Hydrogen adsorption on palladium and palladium hydride at 1 bar

The dissociative sticking probability for H-2 on Pd films supported on sputtered Highly Ordered Pyrolytic Graphite (HOPG) has been derived from measurements of the rate of the H-D exchange reaction at 1 bar. The sticking probability for H-2, S, is higher on Pd hydride than on Pd (a factor of 1.4 at 140 degrees C), but the apparent desorption energy derived from S is the same on Pd and Pd hydride within the uncertainty of the experiment. Density Functional Theory (DFT) calculations for the (111) surfaces of Pd and Pd hydride show that, at a surface H coverage of a full mono layer, H binds less strongly to Pd hydride than to Pd. The activation barrier for desorption at a H coverage of one mono layer is slightly lower on Pd hydride, whereas the activation energy for adsorption is similar on Pd and Pd hydride. It is concluded that the higher sticking probability on Pd hydride is most likely caused by a slightly lower equilibrium coverage of H, which is a consequence of the lower heat of adsorption for H on Pd hydride.

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