

Abstract Submitted  
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**Electron transport simulations through organic adlayers on metal surfaces**<sup>1</sup> MANUEL COBIAN, ICMAB - CSIC, NICOLAS LORENTE, PABLO ORDEJON, CIN2 - CSIC — Molecular entities at the interface with an inorganic surface are the basis for new hybrid functional materials for microelectronics. In most cases, strong bonding of molecules to metal surfaces perturbs the discrete molecular energy levels leading to a broadening of the molecular density of states. Deposition of  $C_{60}$  on a Au(111) surface previously exposed to tetraphenyladamantane give rises to a nanostructured organic layer where the electronic coupling between the  $C_{60}$  and the Au(111) surface is significantly reduced compared to  $C_{60}$  on a clean Au(111) surface. Calculations based on Density Functional Theory reveal that intermolecular interactions lock  $C_{60}$  into a particular orientation in agreement with Scanning Tunneling Microscopy experiments. This system exhibits the presence of negative differential resistance which can be understood by simulations of the transport properties at the ab-initio level using TRANSIESTA.

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