Abstract Submitted
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Manipulation of Single Molecular Hydrogen in a Size-tunable Nanogap[1] HUI WANG, Department of Physics, Fudan University, Shanghai 200433, China, HAIYAN HE, Department of Physics, University Science and Technology of China, Hefei, Anhui 230026, China, SHAOWEI LI, WILSON HO, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575, USA — The determination of weak bonds in physisorption systems remains as a major challenge for modern density functional approaches. In addition, it becomes important to use the tip of scanning tunneling microscope (STM) to manipulate chemical bonds. Here we study the adsorption geometries, translational and rotational motions, and vibrations of a single H2 molecule trapped in the gap of STM-tip and Au (110) reconstructed surface, using the density functional theory calculations. The tip-substrate separation is used as an adjustable parameters. We find that the stable adsorption geometry, H2 bondlength, H-H stretching frequency, and H2-Au bouncing frequency strongly depends on the tip-substrate distance. Computational results agree well with STM data, both indicate the strong role of STM tip on the behavior H2 motions. The new insights established through this work are useful for the understanding of puzzling observations, and should be applicable for the analysis of other physisorption systems.

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