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Atomic-Scale Inelastic Tunneling Probe of Molecular Potentials

WILSON HO, Univ of California - Irvine

The spatial distribution of the electrostatic potential of a molecule adsorbed on a solid surface reflects its structure and composition and further defines its chemistry. This potential can be probed by a carbon monoxide (CO) molecule attached to the tip of a scanning tunneling microscope (STM). In the inelastic tunneling probe (itProbe) with the STM, this CO molecule in the tunneling gap lies in an overall potential energy surface defined by its binding to the tip and its interaction with the potential of the adsorbed molecule. As the CO-tip scans over the adsorbed molecule, its vibrations are perturbed in energy, intensity, and line shape by variations in the three-dimensional landscape of the potential energy surface (PES) in which the CO is immersed. Spatial maps of the soft hindered translational mode of the CO reveal different features of the PES, such as the ridges and valleys, as the vibrational energy is related to the curvature of the PES. Thus the itProbe maps the gradient of the force on the CO molecule as it scans over the potential of the adsorbed molecule. These images reveal line features that reflect the skeletal structure of molecules and perturbations in space due to intermolecular interactions. Examples are given to illustrate such effects that illuminate the nature of chemical interactions when atoms are in close proximity of each other, leading to intramolecular interactions, and in the assembly of extended molecular structures involving weaker intermolecular interactions.