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Rotational Spectroscopy at Sub-Angstrom Level: Rotationaland Vibrational Excitations of Molecular Hydrogen measured by the Scanning Tunneling Microscope SHAOWEI LI, ARTHUR YU, HUI WANG, FREDDY TOLEDO, ZHUMIM HAN, RUQIAN WU, WILSON HO, University of California, Irvine — The power of rotational spectroscopy has long been demonstrated in the frequency domain by microwave spectroscopy, but its application in real space has been limited. Using a scanning tunneling microscope (STM) and inelastic electron tunneling spectroscopy (IETS), we are able to conduct real-space measurements of rotational transitions of gaseous hydrogen molecules physisorbed on Au(110) surface at 10 K. The $j=0$ to $j=2$ rotational transition for para- H_2 and HD as well as the $v=0$ to $v=1$ vibrational transitions for H_2 , D_2 and HD were observed by STM-IETS. By varying the tip-substrate distance, we could precisely investigate how the environmental coupling modifies the structure, including the bond length, of a single molecule with sub-Angstrom resolution. Rotational spectroscopy at the single molecule level provides a powerful tool for chemical identification as well as bond length measurement in both the frequency and space domains.

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