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Molecular Simulations of The Formation of Gold-Molecule-Gold Junctions HUACHUAN WANG, The George Washington University — We perform classical molecular simulations by combining grand canonical Monte Carlo (GCMC) sampling with molecular dynamics (MD) simulation to explore the dynamic gold nanojunctions in a Alkenedithiol (ADT) solvent. With the aid of a simple driving-spring model, which can reasonably represent the long-range elasticity of the gold electrode, the spring forces are obtained during the dynamic stretching procedure. A specific multi-time-scale double reversible reference system propagator (double-RESPA) algorithm has been designed for the metal-organic complex in MD simulations to identify the detailed metal-molecule bonding geometry at metal-molecule-metal interface. We investigate the variations of bonding sites of ADT molecules on gold nanojunctions at Au (111) surface at a constant chemical potential. Simulation results show that an Au-ADT-Au interface is formed on Au nanojunctions, bond-breaking intersection is at 1-1 bond of the monatomic chain of the cross-section, instead of at the Au-S bond. Breaking force is around 1.5 nN. These are consistent with the experimental measurements.

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