Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Objective Molecular Dynamics with Self-consistent Charge Density Functional Tight-Binding (SCC-DFTB) Method[1] TRAIAN DUMITRICA, University of Minnesota, BEN HOURAHINE, University of Strathclyde, BALINT ARADI, THOMAS FRAUENHEIM, University of Bremen — We discus the coupling of the objective boundary conditions [1] into the SCC density functional-based tight binding code DFTB+[2]. The implementation is enabled by a generalization to the helical case of the classical Ewald method, specifically by Ewald-like formulas that do not rely on a unit cell with translational symmetry [3]. The robustness of the method in addressing complex hetero-nuclear nano- and bio-fibrous systems is demonstrated with illustrative simulations on a helical boron nitride nanotube, a screw dislocated zinc oxide nanowire, and an ideal double-strand DNA. [1] T. Dumitrica and R. D. James, J. Mech. Phys. Solids 55, 2206 (2007). [2] B. Aradi, B. Hourahine, and T. Frauenheim, J. Phys. Chem. A 111, 5678 (2007). [3] I. Nikiforov, B. Hourahine, B. Aradi, Th. Frauenheim and T. Dumitrica, J. Chem. Phys. 139, 094110 (2013).

[1]Work supported by NSF CMMI 1332228.

Traian Dumitrica
University of Minnesota

Date submitted: 10 Nov 2016 Electronic form version 1.4