Inelastic electron tunneling spectroscopy on graphene from first principles

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In recent years, phonons and electron-phonon coupling mechanism in graphene sheets have been extensively studied both from a experimental and a theoretical point of view [1–4]. Here we present our first principles calculations of the inelastic electron tunneling spectra (IETS) of a graphene sheet coupled to two monoatomic gold chains using the DFT code Inelastica [6]. Calculations were repeated for increasing size of the graphene supercell and for different positions of the gold electrodes with respect to the surface. Also, different coupling regimes have been analysed. Motivated by recent experimental results [5], we think it could be important to extend the existing model in the next future to include second order emission processes. Also, since calculations were converged just for the Γ-point inside the Brillouin zone, modelling phonons dispersion in the x-y plane could give further insights into the IET spectra of graphene.

References

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