

NW-P033

Origin of Multiple Conductance Peaks in Single-Molecule Junction Experiments

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One of the most important yet unresolved problems in molecular electronics is the controversy over the number and nature of multiple conductance peaks in single-molecule junctions. Currently, there are three competing explanations of this observation: (1) manifestation of different molecule-electrode contact geometries, (2) formation of gauche defects within the molecular core, (3) involvement of different electrode surface orientations [1]. However, the exact origin of multiple conductance peaks is not yet fully understood, which indicates our incomplete understanding of the scientifically as well as techno-logically important organic-metal contacts. To theoretically resolve this problem, we previously applied a multiscale computational approach that combines force fields molecular dynamics (FF MD), density functional theory (DFT), and matrix Green's function (MGF) calculations [2] to a thermally fluctuating hexanedithiol (C6DT) molecule stretched between flat Au(111) electrodes, but could observe only a single conductance peak [3]. In this presentation, using DFT geometry optimizations and MGF calculations, we consider molecular junctions with more realistic molecule-metal contact conformations and Au(111) electrode surface directions. We also conduct DFT-based molecular dynamics for the highly stretched junction models to confirm our conclusion. We conclude that the S-Au coordination number should be the more dominant factor than the electrode surface orientation.

Keywords: Molecular electronics, Single-molecule, Multiple conductance peaks