

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Improving Boundary Conditions for Electronic Structure Calculations** G. A. BENESH, Baylor University, ROGER HAYDOCK, University of Oregon — Boundary conditions imposed on a local system joined to a much larger substrate system routinely introduce unphysical reflections that affect the calculation of electronic properties such as energies, charge densities, and densities of states. These problems persist in atomic cluster, slab, and supercell calculations alike. However, wave functions in real, physical systems do not reflect at artificial boundaries. Instead, they carry current smoothly across the surface separating the local system from the underlying medium. Haydock and Nex have derived a non-reflecting boundary condition that works well for discrete systems [Phys. Rev. B 75, 205121 (2006)]. Solutions satisfying their maximal breaking of time-reversal symmetry (MBTS) boundary condition carry current away from the boundary at a maximal rate—in much the same way as exact wave functions in physical systems. The MBTS approach has now been extended to studies employing continuous basis functions. In model systems, MBTS boundary conditions work well for calculating wave functions, eigenenergies, and densities of states. Results are reported for an Al(001) surface. Comparisons are made with slab calculations, embedding calculations, and experiment.

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Date submitted: 24 Nov 2015

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