Recent Applications of DFTB Objective Molecular Dynamics (OMD) to Nanomechanics of Carbon Nanotubes (CNTs) and Few-layer Graphene (FLG)

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Abstract

In this talk, I will give a brief overview of the implementation of objective molecular dynamics in DFTB+ and a demonstration of its applicability in two recent works:

- Collapsed CNTs are potential building blocks in the development of ultra-strong lightweight composite materials. However, their mechanical properties and packing are not well understood. Atomistic calculations with DFTB OMD allow for the identification of the an elastic beam model of a collapsed CNT, which is further used to derive an ultra-coarse-grained representation useful for simulating a large number of such nanotubes. DFTB is further used to understand packing of collapsed CNTs. In spite of the size dependence of the collapsed loop edges on the number of CNTs walls, high density graphitic packing into a stacking with dislocation mode is possible in single-, double-, and triple-walled CNTs.
- Bent few-layer graphene (FLG) as large-radii (up to 45 nm) are modeled as infinitely-long multi-walled nanotubes in order to uncover its bending rigidity. Bending of ABA-stacked FLG simulated with DFTB OMD allow to evaluate the impact of interstitial defects and interlayer sliding onto FLG flexibility. We reveal a contrasting behavior: On one hand, inter-layer interstitials that bond to four carbon atoms located on two adjacent bent layers are stable and able to preserve the plate-like bending rigidity. Thus, introducing inter-layer interstitials can be an effective way to maintain the plate-like rigidity of FLG by preventing layer sliding. On the other hand, inter-layer sliding dramatically lowers the bending constant and makes FLG nearly as flexible as the on-atom thick graphene. In this process we discovered non-classical low-energy rippling modes characterized by wavelengths as small as a few nm and large local curvatures, which are distributed non-uniformly across the FLG thickness.

The talk will conclude with an example of the applications of OMD DFTB to nanostructures with dislocations and a discussion of the potential applications of the method to understand phonon scattering on dislocations.