Abstract Submitted
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Molecular conductance from density functional theory calculations DANIEL KOSOV, ZHENYU LI, University of Maryland — We will present a plane-wave/pseudopotential implementation of a method to calculate the electron transport properties of nanostructures. We performed density functional theory based electron transport calculations of amine, dithiocarboxylate and dithiiocarbamate anchored junctions. We demonstrated that the stronger molecule-electrode coupling associated with the conjugated dithiocarbamate linker broadens transmission resonances near the Fermi energy. The conductance enhancement factor is as large as 25 is predicted for dithiocarbame anchored junctions. A microscopic origin of the experimentally observed current amplification by dithiocarboxylate anchoring groups is established. We calculated the conductance traces for amine and thiol anchored junctions as the molecules are pulled by the STM tip from the Au electrode. Our calculations show that the stretching of the thiol anchored junction during its formation is accompanied by significant electrode geometry distortion. Oppositely, the electrode for the amine terminated junction remains intact when the junction is stretched by the STM tip. Z. Li and D. Kosov, J.Phys.:Cond.Matt. 18 (2006) p.1347; J.Phys.Chem B 110 (2006) p.19116, ibid p.9893

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