

Abstract Submitted
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The Electronic Structure of Rare-Earth Pnictides. SHOAI B KHALID, ANDERSON JANOTTI, Univ of Delaware — The structural parameters and electronic band structure of rare-earth pnictides are investigated using density functional theory (DFT) with the Heyd, Scuseria, and Ernzerhof (HSE06) screened hybrid functional. The rare-earth pnictides which are the focus of this study include RE-V compounds, where RE=La, Nd, Sm, Gd, Tb, Er, Lu, and V=As, Sb, Bi, in the rock-salt crystal structure. All the calculations include spin-orbit interaction, and we pay special attention to the effects of including the RE f electrons in the valence. The results of HSE06 calculations are compared with DFT within the generalized gradient approximation (GGA) and other previous calculations. Finally, we also investigate the effect of hydrostatic and biaxial strain on the band structure, in special the role of epitaxial strain in lifting degeneracies of the bands near the Fermi level.

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