

Unravelling the hydrogen absorption process in Pd overlayers on a Au(111) surface

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Supporting material

Kinetics and Reaction Paths for the Absorption of Hydrogen

a) Scenario A: Subsurface penetration of adsorbed hydrogen

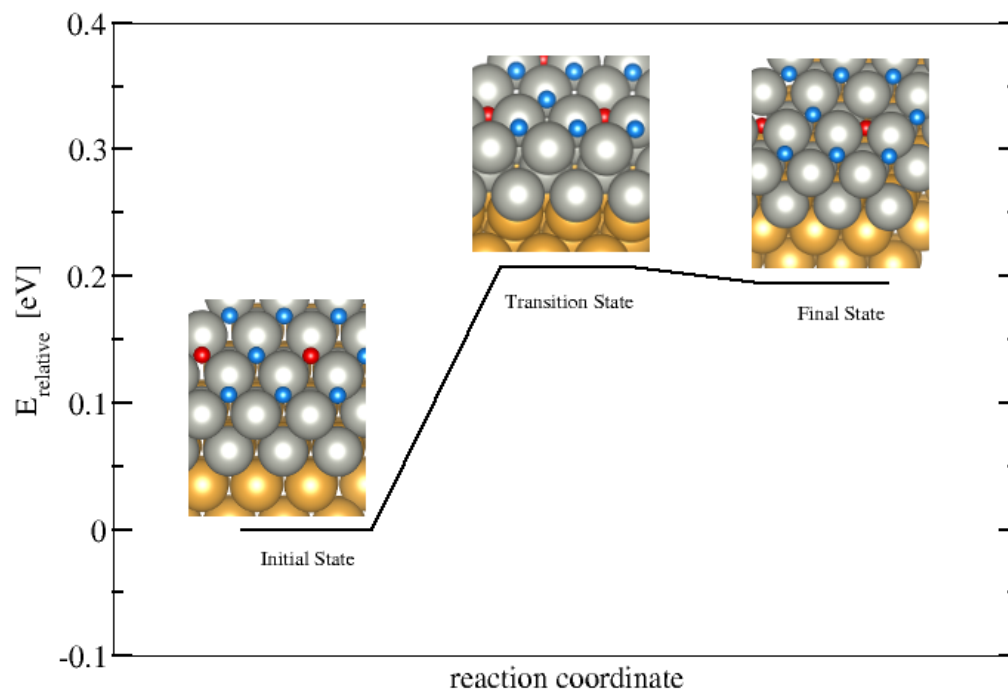


Figure 1: Reaction scheme for the hydrogen subsurface penetration from a monolayer of pre-adsorbed hydrogen or the well known H_{UPD} . Initial, transition and final states are shown. Each type of atom are represented in different colors: H (light blue), Pd(grey) and Au(yellow).

