DFT-NEGF calculations of gated graphene nano-structures

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Abstract

First-principles modeling of electrostatic gating is important for characterization of transistor-like systems at the atomic scale. In 2D materials, such as graphene, one can control the Fermi level and electronic states involved in transport by gating, as well as achieve gate/device separations on the order of a few Angstroms due to the thinness of graphene [1–3].

We use DFT-NEGF calculations by considering a variety of technologically relevant 2D structures of different chemical and physical characteristics. Specifically we focus on the interplay between charge accumulation/depletion and the electric field in these.

To accomplish this task we have implemented a gating feature in the SIESTA package which can be used to simulate homogeneous and inhomogeneous charge distributions, thus allowing us to model electrostatic gates but also trapped charges without resorting to empirical parameters [4–6]. Our implementation gives results consistent with ∞-dielectric medium calculations in the homogeneous case [7].

We consider the effect of gating a graphene nanoconstriction with hydrogen terminated edges connecting two graphene leads. Such constrictions are known to have electronic resonances due to the diffraction barrier at abrupt interfaces [8]. We examine how a gate can be used to tune the position of the electronic resonances, however less linearly than expected, and hereby changing what states drive the current through the device.

In Fig. 1(left figures) we show the charge density redistribution for a non-gated and a gated (p-type) nanoconstriction. Interestingly, the left-right symmetry is broken and the potential profile is concentrated where the resistivity dipoles are mostly dominant as can be seen in Fig. 1(right figures). This effect can be traced back to the difference between the density of states in the two leads when a gate is applied. One can therefore utilize a gate to engineer the local potential drop across such constrictions.

Additionally, we will compare the effect of gating with that of donor and acceptor adatoms and examine the role of a gate on functionalization and adatoms in the device.

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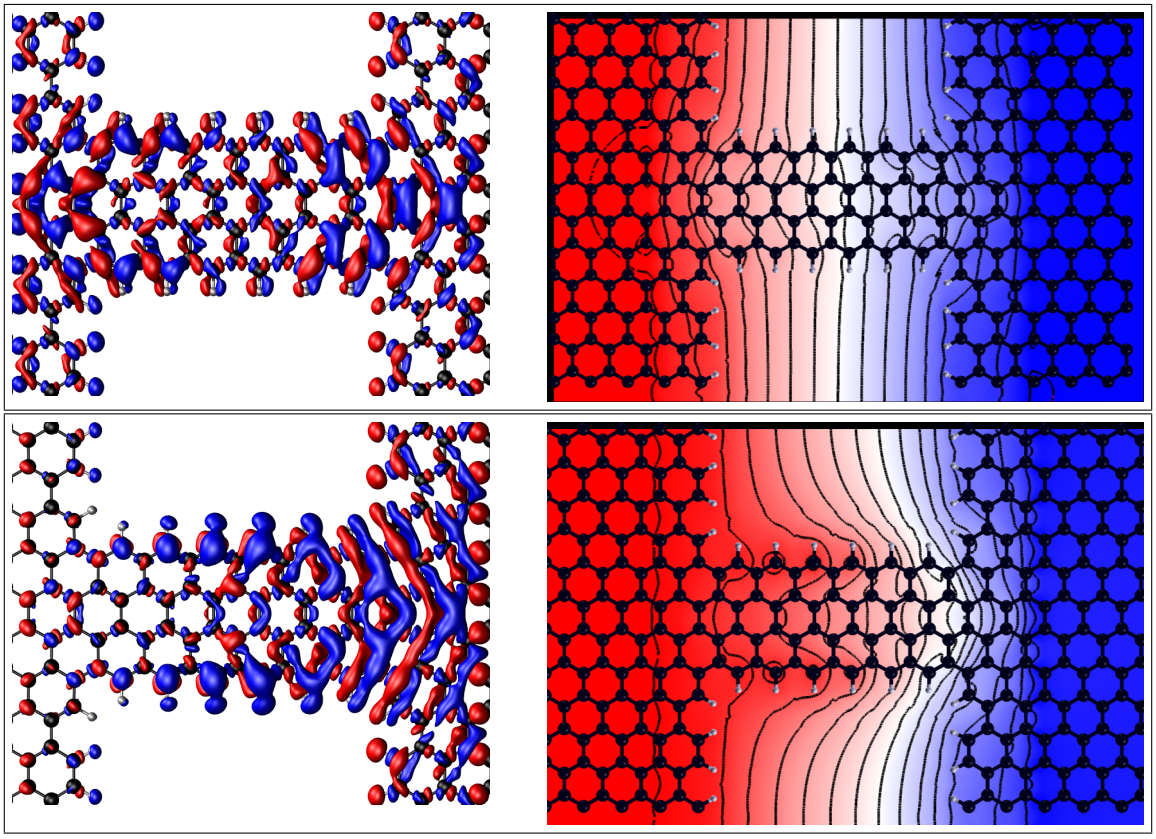

Figure 1: Charge redistribution with respect to $V_{\text{bias}} = 0\,\text{V}$ (left figures) and potential drop (right figures) of the nano-constriction device upon application of a $V_{\text{bias}} = 0.5\,\text{V}$. Top panel shows the case for no doping $n = 0e$ and bottom panel show $n = -0.5e$ (p-type).