Electron-phonon scattering rates in graphene nanostructures

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Monte Carlo device simulators rely on tabulated electron-phonon scattering rates in order to account for the effects of optical and acoustical scattering on the carrier distribution (1). These rates are obtained from Fermi's Golden Rule (FGR), under the assumption of bulk electronic states (Bloch waves) and bulk phonons.
For graphene nanostructures, both assumptions cease to apply, as electron and phonon confinement may play an important role.
We have developed a methodology that couples a Wannier function-based model tight-binding constructed from a first-principles dispersion relation (2) (Figure 1) for the description of electronic properties, to an atomic trajectory obtained from molecular dynamics (3)(4) (Figure 2). From this we can numerically solve the time-dependent Schrödinger equation in tens of thousands of atoms in a graphene nanostructure under the action of a single phonon or a thermal bath, and perform a direct extraction of the electron-phonon scattering rates, as well as a critical appraisal of the validity of FGR at the nanoscale.

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References

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Figures

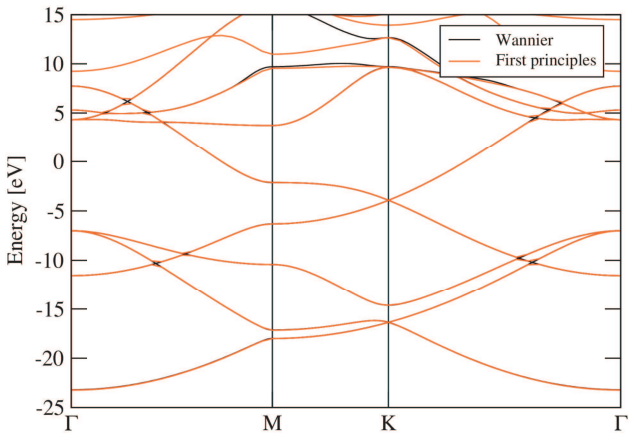

Figure 1: Graphene band structure calculated from first-principles and from Wannier functions.

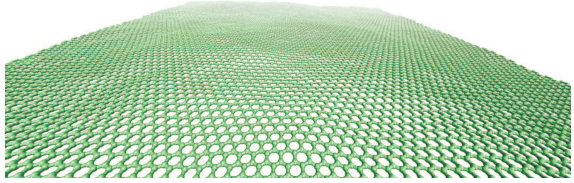

Figure 2: Graphene under a thermal bath.