Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Self-interaction correction in multiple scattering theory – Application to transition metal oxide MARKUS DAENE, Oak Ridge National Lab, WOLFRAM HERGERT, Martin Luther University Halle, Germany, ARTHUR ERNST, Max Planck Institute for Micrstructure Physics, Halle, Germany, MARTIN LUEDERS, ZDZISLAWA SZOTEK, WALTER TEMMERMAN, Daresbury Laboratory, UK — In this work we study the electronic structure of 3d-transition metal oxides as obtained with the self-interaction corrected-local spin density approximation method, implemented within multiple scattering theory. We briefly describe the formalism and discuss important technical issues of its implementation within the KKR band structure method.
We present results of such important properties as lattice constants, local magnetic moments, band gaps and discuss them in comparison with the LSD and the experimental values.

Markus Daene
Oak Ridge National Lab

Date submitted: 21 Nov 2008 Electronic form version 1.4