First principles simulations of inelastic tunnel spectroscopy on graphene

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Experiments employing electron inelastic tunnel spectroscopy (IETS) performed using scanning tunnel microscopy(STM) on pristine graphene has revealed the importance of electron-phonon interactions in STM on graphene[1,3]. However, IETS can in principle also be a powerful tool for obtaining local information about defects such as adsorbates or grain boundaries. Here we present first principles calculations based on density functional theory (DFT) and non-equilibrium Greens functions in order to investigate how IETS can yield local information. Unique to graphene [1-3] the experimental results show a very prominent conductance gap in the tunneling spectra (tunnelling conductance vs. voltage). These spectra have been obtained depending on gate voltage, and the inelastic electron-phonon scattering mechanism has been established through a tight binding approach [4].

We perform first principles transport calculations using the TranSIESTA code in conjunction with SIESTA [5,6] (Fig 1a). Electronic coupling to the vibrations in graphene is included, with a lowest (second) order expansion of the self-consistent Born approximation [7,8]. We first demonstrate how these results on pristine graphene at different gate voltages can be reproduced using our methods for a suspended graphene sheet (Fig. 1b). We find that the conductance gap is independent of change in the gate voltage and increase of the tunnelling distance, as in experiments [1].

We then test the stability of the gap feature with respect to various modifications of the pristine graphene lattice. We find that hydrogen adsorbates on the graphene lattice quenches the gap feature locally, due to the introduction of short range protrusions. This effect is seen for hydrogenation on either side of the graphene sheet (Fig 1c). Near a hydrogen passivated armchair edge, the gap is also quenched. This should lead to local conductance enhancement near edges at low bias energy that cannot be attested to localized electronic states. In the presence of a Stone-Wales defect we find that the gap is only altered slightly due to low energy out-of-plane phonon modes. The low energy modes are a result of the instability of graphene near defect sites which can be related to long-range out-of-plane corrugations of graphene. Thus IETS may yield information about the local vibrational structure and instabilities towards corrugation.

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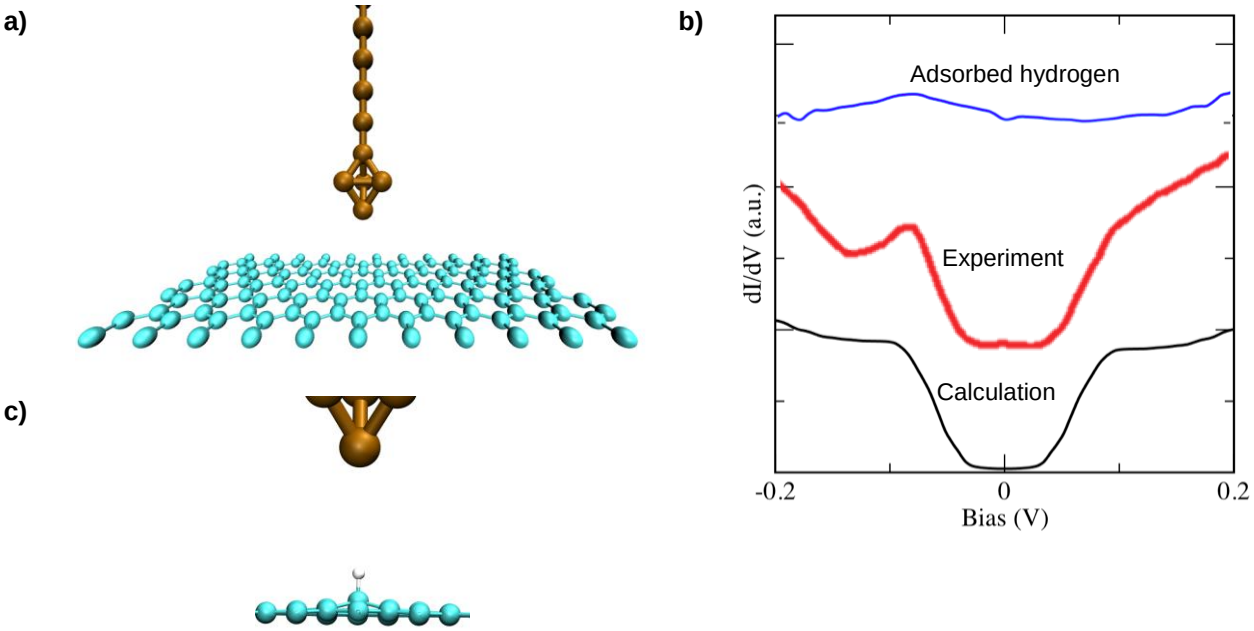

Fig 1: (a) System setup with semi-infinite leads on both graphene ends and a model STM made of a 4 atom gold cluster (b) Differential conductance spectrum for: Experimental results, fitted to the principal axis (red) [1], dI/dV calculation of STM on pristine graphene (black) and graphene hydrogenated system (blue). (c) Graphene with hydrogen impurity.