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Measuring the Quality of Generalized Gradient Approximations in a Density Functional Theory Pseudopotential Environment for Solids
ZACHARY NAULT, ANTONIO CANCIO, Ball State University — Much recent development in DFT has focused on improving GGAs. Two schemes are second order GGA (SOGGA) and the APBE which builds the GGA from atomic systems and not the HEG. Both of these have been tested within an all electron (AE) environment, providing the most accurate results. The focus of many simulations, however, is on large systems using pseudopotentials (PsP's). Are these PsP calculations, which rely on functionals tested in an AE environment, accurately reproducing the AE ground state properties? If not, can the deficiencies be identified? To assess this, we use the PsP generator APE, using the functional library libXC which works with the PsP package ABINIT and the AE package Elk. We generate standard Troullier-Martin PsP's based on common and new XC functionals (LDA, PBE, PBEsol, APBE, SOGGA) and test their performance in 13 solids (Na, Li, Al, C, Si, GaAs, NaCl, LiF, LiCl, Cu, Pd, Rh, and Ag). We measure how well three ground state properties (lattice constant, bulk modulus, and cohesive energy) are calculated with PsP's as compared to the corresponding AE calculations.

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