

## Bipolar conductance switching of single anthradithiophene molecules

R. Pétuya<sup>1</sup>, B. Borca<sup>2</sup>, V. Schendel<sup>2</sup>, I. Pentegov<sup>2</sup>, T. Michnowicz<sup>2</sup>,  
U. Kraft<sup>2</sup>, H. Klauk<sup>2</sup>, P. Wahl<sup>2,3</sup>, U. Schlickum<sup>2</sup>, K. Kern<sup>2,4</sup> and A. Arnau<sup>1,5</sup>

<sup>1</sup> *Donostia International Physics Center, E-20018 Donostia-San Sebastián, Spain  
(corresponding author: R. Pétuya, e-mail: remipetuya@gmail.com)*

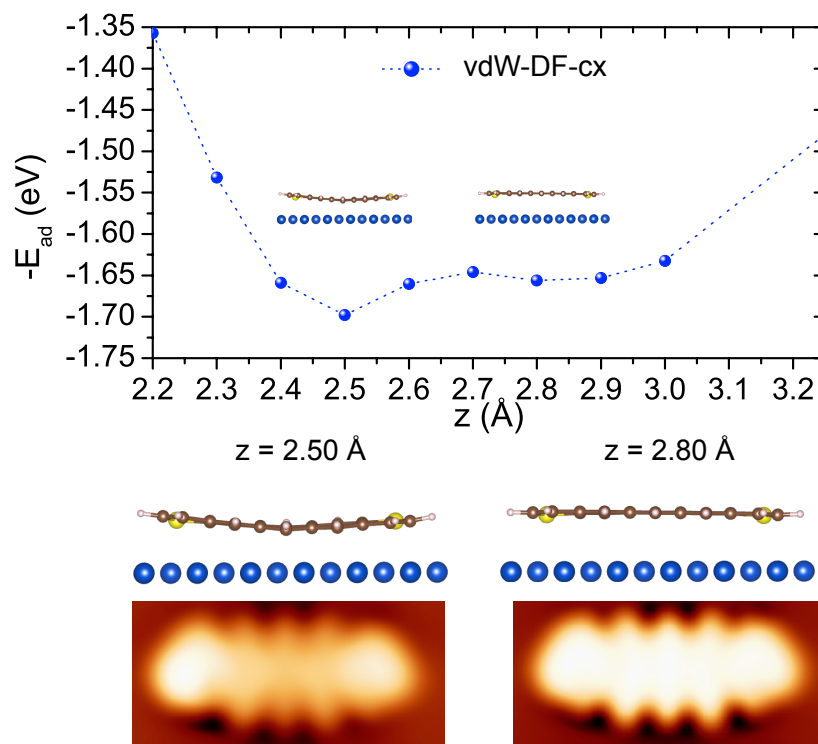
<sup>2</sup> *Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany*

<sup>3</sup> *SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16  
9SS, United Kingdom*

<sup>4</sup> *Institut de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne (EPFL),  
CH-1015 Lausanne, Switzerland*

<sup>5</sup> *Departamento de Física de Materiales UPV/EHU and Material Physics Center (MPC), Centro  
Mixto CSIC-UPV/EHU, E-20018 Donostia - San Sebastián, Spain*

Molecular electronics appears to be one of the great challenges in the nanoscience field of investigation [1]. Functional molecules, with ability to switch between two or more stable states, may have a promising future as logical component or for data storage purpose. Scanning Tunneling Microscope (STM) measurements have evidenced bipolar conductance switching process of anthradithiophene (ADT) molecules (pentacene analogue) corresponding to bistable molecular adsorption conformations on Cu(111). First principle calculations using a vdW-DF-cx [2,3] approach are performed to investigate the switching mechanism locally activated by the STM tip apex. In agreement with a recently proposed model [4] of switching between different adsorption conformations of molecules on a metallic surface, we found that the two conductance states correspond to two different adsorption geometries [5]. In the “off” state, obtained upon evaporation, the molecules adsorb at short distance and adopt a bent geometry whereas in the “on” state, the molecule adsorb at larger distance from the surface with a flat geometry. In addition, the competing effects of the sulfur groups and the acene rings position with the substrate atoms in the adsorption geometry is scrutinized for the *cis* and *trans*-ADT isomers.



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