

Abstract Submitted
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Isomerization of one molecule observed through tip enhanced Raman spectroscopy¹ YANXING ZHANG, Department of Physics and Astronomy, University of California, JOONHEE LEE, VARTKESS A APKARIAN, Department of Chemistry, University of California, RUQIAN WU, Department of Physics and Astronomy, University of California, RUQIAN WU, YANXING ZHANG TEAM, JOONHEE LEE, VARTKESS A. APKARIAN TEAM — While exploring photoisomerization of azobenzyl thiols (ABT) adsorbed on Au(111), through joint scanning tunneling microscopy (STM) and tip-enhanced Raman scattering (TERS) studies, the reversible photoisomerization of one molecule is captured in TERS trajectories. The apparently heterogeneously photo-catalyzed reaction is assigned to cis-trans isomerization of an outlier, which is chemisorbed on the silver tip of the STM. In order to clarify the role of the silver tip of the STM, we perform systematic density functional theory (DFT) calculations. The results show that compared with the case on the flat Ag(111) surface, the energy difference between trans and cis states of ABT decrease as we add one silver atom or a tetrahedron silver cluster on Ag(111) surface which mimic the geometry of a silver tip. In particular, the trans stretches away from the surface on the tetrahedral silver cluster, and the energy difference between trans and cis decreases to 0.27 eV, from ~ 1 eV for ABT on the flat Ag(111) surface. This significantly increases the possibility of cis-trans isomerization, as observed in our experiments.

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