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First principles study of absorption of Hydrogen into Pd(111) SAMPYO HONG, TALAT RAHMAN, Kansas State University — It is well known that Hydrogens interact with Palladium to form a hydride PdH, and numerous studies both experimental and theoretical have been devoted to the system. However, important data such as the energy barriers for hydrogen absorption in the Pd substrate which eventually leads to formation of the hydride are not well known. In order to understand the rationale for hydrogen absorption process, we have carried out first-principles electronic structure calculations for high and low coverages of H on Pd(111). We have found that for subsurface H which is absorbed in the octahedral position below the top layer on Pd(111) the energy barrier to be overcome is 0.6 eV for low coverage and increases for high coverage. For a comparative study we have carried out our additional calculations for H on Pt(111). In this talk, we will compare the coverage dependent barriers for H on Pd(111) with those on Pt(111) and obtain insights from first-principles calculations about how they differ. *Work supported in part by US-DOE under grant DE-FGO2-03ER154645.

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