Simulation of nanostructures with helical symmetry using helical boundary conditions

David Teich[1]*, Gotthard Seifert[1], David Tománek[2], Zacharias G. Fthenakis[2]

1 Physikalische Chemie, Technische Universität Dresden, Germany
2 Physics and Astronomy Department, Michigan State University, USA

Quantum mechanical calculations of periodic structures are usually performed by using translational periodic boundary conditions. However, ab initio methods formulated in the typical periodic boundary condition context are computationally very time consuming for helical structures consisting of a large unit cell. A more elegant way is to utilize the helical symmetry of helical structures by introducing helical boundary conditions. This leads to a reduction in the system size to an objective domain containing a minimum of atoms. We present the combination of helical boundary conditions with the density functional based tight binding method by using symmetry-adapted Bloch functions. Instead of translational k-points, the orbital symmetry is described with helical quantum numbers. As an example, the calculation of the deformation energy of a twisted carbon nanotube rope is shown [1].

* Email of the corresponding author: david.teich@chemie.tu-dresden.de

[1] David Teich, Zacharias G. Fthenakis, Gotthard Seifert, and David Tománek, *Nanomechanical energy storage in twisted nanotube ropes*, Phys. Rev. Lett. **109** (2012) 255501.