Transport in and into graphene: Insights from transport calculations

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Devices based on stacked van der Waals heterostructures of two-dimensional (2D) materials are promising candidates for future atomically thin, flexible electronics. A key advantage is precise control of the carrier density by a gate. Atomistic first principles transport calculations, which can take voltage biases, currents, and gate potentials into account, can yield important insights into the behaviour of the novel device architectures and phenomena based on the 2D materials.
I will in the talk illustrate this point by presenting examples of transport calculations based on Density Functional Theory combined with non-equilibrium Green's functions (DFT-NEGF) [1], or the Boltzmann equation [2].

The examples include the role of the gate potential for the contact resistance between 2D materials, and how it depends on the stacking order and gate position (see Fig. 1)[3], gate-induced flexural electron-phonon scattering mechanism in graphene[4], the critical role of phonon-scattering in point-contacts to graphene[5], and finally, the dependence of contact resistance on the metal used for contacting graphene edges[6]

References

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Figures

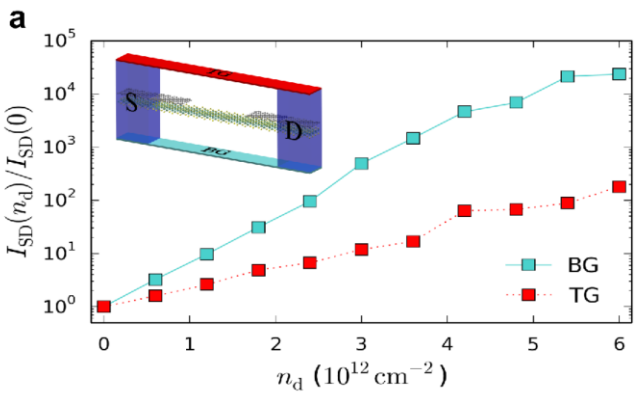

Figure 1: Source-drain current as a function of gate-induced carriers in a graphene-contacted MoS2 channel for gate at top or bottom (insert). From Ref. [3].