Abstract Submitted
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Electronic structure of PbTiO3-based ferroelectric materials determined from LDA+U study[1] GAOYANG GOU, HIROYUKI TAKENAKA, JOSEPH BENNETT, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323 — We perform a systematic theoretical study of the electronic structure of $PbTiO_3$ and related ferroelectric materials, using LDA+U calculations. The effective on-site correlation terms U for the localized electronic states of $PbTiO_3$ are determined with a linear-response method. Compared to the DFT- LDA method (where the band gap values are greatly underestimated), band gap values for $PbTiO_3$ obtained by LDA+U calculations are much closer to the experimental results. Special focus has been paid to solid-state solutions formed by doping $PbTiO_3$ with a d^8 cation (Ni, Pd, Pt) and accompanying O vacancy, which have recently been proposed. We re-examine the dopant states of these materials, and also recalculate their electronic structures using the LDA+U method. The improvement achieved with the LDA+U method and comparison with experimental results will be presented.

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