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Influence of xc functional on thermal-elastic properties of metal oxides: A DFT-based Debye-Grüneisen model approach TAEHUN LEE, ALOYSIUS SOON, Yonsei University, Seoul, Korea — For high-temperature applications, the chemical stability, as well as the mechanical integrity of the oxide material used is of utmost importance. Solving these problems demands a thorough and fundamental understanding of their thermal-elastic properties. In this work, we report density-functional theory (DFT) calculations to investigate the influence of the xc functional on specific thermal-elastic properties of some common oxides CeO_2, Cu_2O, and MgO. Namely, we consider the local-density approximation (LDA), the generalized gradient approximation due to Perdew, Burke, and Ernzerhof (GGA-PBE), as well as a recently popularized hybrid functional due to Heyd-Scuseria-Ernzehof (HSE06). In addition, we will also report DFT+U results where we introduce a Hubbard U term to the Cu $3d$ and the Ce $4f$ states. Upon obtaining the DFT total energies, we then couple this to a volume-dependent Debye-Grüneisen model [1] to determine the thermodynamic quantities of these oxides at arbitrary pressures and temperatures. We find an explicit description of the strong correlation (e.g. via the DFT+U approach and using HSE06) is necessary to have a good agreement with experimental values. [1] A. Otero-de-la-Roza, D. Abbasi-Pérez et al. Com. Phys. Com. 182 (2011) 2232

Taehun Lee
Yonsei University, Seoul, Korea

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