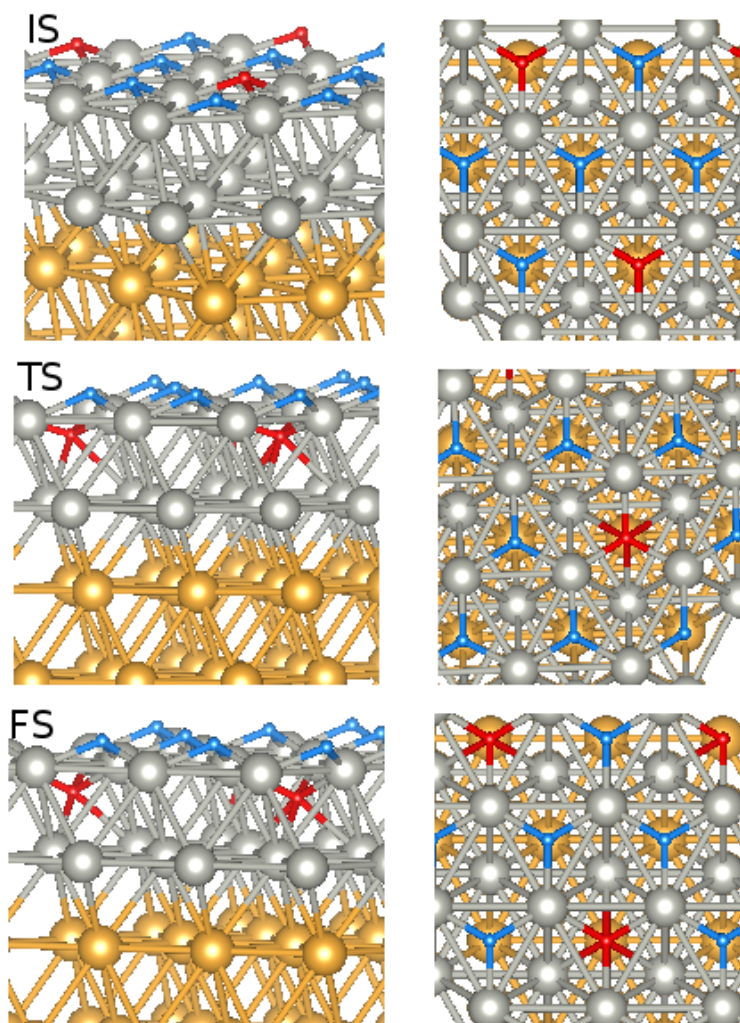


Figure 2: Initial, transition and final states for the scenario A. Each type of atom are represented in different colors: H (light blue), Pd(grey) and Au(yellow). Top and side views of the initial (IS), transition (TS) and final (FS) states are shown in ball-and-stick model.

b) Scenario B: Approach and subsurface penetration of a H_2 molecule

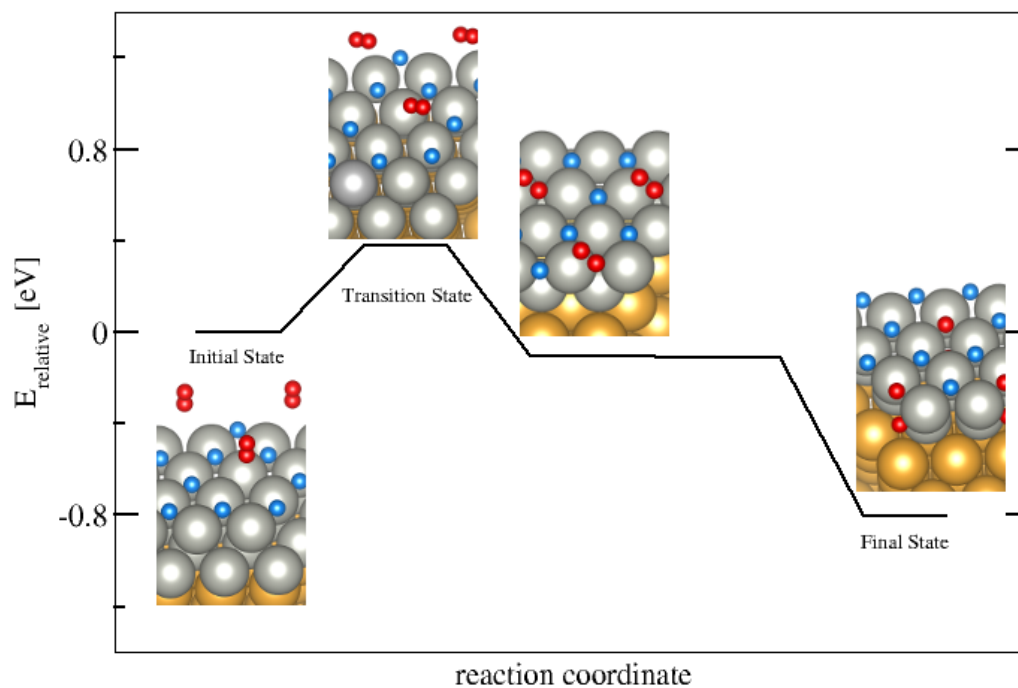


Figure 3: Reaction scheme for the hydrogen subsurface penetration upon H_2 adsorption and bond breaking. Initial, transition and final states are shown. Each type of atom are represented in different colors: H (light blue), H_2 molecule (red), Pd (grey) and Au (yellow).

