Relativistic Optimized Norm-Conserving Vanderbilt Pseudopotentials

D.R. HAMANN, Dept. of Physics and Astronomy, Rutgers University — Two-projector fully non-local pseudopotentials obeying the generalized norm-conserving condition\(^1\) and incorporating systematic convergence optimization\(^2\) have been shown to accurately reproduce all-electron results with high computational efficiency.\(^3\) The generalized norm-conservation theorem guarantees exact reproduction of all-electron norms, radial log-derivatives, and first energy derivatives of radial log derivatives at several energies, as well as the hermiticity of the non-local pseudopotential operator. This theorem is exact only for non-relativistic all-electron wave functions.\(^4\) Averaging out small asymmetries of the non-local operators generated using scalar-relativistic Schrödinger equation solutions preserves agreement of these quantities to order \(10^{-4}\), and yields excellent results for solids.\(^5\) I show that fully-relativistic Dirac-equation solutions can be treated in the same manner, with comparably small errors. Spin-orbit band splittings as well as other properties of several solids calculated with these pseudopotentials will be compared to fully-relativistic all-electron results.

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