ATOMIC LEVEL STUDIES OF SURFACE REACTIONS: THE NATURE OF ACTIVE SITES, ADSORBATE DIFFUSION AND THE ROLE OF IMPURITIES AND POISONS

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We have studied a number of surface processes involving adsorption, diffusion and chemical reactions of simple molecules. The studies are carried out in ultra-high vacuum using a variable temperature scanning tunneling microscope (STM). The STM provides a unique way to study diffusion pathways and to measure the diffusion parameters of atoms and molecules, which is an important step in any reaction. Because of its high spatial resolution, STM makes it possible to determine the influence of surface defects and impurities as they influence the diffusion. An interesting class of defects that has not been received sufficient attention is that of subsurface impurities. Such impurities are for example C and O, can be present as interstitial or substitutional defects in the second layer of metal atoms. We will show how they can strongly modify the diffusion and the binding of other adsorbates. In the same line, we will discuss another the important topic of the interaction between adsorbed species and the formation of interaction pairs and clusters. I will present several examples including CO, H2O, H2 and O2 on Pd(111), Ru(0001) and Ni(110). Finally I will present a study of the dissociative adsorption of H2 to answer the question of the nature of the active sites, in particular the number of empty sites required to dissociate a molecule.

Figure. Left illustration of the STM tip imaging a diatomic molecule. Right: STM image of Pd(111) at 40K with a nearly saturated monolayer of H atoms. The H atoms appear as small 5 pm depressions forming a 1x1 lattice. They form the small maxima and minima in the image. The large bright maxima are due to H vacancies in the saturated 1x1 surface. They are bright (about 25 pm protrusions) because the tunnel current is much larger when the tip is over an empty Pd site.