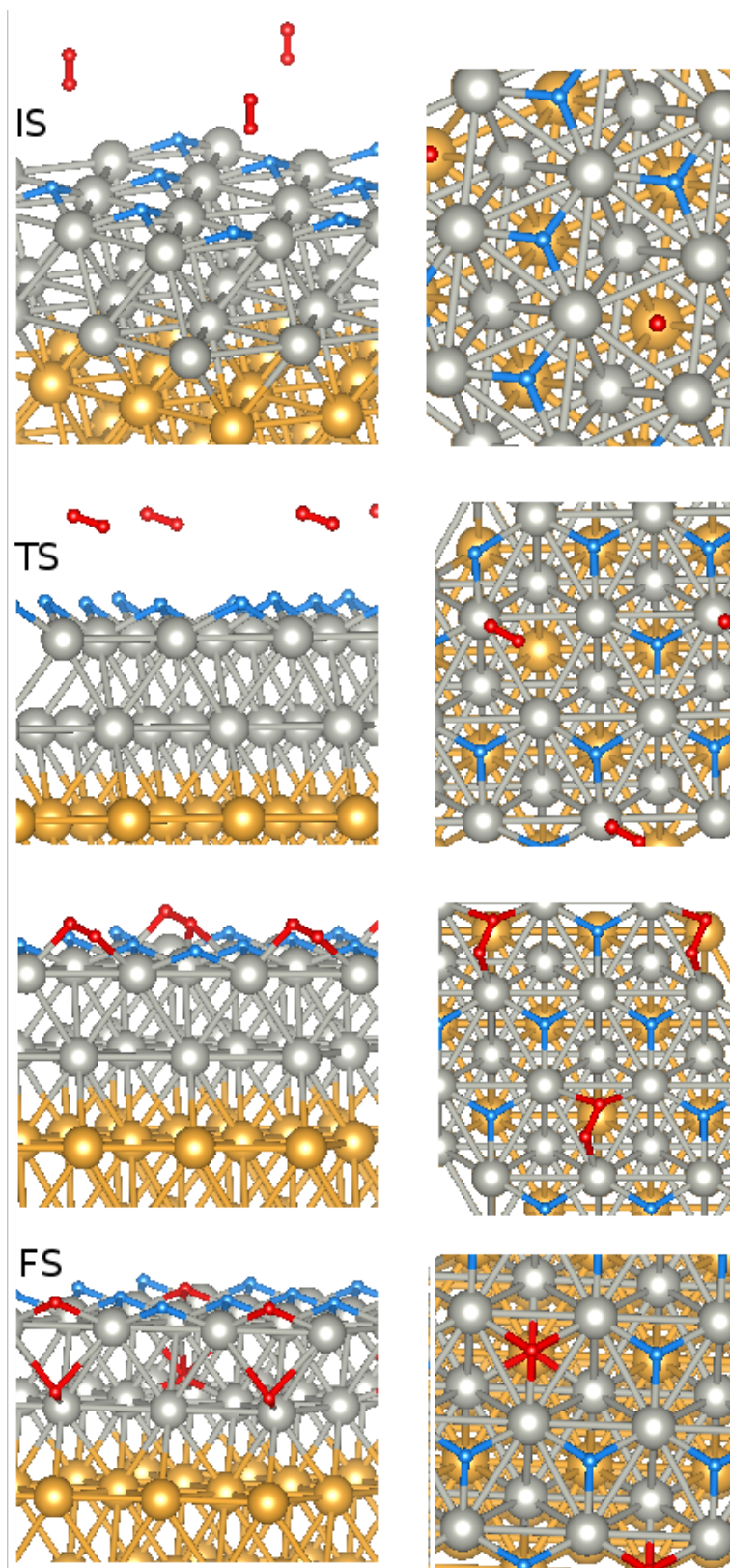


Figure 4: Initial, transition and final states for scenario B. Each type of atom are represented in different colors: H (light blue), H molecule (red), Pd(grey) and Au(yellow). Top and side views of the initial (IS), transition (TS) and final (FS) states are shown in ball-and-stick model.