How hydrogen atoms bind to metal surfaces

Chemical reactions at surfaces are exceptionally complex as they require a multitude of elementary steps. The first step in every surface reaction is the adsorption of the participating atoms and molecules to the surface. Only if the translational energy carried by the particles and the binding energy are efficiently dissipated, adsorption can take place. A detailed understanding of the adsorption mechanism is an important step towards the development of a predictive theory of chemical reactions on surfaces.

In surface dynamics molecular beam methods combined with laser methods and ultra-high vacuum apparatuses are used to study this processes in detail. Commonly, adsorption is not studied directly but inelastic scattering. Such experiments give detailed information about the energy exchange between particle and surface. Scattering of atoms from surfaces is the simplest system one can investigate in surface dynamics. From all reactive atoms hydrogen is the simplest. These reasons make H-atom scattering from surfaces especially attractive for detailed comparisons between experiment and theory.

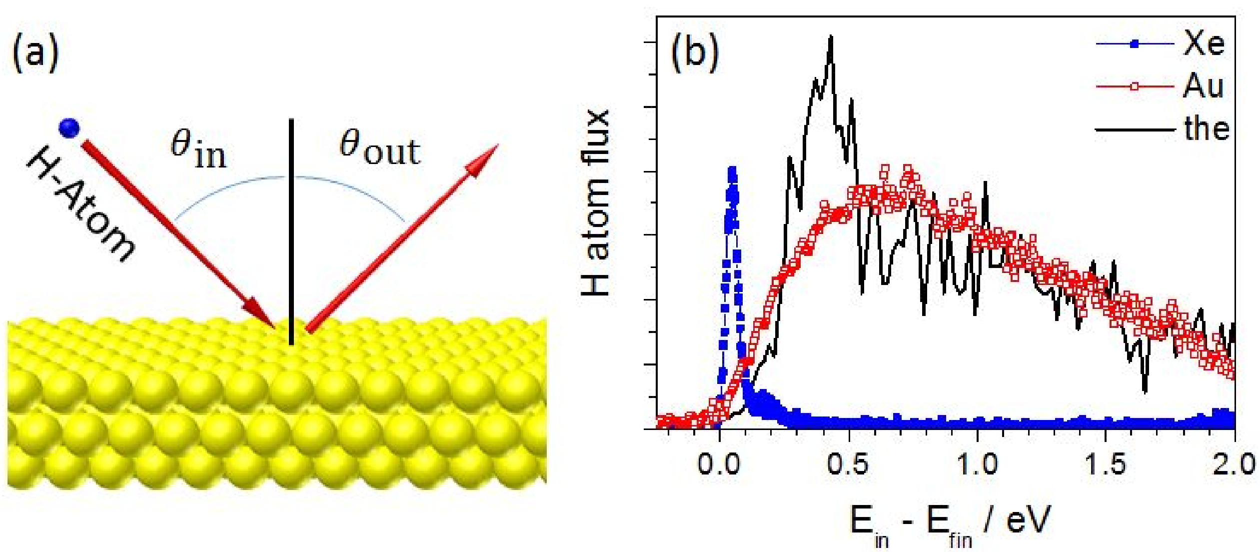

Fig. 1. (a) Experimental Concept. (b) Energy loss spectra for H-atoms scattered from a xenon and a gold surface in comparison to the theoretical model.

Furthermore, the efficient adsorption of hydrogen was a conundrum for a long time. Imagine a ping-pong ball strikes against a billiard ball. Everyone knows intuitively what happens: The ping-pong ball bounces back from the billiard ball while the billiard ball does not move. This is due to the large mass difference between the two balls. It prevents the ping-pong ball from effectively transferring its kinetic energy to the heavier billiard ball. When applying this simplistic picture to light hydrogen atoms striking heavy metal atoms at the surface of a solid metal, one would expect the hydrogen atom to bounce back from the surface. However, a completely different behavior is observed in experiments: The light hydrogen atom has a high probability to stick to the surface. It is this adsorption of atoms which makes chemical reactions at surfaces possible in the first place. Of course, scattering from a surface is much more complex than scattering from one atom. Furthermore, it was speculated for a long time that the energy can not only be transferred to the motion of the metal surface atoms but also to the electrons in the metal surface. In order to understand in principle how H-atoms adsorb to metal surfaces a new experiment was developed alongside a theoretical model.

Figure 1 (a) shows a schematic of the performed experiments. Hydrogen atoms with a defined speed and direction are shot at a surface. The speed as well as the direction of the scattered H-atoms is measured afterwards. Based on the speed lost in the collision one can calculate how much energy had been transferred from the hydrogen atoms to the surface. Two different surfaces were chosen: Gold and xenon. Both elements have completely different properties: Gold is an electric conductor harboring free electrons. The inert gas xenon, on the other hand, is an insulator without free electrons. It was found that hydrogen and xenon atoms behaved quite similarly to ping-pong and billiard balls. The hydrogen atoms bounced back from the much heavier xenon atoms and hardly lost any energy during the collision (Fig. 1 (b) blue). However, hydrogen atoms shot at heavier gold atoms behaved in a different way. They lost most of their energy (Fig. 1 (b) red). The reason is that gold – in contrast to xenon – has free electrons. They affect the hydrogen atoms like a viscous liquid and slow them down. Comparison to the theoretical model confirms the finding that electronic excitation of the surface is the dominant dissipation channel (Fig. 1 (b) black) and makes H-atom adsorption on metals surfaces efficient.

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