

Abstract Submitted
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Single Molecule Mechanochemistry¹ SHAOWEI LI, Dept. of Chemistry, University of California, YANXING ZHANG, Dept. of Physics and Astronomy, University of California, WILSON HO, Dept. of Chemistry, University of California, RUQIAN WU, Dept. of Physics and Astronomy, University of California, RUQIAN WU, YANXING ZHANG TEAM, WILSON HO, SHAOWEI LI TEAM — Mechanical forces can be used to trigger chemical reactions through bending and stretching of chemical bonds. Using the reciprocating movement of the tip of a scanning tunneling microscope (STM), mechanical energy can be provided to a single molecule sandwiched between the tip and substrate. When the mechanical pulse center was moved to the outer ring feature of a CO molecule, the reaction rate was significantly increased compared with bare Cu surface and over Au atoms. First, DFT calculations show that the presence of CO makes the Cu cavity more attractive toward H₂. Second, H₂ prefers the horizontal adsorption geometry in the Cu-Cu and Au-Cu cavities and no hybridization occurs between the antibonding states of H₂ and states of Cu atoms. While H₂ loses electrons from its bonding state in all three cavities, the filling of its anti-bonding state only occurs in the CO-Cu cavity. Both make the CO-Cu cavity much more effectively to chop the H₂ molecule.

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