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DFT-NEGF calculations of gated graphene nano-structures
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Abstract
Two dimensional (2D) materials such as graphene are expected to be prominent candidates for nanoscale electronics applications. In particular the possibility to electrostatically gate 2D atomic scale structures is a key feature. Here we present non-equilibrium simulations of graphene nanostructures to illustrate a novel electrostatic gating implementation in SIESTA [1]. We test this model on a graphene nanocostruction and investigate the doping and the applied bias dependence on the transmission.

Implementation details
- Different gate geometries possible
- 2D materials only
- Electric field obtained from Poisson
- Self-consistent solution in SIESTA [1]

Transmission properties of gating nanoconstriction [2]
- Intrinsic transmission at 0 V
  - 1st peak
  - 2nd peak
- \( n = -2e^- \) transmission at different applied bias \( (V \text{ shifted vertically}) \), symmetric about applied bias
- 0.5 V transmission at different doping levels \( (n \text{ shifted vertically}) \)
- Transmission peak doping compared to graphene doping

Doping via adsorbates
- New electrostatic gating model implemented for SIESTA/TransSIESTA
- Investigating the model on a graphene nanocostruction
  - Gating is not the same as shifting Fermi-level
  - Features of transmission spectra does not shift linearly with \( \Delta V \)
  - Electronic structure can be tuned via doping
  - Potential drop across construction changes with doping, we can therefore tune the local potential drop by gating

Conclusion
- Localised potential drop could influence the reactivity
- Gating other graphene nanostructures could also show non-linear effects
- Currently investigating oxygen terminated nanocostruction

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