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Density Functional Study of a Typical Thiol on Perfect Au(111) Surfaces GUAN WANG, National Research Council Research Associate, WILLIAM SANDBERG, Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory, Washington, DC, STEVEN KENNY, Univ. of Loughborough, U. K. — We investigated systematically the static, dynamical and mechanical properties of a typical thiol-Au surface system at the density functional level. The computational approach uses optimized atomic-like orbits for efficiency and parallel computation. Ab initio results show the equilibrium configuration of the thiol on gold surfaces is in agreement with other computational methods. We found, from ab initio molecular dynamics simulations, that this tethering system keeps stable at 300, 350, and 370 degrees K. We studied the energy profiles that reflect the behaviors of the tethered thiol under normal and parallel stretches. The obtained rupture force is comparable with AFM measurements. We found the rupture force of thiols on gold surfaces is directional. We also show the process by which multiple successive ruptures of the tether occur with the surface. These results should be useful in understanding failure dynamics of tailored biosurfaces in microfluidic devices where fluidic sheer and normal forces are of concern.

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