Atomic-scale engineering of electrodes for single-molecule contacts

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The transport of charge through a conducting material depends on the intrinsic ability of the material to conduct current and on the charge injection efficiency at the contacts between the conductor and the electrodes carrying current to and from the material. To explore if this remains valid down to the limit of single-molecule junctions, experiments with atomic-scale control of the junction geometry is required.

Here we present a method for probing the current through a single C_{60} molecule while changing, one by one, the number of atoms in the electrode that are in contact with the molecule [1]. We show quantitatively that the contact geometry has a strong influence on the conductance. We also find a crossover from a regime in which the conductance is limited by charge injection at the contact to a regime in which the conductance is limited by scattering at the molecule. Thus, the concepts of ‘good’ and ‘bad’ contacts, commonly used in macro- and mesoscopic physics, can also be applied at the molecular scale.

To interpret the experimental observations we performed electronic structure calculations for different contacting configurations to a C_{60} molecule sandwiched between Cu(111) electrodes [1,2]. The calculations reproduce the experimental behavior and explain the crossover from cluster-size limited to molecule limited transport regimes in terms of projected density of states and position of the molecular resonances.

References:

[1] G. Schull, T. Frederiksen, A. Arnau, D. Sanchez-Portal, and R. Berndt, Nature Nanotechnology **6**, 23-27 (2011).
[2] G. Schull, T. Frederiksen, M. Brandbyge, and R. Berndt, Phys. Rev. Lett. **103**, 206803 (2009).