Atomistic far-field currents in graphene using DFT-precision regions - how to couple DFT and 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]. These simple empirical models, however, cannot capture the chemical details of the injection region and/or defects, which is of highest importance due to localized effects such as e.g. charge-effects and deformations.
Here we present an atomistic multi-scale method for including regions treated with Density Functional Theory (DFT) into large-scale parametrized TB models. We will show how the far-field currents look by injecting electrons from DFT-precision STM tips in atomic contact with graphene 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 [4,5], whose combination allows for extreme scale non-equilibrium Green’s function transport calculations.

References

[1] Banszerus et al., Nano Letters 16 (2016) 1387
[2] Bøggild et al., Nature Communications, 8 (2017)15783
[3] Liu et al., Phys. Rev. Lett. 118 (2017) 066801
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[5] Papior, sisl, 10.5281/zenodo.597181

Figures

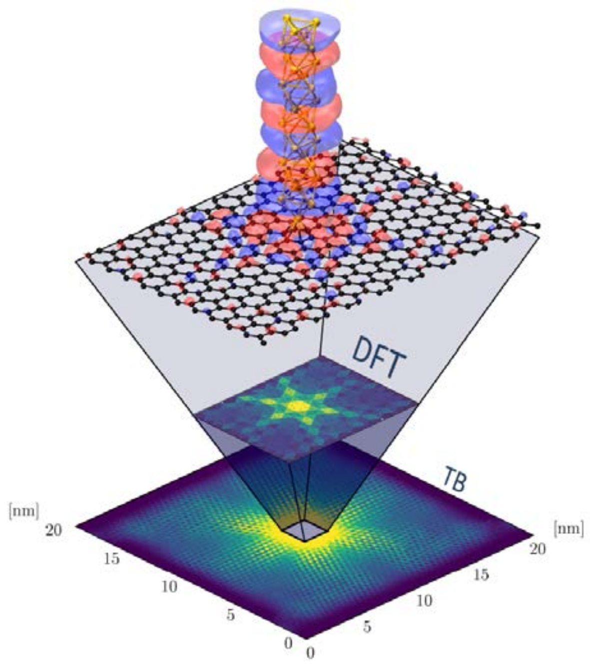

Figure 1: DFT-precision region with STM tip in atomic contact with graphene, embedded into a larger TB pristine graphene region. The six-fold symmetry of the transmission eigenchannel (top) is reflected in the near- and far-field currents observed in DFT (center) and in the larger TB (bottom).