different edges of MgO. This study is a comparison with previous work. However, the article can not be published in the Journal of Materials Science Research and Reviews for the following reasons: 1- First, the work of the authors does not bring any novelty MgO has been extensively studied. 2- The authors do not give enough details on the calculation method used, for example the values of Rmt, the structure of the compound MgO, the value of U since they performed a calculation with LDA + U 3- The list of references is incorrect, for example: Ref 5 put the reference of the LDA * J.P. Perdew, Y. Wang, Phys. Rev. B, 45 (1992) 13244. Ref 9 put the reference for density functional theory * Hohenberg, P., Kohn, W. : Phys. Rev. 136, B864-871 (1964) * Kohn, W., Sham, L.J. : Phys. Rev. 140, A1133-1138 (1965) 4- The authors do not discuss anything about the ground state properties for the studied material. The authors should refer the more recent published papers. Bibliographic research is insufficient on the studied material. I invite the authors to read the article by H. Baltache et al. / Physica B 344 (2004) 334-342. 5- The authors applied pressures on the material to study the contribution of states s and d. The application of a pressure implies a break of the bonds and thus a structural phase transition. I wonder if the authors have taken into consideration the effect of the pressure on the volume!!!!	1) We consider there are calculations and results not previously shown for MgO, such as: In this work MgO X-ray absorption near-edge spectra and X-ray emission spectra were calculated selfconsistently using different potentials: PBE and TB-mBJ and were compared with the projected DOS and experimental results. XANES spectra for different fractional core holes, as proposed by Slater, were obtained to find the best agreement with the experiments. PBE and TB-mBJ XES calculated spectra and projected partial densities of states (DOS) are compared with XES and XPS experiments. Besides, the partial DOS were analysed as a function of the volume of the unit cell. The PBE and TB-mBJ potentials were used to obtain MgO band gap. The Bader's topological method was employed to analyze the ionic behavior in MgO, finding a charge transference about of 1.72 electron units. Using this value, we calculated Lattice Energy that was compared with the value obtained by the Born-Haber cycle, obtaining a very good result. The wannierization procedure was implemented selecting a group of Bloch bands for which the maximally localized Wannier functions (MLWF) are calculated using Wannier90 according to the Marzari and Vanderbilt method. 2) The details of the ab initio calculations were included in Theoretical Method and the three U values 3.5, 5 and 7 eV, were included in Results and discussion. Pages 2 and 3. 3) Perdew, Wang was included and the other references were corrected. Page 6.



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		4) We added Baltache et al. reference and other newer references to the Bibliography. Page 7. 5) We do not show calculations with applied pressures, to the contrary we show results expanding the cell, to analyse what would have happened to the orbitals in the case the atoms were further away and less interaction would be present between them. We tried to be clear about the evolution of the volume of the unit cell from bigger values, starting with 100% bigger, to the equilibrium value. Page 4.
Minor REVISION comments		
Optional/General comments		

PART 2:

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	