Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Transferable tight-binding description of the Fe-C interaction NICHOLAS HATCHER, GEORG K.H. MADSEN, RALF DRAUTZ, ICAMS, Ruhr-Universität Bochum — A coherent transferable tight-binding (TB) parameterization including magnetism has yet to be developed for the Fe-C interaction. Although interatomic potentials have been obtained for this system, recent findings show that the results from these potentials are inconsistent with DFT calculations and do not give an accurate portrayal of chemical bonding in the system. Using dual DFT grid and LCAO calculations within GPAW, we obtain one electron wave functions expanded in a multiple-ζ LCAO basis. This is then down-folded onto an optimal minimal basis, giving a continuous and transferable description of Fe-C bonding. By constructing a TB energy functional using these bond integrals and a parameterized interatomic repulsion, we show how an accurate description of the energy hierarchy of interstitial carbon in Fe-structures can be achieved. Furthermore, we use the model to calculate elastic properties and energies of a variety of Fe-carbides, defects, and carbon diffusion paths. This simple model based on physical insights may be used to study systems containing thousands of atoms.

Nicholas Hatcher
ICAMS, Ruhr-Universität Bochum

Date submitted: 19 Dec 2011 Electronic form version 1.4