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**Quantum Delocalization and Hydrogen Adsorption on Pd (111) Surface** SEONG-GON KIM, Mississippi State University, SUNGHO KIM, Mississippi State University, STEVEN C. ERWIN — The quantum delocalization of hydrogen atoms near the hydrogen atom vacancies on a palladium (111) surface is studied using density functional theory (DFT). Our quantum delocalization model elucidates the puzzle presented by a recent experiment [T. Mitsui, *et al*, Nature **422**, 705 (2003)]. In this experiment, Salmeron and his coworkers reported, contrary to conventional belief, that two-vacancy sites are inactive and that aggregates of three or more hydrogen vacancies are required for efficient hydrogen molecule dissociation and adsorption on a palladium (111) surface. Our total energy calculation shows that one or two hydrogen atoms are delocalized over three available adsorption sites. We found that delocalized vacancies provide a very compelling mechanism to explain the ineffectiveness of two-vacancy sites.

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