Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Zero-bias anomaly in thiol-bound molecular junction on Ag(111)
KEES FLIPSE, ERWIN ROSSEN, Eindhoven University of Technology, Eindhoven, The Netherlands, JORGE CERDA, Instituto de Ciencia de Materiales de Madrid, Madrid, Spain — Single molecule transistors are widely regarded as the successor of current silicon-based technology. To investigate the electronic properties of single molecules, they must be connected to the macroscopic world via electrodes. The most used linker group to connect the molecule to the metal leads is a thiol group. One feature that is often observed in these systems is a significant reduction (10-20%) in the conductance in a narrow region around the Fermi-level. While most authors choose to ignore this feature, it is in general attributed to excitations of the metal-sulphur mode and phonon interactions in the metal leads. We will discuss the origin of this zero-bias anomaly (ZBA) by presenting ab-initio calculation results in a Scanning Tunnelling Microscopy (STM) geometry for thiophenol molecules adsorbed on Ag(111), indicating the important role of the inelastic contributions of low energy vibrational modes in charge transport.

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Date submitted: 14 Dec 2012 Electronic form version 1.4