A Molecular Platinum Cluster Junction: A Single-Molecule Switch

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Abstract

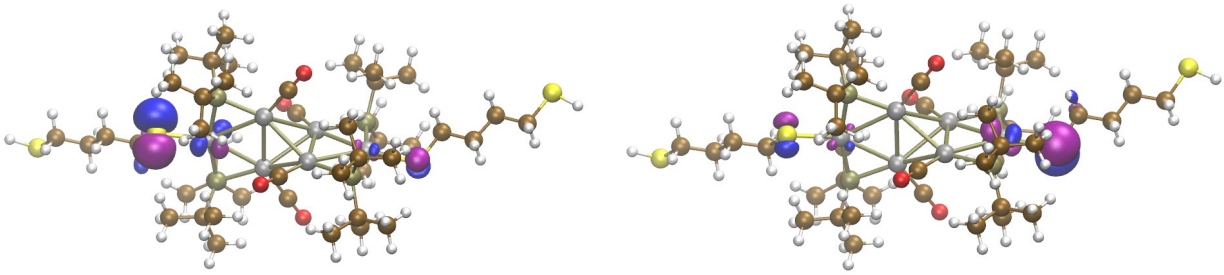
We present a theoretical study of the electronic transport through single-molecule junctions incorporating a Pt6 metal cluster bound within an organic framework ($(SC_4S)_2Pt_6$). In a previous experimental study [1] it was suggested that the presence of the Pt6 cluster creates an indentation in the potential barrier, giving a molecular analog of an inorganic double tunnelling barrier. This was, however, a speculative argument which was never fully proven, and neither was the nature of these states identified. In this study, we show that the insertion of this molecule between a pair of electrodes leads to a fully atomically engineered nano-metallic device with high conductance at the Fermi level and two sequential high on/off switching states [2]. The origin of this property can be traced back to the existence of a HOMO which consists of two degenerate and asymmetric orbitals, lying close in energy to the Fermi level of the metallic leads. Their degeneracy is broken when the molecule is contacted to the leads, giving rise to two resonances which become pinned close to the Fermi level and display destructive interference due to multiple electronic pathways through the molecule. These states, however, do not stem from the Pt unit alone, but specifically from two apical Pt atoms and their neighboring S atoms.

References

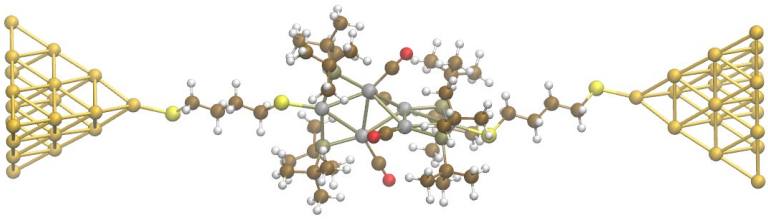
[1] Leary, E.; van Zalinge, H.; Higgins, S. J.; Nichols, R. J.; de Biani, F. F.; Leoni, P.; Marchetti, L.; Zanello, P. Phys. Chem. Chem. Phys., **11** (2009), 5198.

[2] L. A. Zotti, E. Leary, M. Soriano, J. C. Cuevas, and J. J. Palacios, J. Am. Chem. Soc., **135** (2013), 2052**.**

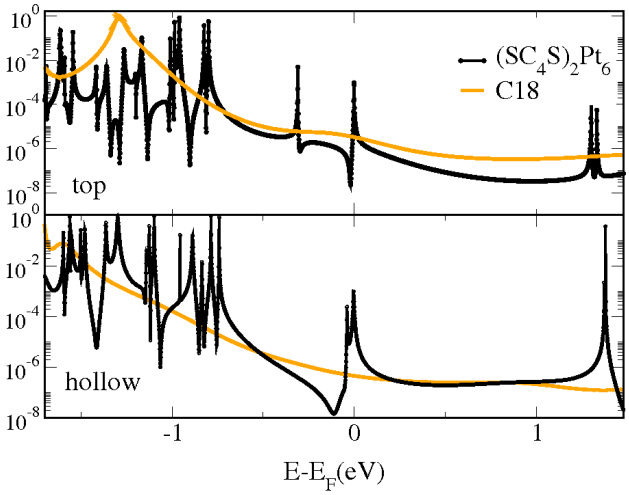
Figures



Optimized geometry of $(SC_4S)_2Pt_6$ with its two degenerate HOMO orbitals.



$(SC_4S)_2Pt_6$ embedded between two gold clusters.



Transmission as a function of energy for $(SC_4S)_2Pt_6$ and for an alkyl chain of the same length (C_{18}).