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Dielectric properties of correlated oxides: a GGA+U electric-enthalpy approach OSWALDO DIEGUEZ, Massachusetts Institute of Technology, PAOLO UMARI, INFM Democritos, MATTEO COCOCCIONI, University of Minnesota, NICOLA MARZARI, Massachusetts Institute of Technology — The dielectric response of correlated-electron oxides is often overestimated in common density-functional theory approaches, such as the local-density or the generalized-gradient approximations, in a failure that closely mirrors the underestimation of the Kohn- Sham band gap. A Hubbard U correction can greatly improve the description of the electronic ground-state for these difficult systems; in addition, U can be derived fully from first-principles using a linear-response approach,[1] making the approach parameter-free. Here, we show that an electric-enthalpy formulation allows to straightforwardly calculate the dielectric properties in the presence of a Hubbard U term, leading to much closer agreement with experiments for the paradigmatic case of $3d$ transition-metal oxides.

[1]M. Cococcioni and S. de Gironcoli, Phys. Rev. B **71**, 035105 (2005)

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