Theoretical investigation of carrier mobility in new carbon electronic materials - a first-principle Boltzmann approach

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New carbon electronic materials include carbon nanotube, graphene, graphdiyne, etc. Charge mobility up to a few hundred thousand to million cm^2/Vs can be realized in such materials, which are the promising key component for the next generation electronics. The electron is well delocalized in such materials, with electron coherence length matching with acoustic phonon wavelength. We apply the Boltzmann Equation under the relaxation time approximation coupled with first-principles calculation to calculate the room-temperature charge mobility in graphene [1], graphdiyen, and carbon nanotubes. The relaxation time arises from the electron-acoustic phonon scattering and can be evaluated through Shockley-Bardeen's deformation potential theory. Exotic size-dependent mobility and polarity have been numerically observed for the graphene nano-ribbon, which can be well justified through the frontier orbital picture for the confined system.

[1] Mengqiu Long, Ling Tang, Dong Wang, Linjun Wang Zhigang Shuai, J Am Chem Soc 131, 17728 (2009).