Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

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.

[1]D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).
[2]A. M. Rappe *et al.*, Phys. Rev. B **41**, 1227 (1990).
[3]D. R. Hamann, Phys. Rev. B **88**, 085117 (2013).
[4]Vanderbilt
[5]Hamann

D.R. Hamann
Dept. of Physics and Astronomy, Rutgers University

Date submitted: 08 Nov 2013 Electronic form version 1.4