Abstract Submitted
for the TSF15 Meeting of
The American Physical Society

Minimizing Reflections from Artificial Boundaries in Electronic Structure Calculations G. A. BENESH, Baylor University, ROGER HAYDOCK, University of Oregon — Boundary conditions imposed on a local system that is joined to a larger substrate system often introduce unphysical reflections that affect the calculation of electronic properties. These problems are common in atomic cluster, slab, and supercell calculations alike. However, solutions of the Schrödinger equation for a physical system carry current smoothly across the (artificial) boundary between the local system and the underlying medium. Previously, Haydock and Nex derived a non-reflecting boundary condition for discrete systems [Phys. Rev. B 75, 205121 (2006)]. Solutions satisfying this 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 the exact wave functions for the physical system. The MBTS boundary condition has proved useful in discrete systems for constructing densities of states and other distributions from moments or continued fractions. The MBTS approach has now been extended to studies employing continuous spatial wave functions. Results are presented for a model system and an Al(001) surface. Comparisons are made with slab calculations, embedding calculations, and experiment.

G. A. Benesh
Baylor University

Date submitted: 12 Oct 2015 Electronic form version 1.4