

The promise and challenge of Multiple scattering based large scale simulation within density functional theory

Don Nicholson

Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

Multiple Scattering Theory (MST) for electrons will be reviewed. Examples of calculations performed with the Locally Self-consistent Multiple Scattering (LSMS) code will be given. Many of these examples will be for systems containing thousands of atoms and in a coarse-grained approach system sizes as large as a million atoms will be illustrated. Limitations and future directions for LSMS will be discussed.