



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:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

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)
Compulsory REVISION comments		
Minor REVISION comments	The article is generally well thought out and written. Topic is up to date and important in the community. Authors made some language errors of minor importance, which are listed below. The figure 11 (a) is not well prepared. The lack of colour scaling legend and the range of scale is not well chosen. Please take care for choosing better scale range or present this in gray scale with appropriate legend. Authors should consider removing of 11.b part of figure as it is almost not described in the text (the wannier plot part) or write an explanation and conclude for such a shape/configuration of this function. Some part of manuscript is not translated to English (for eg. ABSTRACT instead of Resumen and FIGURE instead of figura, REFERENCES instead of referencias). Authors write that they use a supercell approach (the last sentence of introduction). Supercell parameters are never shown in article. "The calculations were produced with core holes 0.0, 0.5 [...]" – 0.0 is not a hole. "resulting in a kpoint sampling in the Brillouin zone (BZ) of about 500 points." – about 500 points? Please provide exact number. "Using the electronic charges obtained with the Bader's topological Method, the Coulomb potential and the Madelung constant of 1.74756 we obtained the Lattice Energy 3377 kJ/mol for the equilibrium lattice parameter and 3429 kJ/mol for the experimental lattice parameter, we compared them with the 3890 kJ/mol value obtained by the Born-Haber cycle." – please specify used equations for Coulomb and Madelung calculations as for now their correctness can't be evaluated! Language corrections: Introduction, first sentence: "[...] most important tools for the characterization of the electronic structure of the materials through the analysis OF the densities of states, the	1) Figure 11 (a) was improved and 11(b) the Wannierization procedure was better described to obtain the MLWF. Page 4. 2) We corrected the titles that were not in english in the latex file. It was a usepackage from latex badly included. 3) We added supercell details. Page 2. 4) We replaced 0 core hole, by no core hole, and removed "about" when describing the number of k points. Pages 2, 3 and 5. 5) The calculation of the Born Haber cycle was included in detail in the paper. Pag 5. 6) The wrong expressions were corrected. Pages 1 and 4.



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	valence and conduction bands and OF the optical properties.” 3.2 X-ray emission spectroscopy: “To show this effect is more important when the volume OF THE cell decreases and the oxygen atom is”, again in the last sentence of this paragraph.	
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>	