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Electron Transport in Single Molecule Junctions: Stability, Electron-Phonon Interactions and Current-Induced Local Heating

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Understanding electron transport in a single molecule connected to two electrodes is as basic task in molecular electronics. A widely used approach is to attach the molecule with two linkers that can bind to the electrodes. Thiol is the most studied linker because of its well known capability to bind strongly to metal electrodes, such as Au, although several other linkers, such as isocyanide, amine, pyridine, carbon-carbon and carboxylic acid, have also been used to establish a molecule-electrode contact. It has been concluded that the linkers can play an important or even dominant role in the conductance and other electron transport properties of molecular junctions. Since the molecule-electrode contact is often the weakest link in a molecular junction, an important question that has not yet been well studied is: *How stable is a molecular junction due to the finite lifetime of the linker-electrode bond?* Another important question is: *How hot does a molecular junction get when passing a current through it?* In the present work, we investigate the stability and breakdown mechanism of a single molecule covalently attached to two gold electrodes via Au-S bonds. We report on an experimental study of current-induced local heating in single molecules covalently attached to two gold electrodes as a function of applied bias and molecular length. We also discuss the related electron-phonon interactions in single molecule junctions.