



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)
<u>Compulsory</u> REVISION comments	According to the band gap calculated by TB-mBJ it is 7.16 eV for the MgO, it will be better bought with the experimental result 7.83 eV. Since this value of the band gap is very large what type of semiconductor is the MgO. Semiconductor of direct or indirect band. Why does the TB-mBJ spectrum show a better fit with the experimental spectrum for high energies and not for low energies? Argument more the discussion of each one of the figures 1, 2, 3, and 4. Likewise describe the physical behavior of the theoretical calculations obtained with the experimental part.	1) According to the value of band gap MgO is an insulator. We add a graphic to the paper with the bandstructure plot for TB-mBJ calculation, there it is shown the 7.16 eV direct gap in Gamma point. Page3. 2) We do not consider that the TB-mBJ shows a better fit only for high energies, it depends on the case. The paragraph that was leading to a misunderstanding was modified. Page3. 3) We added a description of the XANES spectra calculated with Wien2k and compared to the experimental results. Page 3.
<u>Minor</u> REVISION comments	It is recommended to include more current references.	4) We added more references to the paper.
<u>Optional/General</u> 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>	