Abstract Submitted
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Influence of xc functional on thermal-elastic properties of Ceria: A DFT-based Debye-Grüneisen model approach[1] JI-HWAN LEE, YOUNGJOO TAK, TAEHUN LEE, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Ceria (CeO_{2-x}) is widely studied as a choice electrolyte material for intermediate-temperature ($\sim 800\,\mathrm{K}$) solid oxide fuel cells. At this temperature, maintaining its chemical stability and thermal-mechanical integrity of this oxide are of utmost importance. To understand their thermal-elastic properties, we firstly test the influence of various approximations to the density-functional theory (DFT) xc functionals on specific thermal-elastic properties of both CeO_2 and Ce_2O_3. Namely, we consider the local-density approximation (LDA), the generalized gradient approximation (GGA-PBE) with and without additional Hubbard U as applied to the $4f$ electron of Ce, as well as the recently popularized hybrid functional due to Heyd-Scuseria-Ernzehof (HSE06). Next, we then couple this to a volume-dependent Debye-Grüneisen model to determine the thermodynamic quantities of ceria at arbitrary temperatures. We find an explicit description of the strong correlation (e.g. via the DFT+U and hybrid functional approach) is necessary to have a good agreement with experimental values, in contrast to the mean-field treatment in standard xc approximations (such as LDA or GGA-PBE).

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Ji-Hwan Lee
Department of Materials Science and Engineering, Yonsei University

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