Molecular electronics: controlled manipulation, noise and graphene architecture

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propositions

Molecular electronics: Controlled manipulation, Noise and Graphene architecture

1. Controlled lifting of a monoatomic gold chain shows conductance parity-oscillations, fixing its phase to give a maximum for even numbers of atoms in the chain. (*Chapter 2 of this thesis*)

2. The real-time molecular manipulation simulator using a graphics processing unit will be useful not only for molecular electronics but also for other scanning probe microscope based manipulation experiments. (*Chapter 3 of this thesis*)

3. Inelastic electron-phonon interactions are not unique in giving rise to non-linearities in the shot noise. Even purely elastic electronic interactions with defect sites can give rise to non-linear, asymmetric shot noise as a function of bias. (*Chapter 5 of this thesis*)

4. The measurement of noise due to two-level fluctuations excited at the vibrational energies of a molecule can be useful when elastic interactions dominate the differential conductance spectra. (*Chapter 6 of this thesis*)

5. The principle of scanning tunnelling microscope based cutting of graphene by current pulses is a result of controlled localized electro-burning. (*Chapter 7 of this thesis*)

6. In the absence of spectral information, the observed enhancement in noise reported by Chen *et al.* cannot be uniquely attributed to inelastic interactions. (*Nature Sci. Rep.* ***4****, 4221, (2014)*)

7. The three electrodes implementation using graphene to study single molecules shown by Puczkarski *et al.* provides an attractive idea of scaling to multi-molecule circuits. (*App. Phys. Lett.* ***107****, 133105, (2015)*)

8. Recently, Green *et al*. have demonstrated controlled lift-off of single molecules by using a scanning tunnelling microscope. This method requires statistics on different possible trajectories. Use of real-time force-field simulations to aid experiments for controlled lift-off of single molecules as demonstrated in this thesis will avoid the need to collect such statistics. (*Beilstein J. of Nano.* ***5****, 1926, (2014)*)

9. Recent experiments done on a free-standing single molecule using scanning tunnelling microscopy shows that the changes in the symmetry of molecular orbitals with respect to the corresponding orbitals of the metallic leads can strongly affect the conductance measurement. This is something which

cannot be controlled or monitored using break-junction measurements. (*Phy. Rev. Lett.* ***119****, 066801 (2017)*)

10. Control of the positions of scattering sites by a designed molecular system can provide tuneable functionalities.
11. The numeric height of a gold atomic step on a Au(111) surface (in Ångström) to good approximation equals the ratio between the full width half maximum to the standard deviation of a Gaussian distribution *i.e.,* $2\sqrt{2\ln 2}$.
12. Progress in molecular electronics would benefit from international coordination analogous to the International Technology Roadmap for Semiconductors (ITRS).
13. It is widely believed that the last year of a PhD research project is the most productive. However, the time elapsed also helps in getting a better feel for the value of the results obtained in the earlier years.

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