Resonant transport and electrostatic effects in single-molecule electrical junctions

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In this contribution, we show a combined theoretical and experimental study on the electronic transport through metal–molecule–metal junctions. The molecules consist of a benzene ring held between alkanethiol chains of four different lengths. The Breit-Wigner resonance was found to originate from one of the arene–bonding orbitals, which sharpens and moves closer to the contact Fermi energy as n increases. Varying the number of methylene groups thus leads to a very shallow decay of the conductance with the length of the molecule. By DFT (Density Functional Theory)+NEGF (Non Equilibrium Green’s Function) techniques and cDFT (Constrained DFT) we demonstrate that the electrical behaviour observed here can be straightforwardly rationalized by analyzing the effects caused by the electrostatic balance created at the metal–molecule interface [1]. Such resonances offer future prospects in molecular electronics in terms of controlling charge transport over longer distances, and also in single molecule conductance switching if the resonances can be externally gated.