Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

New approach on calculating Green's functions in Full-Potential Multiple Scattering Methods.[1] AURELIAN RUSANU, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, G. M. STOCKS, Oak Ridge National Laboratory, JOHN S. FAULKNER, Florida Atlantic University — The most common methods of computing Green's functions in modern full-potential multiple scattering applications rely on solving Schrödinger (Dirac) equations for regular and irregular solutions of a single-site scatterer over an energy contour in the complex plane. While, for spherical potentials, the standard formulae for calculating the Green's function are numerically stable they often result in unphysical behavior for non spherical potentials, particularly close to the nucleus and for large angular momentum quantum numbers. Here we use a new analytical and numerical method that does not require calculation of the irregular solution, to which the numerical instability can be traced. The new approach results in the correct analytic behavior and numerical stability.

[1]Research sponsored by the Division of Materials Science and Engineering, U.S. DOE, Oak Ridge National Laboratory with UT-Battelle, LLC.

Aurelian Rusanu
Oak Ridge National Laboratory

Date submitted: 21 Nov 2008 Electronic form version 1.4