

Abstract Submitted
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The Nature of the Dissociation Sites of Hydrogen¹ FRANCK ROSE, MOUS TATARKHANOV, EVGENI FOMIN, D. FRANK OGLETREE, MIQUEL SALMERON, Lawrence Berkeley National Lab — Previously, we have demonstrated [1] that pairs of neighboring monoatomic hydrogen vacancies (HVs) on Pd(111) are totally unreactive toward H₂ dissociative adsorption and that active sites for the catalytic reaction can only be constituted of ensembles of at least three aggregated HVs. Thanks to LT-STM atomic observations, we show that this new description of H₂ dissociative adsorption onto transition metal surfaces is not an exotic particular catalytic case relevant only to Pd(111) and close-packed faces of fcc metals, but that it also applies to close-packed faces of hcp metals such as Ru(001) [2, 3]. Close to saturation of 1 ML, HVs were observed either as single entities or forming transient aggregations. Vacancies diffuse and aggregate to form active sites for the dissociative adsorption of H₂. We have found that H₂ dissociation takes place only on Ru sites where the metal atom is not bound to any H atom [3]. Such active sites are formed when at least 3 HVs aggregate by thermal diffusion. Sites formed by single HV or pairs of adjoining HVs were found to be unreactive toward H₂. [1] T. Mitsui, et al., *Nature* **422** 705 (2003) [2] M. Tatarkhanov, et al., *Surf. Sci., in Press* (2007) [3] F. Rose, et al., *J. Phys. Chem. C, Accepted* (2007)

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