Electronic structure of PbTiO$_3$-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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