Atomistic far-field currents in graphene – how to include DFT-precision regions in large-scale tight-binding

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Graphene has proven to host outstanding mesoscopic effects involving massless Dirac quasiparticles travelling ballistically over several μm [1]. Atomistic large-scale simulations of the current distribution far from the injection source ("far-field currents") in graphene are accessed via the tight-binding (TB) model for π-orbitals, where specific parametrizations can be used to include a wide variety of effects such as p-n junctions, magnetic fields or absorptive apertures [2,3,4]. These simple empirical models, however, cannot capture the chemical details of the injection region and/or defects, which are of highest importance due to localized effects such as e.g. charging effects and deformations.

Here we present an atomistic multi-scale method to include regions treated with Density Functional Theory (DFT) into large-scale parametrized TB models within the context of non-equilibrium Green's function (NEGF) transport calculations. We will show how the far-field currents look by injecting electrons from DFT-precision STM tips in atomic contact with graphene-based devices and highlight how the symmetry of the states at the point contact are reflected in the far-field. We will also provide an overview of the used computational methods, based on the TranSiesta, TBtrans and sisl toolboxes [5,6], whose combination allows for extreme scale NEGF transport calculations.

References

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Figures

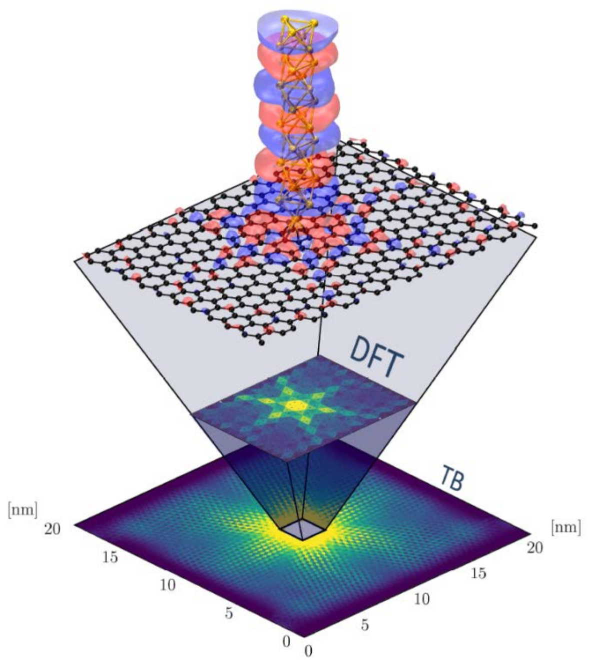

Figure 1. DFT-precision region with STM tip in atomic contact with graphene, embedded into a larger TB pristine graphene region. The six-fold symmetry of the transmission eigenchannel (top) is reflected in the near- and far-field currents observed in DFT (center) and in the larger TB (bottom).