

**Abstract Submitted
for the MAR98 Meeting of
The American Physical Society**

Sorting Category: 7-c

Energy Convergence of LSDA Calculations using the Locally Self-consistent Multiple Scattering Method¹ A. B. OPARIN, University of Tennessee Knoxville, D. M. C. NICHOLSON, Oak Ridge National Laboratory - In the multiple scattering approach to solving the Schrodinger equation, contributions to the electron density at a site can be divided into those arising from multiple scattering paths within a local interaction zone surrounding the site and paths involving scattering from more distant atoms. Accurate energies can be obtained if the second category of multiple scattering events is approximated or even taken to be zero. Convergence properties of the energy will be compared for several approximations to the distant scattering. Results for random alloys and inhomogeneous magnetic materials will be used to illustrate the approximations.

¹Work supported by Office of Basic Energy Sciences, Division of Materials Science, and Office of Computational and Technology Research, Mathematical, Information, and Computational Sciences Division, U.S. DOE, under subcontract DEAC05-96OR22464 with Lockheed Martin Energy Research Corporation.

G. M. Stocks
Prefer Oral Session
gms@ornl.gov
Prefer Poster Session
Ridge National Laboratory

Oak

Date submitted: February 5, 1998
Electronic form version 1.2