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Davisson-Germer Prize Talk: Structure and Reactivity of Surfaces in Vacuum and Under Ambient Gas Pressures

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The goal of surface science research is to provide atomic level understanding of the structural and dynamic properties of surfaces, a goal particularly relevant for chemical applications, including catalysis, photochemistry, batteries and fuel cells. With X-ray Photoemision Spectroscopy (XPS) we can determine the composition and electronic structure. With Scanning Tunneling Microscopy (STM) we can image atoms and molecules as they adsorb, diffuse and react on single crystal surfaces. STM uniquely permits to visualize and determine adsorbate-adsorbate interactions by making movies of their motion. I will show how water molecules diffuse, H-bond to each other, and wet the surface forming 2D films. We also imaged how H2 molecules adsorb and dissociate on a Pd surface, and how the movies revealed that a particular arrangement of substrate atoms is required to generate the active sites through fluctuations. To study surfaces in the presence of gases, in the Torr to Atmospheres range, which is relevant to practical catalysis, new instrumentation is needed. Over the last years we developed high pressure STM and XPS, which allowed us to study surfaces under high coverage of adsorbates in equilibrium with gases near ambient pressures and temperature. I will show how under these conditions the structure of surfaces can be very different from that at low coverage, or even at high coverage but at low temperature. Adsorbates can induce dramatic restructuring of the surface, as I will show in the case of CO on Pt and Cu. Equally important, reactions on catalyst surfaces can now be followed in real time, by measuring composition with XPS, and structure with STM, during the reactions to extract kinetic parameters.