Reinvigorating Norm Conservation: the ONCVPSP Project

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ABSTRACT

Recent interest in high-throughput materials discovery has led to a critical reexamination of some published sets of pseudopotentials. While the creation of improved sets has focused on ultrasoft and PAW potentials for consistent accuracy and convergence, norm-conserving potentials remain attractive for the relative algorithmic simplicity they offer, especially for more complex calculations. The open-source ONCVPSP code has been developed to foster the creation of improved norm-conserving potentials with competitive accuracy and convergence capabilities. The principal of generalized norm conservation will be reviewed, which permits norm-conserving potentials to accurately reproduce the scattering properties of all-electron potentials at several energies. We will then show how this can be combined with systematic convergence optimization based on minimizing the kinetic energy error produced by the plane-wave expansion cutoff. A transparent reformulation of this optimization will be introduced, along with a means of applying it to positive-energy scattering states.[1] A series of tests comparing all-electron and two-projector norm-conserving results for lattice constants and bulk moduli show encouraging agreement for a group of solids chosen to represent a variety of types of bonding and a sampling of the periodic table. A few comparisons for magnetic systems and spin-orbit band structures have also been made. The open-source code, which can produce potentials for QUANTUM ESPRESSO and ABINIT, will be briefly discussed, along with possible paths for the evolution of the code and its datasets.

[1] D. R. Hamann, Phys. Rev. B **88**, 085117 (2013).