Elastic and inelastic electron transport simulations from first principles - new methods and effects

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The effects of electronic current on the atomic structure of nano-scale conductors have become accentuated with the continued down-scaling of electronics. In the extreme scaling limit the position of a few atoms may control the operation of a nano-scale device. Thus it is important to be able to investigate the effects of atomic geometry on the transport and of the current on the atomic geometry. Due to the complexity of the problem computer simulations play an important role. We present theory based on non-equilibrium Greens functions (NEGF) in combination with density functional calculations as implemented in the SIESTA, TranSIESTA, and Inelastica packages [1]. We present examples of first principles simulations of the interplay of the electronic current and atomic dynamics and in metallic and molecular contacts, as well as in graphene-based nano-junctions in the presence of electrostatic gating.

The energy exchange between electrons and vibrations which can be detected in current spectroscopy, and yield information about the electronic resonance structure in the junction [2]. This provides an opportunity for direct comparison between experiments and theory. On the other hand, we demonstrate how a high current density can lead to other energy-transfer mechanisms than the local Joule heating in the junction. In particular, the current can cause several types of instabilities [3,4,5,6,7].

References

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