Tight-Binding Parametrizations for Large Scale Materials Science Computations

Michael Mehl
Naval Research Laboratory
Washington DC
mehl@dave.nrl.navy.mil

Quantum mechanically accurate first-principles calculations for real materials are computationally limited to no more than 100-1000 atoms. While atomistic potentials can handle much larger systems, they may miss some physics where changes in the electronic structure are important, e.g. at cracks and defects. Parametrized tight-binding (TB) methods exist between these two extremes. Unlike atomistic potentials, the quantum mechanical behavior of the electrons is maintained, but the computational effort is much less than needed for comparably sized first-principles calculations, though larger than required for atomistic potential methods. The NRL Tight-Binding Method (NRL-TB) maps the results of a limited set of first-principles calculations to a two-center non-orthogonal Slater-Koster TB Hamiltonian with on-site Hamiltonian parameters which are sensitive to the local environment. The method has been shown to successfully determine elastic constants, phonon frequencies, vacancy formation energies, and surface energies. In addition, TB molecular dynamics simulations are used to study thermal expansion and atomic diffusion. We will discuss applications to spin-polarized systems, non-collinear magnetization, and multi-component systems, including MgB_2. The NRL-TB parameters and codes are available as part of the U.S. Department of Defense Common High Performance Computing Software Support Initiative (CHSSI).