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Identification of the Atomic Scale Structures of the Molecule-Metal Interfaces of Single-Molecule Nanowires[1] FIRUZ DEMIR, GEORGE KIRCZENOW, Simon Fraser University, Burnaby, Canada — We show theoretically how inelastic tunneling spectroscopy can identify the atomic scale structures of the molecule-metal interfaces of single-molecule nanowires bridging pairs metal electrodes, and thus resolve a long standing problem that is central to the field of single-molecule nanoelectronics. As an example we consider the propanedithiol (PDT) molecules bridging gold nanocontacts in the recent experiment of Hihath *et al.* [Nano Lett. **8**, 1673 (2008)]. Based on *ab initio* density functional and semi-empirical calculations we identify the features observed in the experimental inelastic tunneling spectra of these molecules at phonon energies near 46, 40 and 42 meV as arising from sulfur atoms (that have lost their thiol hydrogen atoms) bonding to the gold contacts in top site, bridge site and mixed bridge-top site geometries respectively. PDT molecules in which the sulfur atoms retain their thiol hydrogen atoms and bond strongly to gold in the top site geometry give rise to an IETS feature in the phonon energy range 54-57 meV.

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