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Electronic and Optical Properties of Orthorhombic NdMnO3 with the Modified Becke-Johnson Potential

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Abstract : We investigate the electronic structure, magnetic and optical properties of the orthorhombic NdMnO3 through density-functional-theory (DFT) calculations using both generalized gradient approximation GGA and GGA+U approaches, the exchange and correlation effects are taken into account by an orbital independent modified Becke Johnson (MBJ). The predicted band gaps using the MBJ exchange approximation show a significant improvement over previous theoretical work with the common GGA and GGA+U very closer to the experimental results. Band gap dependent optical parameters like dielectric constant, index of refraction, absorption coefficient, reflectivity and conductivity are calculated and analyzed. We find that when using MBJ we have obtained better results for band gap of NdMnO3 than in the case of GGA and GGA+U. The values of band gap founded in this work by MBJ are in a very good agreement with corresponding experimental values compared to other calculations. This comprehensive theoretical study of the optoelectronic properties predicts that this material can be effectively used in optical devices.

Keywords : DFT, optical properties, absorption coefficient, strong correlation, MBJ, orthorhombic NdMnO3, optoelectronic
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