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Metallic conductance in single-molecule junctions

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Through break junction techniques it has become possible to attach metallic wires to individual molecules. The actual presence of the molecule, its identity, and the numbers of molecules involved in the transport in many cases need to be deduced from measurements of current and voltage only. In parallel, several implementations of non-equilibrium Greens function approaches in combination with density functional theory have been developed in order to compute the properties of molecular junctions. For a sensitive test of the computational models there is a need for more detailed experimental observations on well-characterized model systems. In our experiments we focus on such model systems. They are simple, small molecules which have the advantage that they are relatively easy to handle in computations and they allow for more precise experimental tests at low temperatures. The molecules we have studied include H₂, H₂O, CO, CO₂, C₆H₆ (benzene), and C₆₀ contacted between Pt leads. The molecular levels hybridize strongly with the Pt metal giving rise to a high conductance. The presence of the molecules can be confirmed by the detection of vibration modes. These modes are visible in the differential conductance, dI/dV , as a function of voltage bias as fine steps at the energies $eV = \hbar\omega_n$ corresponding to those of the vibration modes. Further test involve isotope-substituted molecules and stretching of the molecular bridge in order to detect shifts in the energy of the modes. The conductance of a single-molecule bridge cannot be uniquely distinguished from bridges due to several parallel channels. However, by measuring shot noise, i.e. the intrinsic noise in the electron current, it is possible to show that the current is carried by a single molecule. For other molecules the measurement gives evidence that the molecule provides two, or sometimes more channels for conductance. The results are compared with state of the art non-equilibrium DFT calculations.