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**Structural, Electronic and Magnetic Properties of doped-LaPO<sub>4</sub>**

JAN ANDZELM, US Army Research Lab - Aberdeen, MAHESH NEUPANE, GREGORY GARRETT, US Army Rsch Lab - Adelphi — Lanthanum orthophosphates (LaPO<sub>4</sub>) are a very interesting class of host lattices of activator ions due to their high insolubility and high thermal stability, thus providing durable phosphors for optical applications. When substitutionally doped with other rare-earth (RE) elements, RE-doped LaPO<sub>4</sub> exhibits intriguing dopant-induced electronic and optical properties. Recent experimental studies have also achieved efficient optical luminescence in LaPO<sub>4</sub> by varying RE concentration. Theoretical or computational study of the concentration dependent RE-doped LaPO<sub>4</sub> so far has been limited. In this study, we present a detailed DFT-based theoretical study of RE-doped LaPO<sub>4</sub> by varying the RE-dopant types and concentration from 25% to 3%. The importance of the inclusion of electron-electron interactions during the theoretical study of RE-doped LaPO<sub>4</sub> systems will be highlighted by comparing the results from the local and hybrid functionals. Finally, an analysis on the effect of RE-dopant type and concentration on structural, electronic and magnetic properties of RE-doped LaPO<sub>4</sub> systems will be presented, which might expand the applicability of these materials to other domains such as spintronics and magnonics.

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