Abstract Submitted
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Ab initio study of complex defects and optical transitions in $MgAl_2O_4$[1] J.C. GARCIA, P.D. BORGES, Texas State University, USA, F.G. PINTO, J. TRONTO, Universidade Federal de Vicosa, Brazil, L. SCOLFARO, Texas State University, USA — The excellent optical properties of the Magnesium aluminate (MAO) spinel makes it an important material for novel technological applications. Considering that a presence of native defects can promote important changes in those properties, we present in this work a study of the structural, electronic and thermodynamic properties of the MAO. The calculated formation energy for isolated defects, such as the vacancies of manganese, aluminum and oxygen, oxygen interstitial, manganese and aluminum antisites, as well as the complexes in the most stable charge states are shown. In good agreement with experimental data, we obtained that complex centers, such as oxygen vacancies in conjunction with oxygen interstitial, manganese or aluminum antisites at different charge states are good candidates for the observed optical transitions at 4.75, 5.3, and 6.4 eV. Our findings were obtained from ab initio electronic structure calculations performed within the Density Functional Theory. For the exchange-correlation potential, the generalized gradient approximation was used. Furthermore, a modified Becke-Johnson correction to the exchange potential was applied to obtain a suitable value for the band gap energy, 7.40 eV, in good agreement with the experimental one of 7.8 eV.

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