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Phase dependent structural and electronic properties of Lanthanum Orthophosphate ($LaPO_4$) MAHESH NEUPANE, US Army Research Laboratory, Aberdeen Proving Ground, MD, GREGORY GARRETT, SERGEY RUDIN, US Army Research Laboratory, Adelphi, MD, JAN ANDZELM, US Army Research Laboratory, Aberdeen Proving Ground, MD — Lanthanum orthophosphate ($LaPO_4$) belongs to the family of rare-earth (RE) orthophosphates. The La-ion lacks valence 4f-electron, so for it to exhibit f-electron dependent physics, it must be doped with additional RE elements. In the bulk form, $LaPO_4$ exist in both a stable monoclinic and a metastable hexagonal phase, which both possess indirect energy transition characteristics. Though the overall optoelectronic properties of the RE-doped $LaPO_4$ depend on the accuracy of the observed bulk energy gap, the reported experimental and theoretical energy gaps varies between ~$8^{1,2}$ and ~5^3 eV, respectively. Through this theoretical study, we attempt to establish a correlation between electronic properties of bulk $LaPO_4$ and various levels of first principle theories. Compared to experimental data, the PBE0 functional over-predicts energy gaps and the energy differences between the indirect-to-direct transition energies by 25%. The HSE06 gives a good description of electronic properties and predicts the energy gaps to be 7.68 (monoclinic) and 7.29 eV (hexagonal). Analysis on the structural stability also reveals that the total energy difference between the two phases is 6meV, consistent with the experimentally observed instantaneous pressure and temperature dependent phase transition. [1] J. Lumin. 72–74, 255, 1997, [2] J. Lumin. 15-18, 255, 1977, [3] App. Surface Science, 268, 458-463, 2013.

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