Atomistic large-scale simulations of transport in ballistic graphene

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Graphene exhibits astonishing mesoscopic effects hosting massless Dirac quasiparticles that can travel with little scattering and behave like light rays [1]. Electrons in graphene devices undergo negative refraction when passing p-n junctions and can be manipulated by external electromagnetic fields, paving the way to a new concept of electronics based on the principles of optics [2]. One interesting perspective is a "2D Dirac fermion microscope" (DFM), where electron guns, tunable lenses, deflectors, and detectors are combined in a graphene "vacuum chamber" to image different types of targets [3]. We perform multi-scale simulations of ballistic graphene devices starting from atoms, combining density functional theory (DFT) and large-scale tight-binding (TB) models in a non-equilibrium Green's functions (NEGF) framework. Using NEGF+TB we reproduce key features of electron transport in a DFM, such as electron beam collimation, deflection and scattering off circular p-n junctions, supporting and extending the results of semiclassical simulations [3]. Pushing towards full atomistic detail, we develop a simple multi-scale approach to locally couple accurate DFT and large-scale TB+NEGF models, based on coupling through a real-space-projected self-energy. We adopt this method to calculate and visualize far-field currents injected from a DFT model of a gold tip in atomic contact with graphene.

References

[1] Cheianov et al., Science, 315 (2007) 1252
[2] Chen et al., Science, 353 (2016) 1522
[3] Bøggild et al., Nature Communications, 8 (2017) 15783

Figures

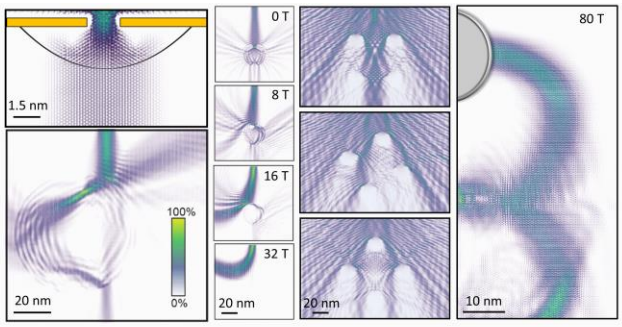

Figure 1: NEGF+TB simulations of a DFM: geometry and bond-currents for various beams and targets [3].

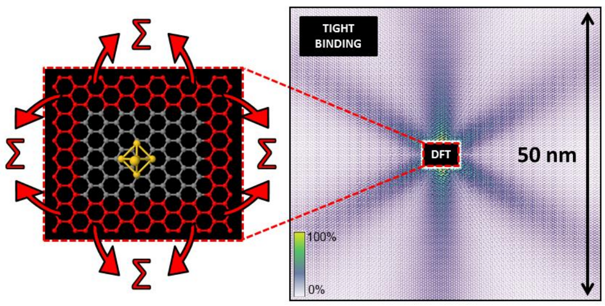

Figure 2: Far-field currents injected from a gold tip in atomic contact with graphene, obtained by coupling DFT with large-scale TB+NEGF models.