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Quantum Delocalization and STM Image Simulation of Hydrogen Atoms Adsorbed on Pd(111) Surface SUNGHO KIM, Mississippi State University, SEONG-GON KIM, Mississippi State University, STEVEN C. ERWIN, Naval Research Laboratory — Dissociative hydrogen adsorption process on noble metal is one of the most crucial catalytic processes in the fuel cell technology. Quantum delocalization model is proposed to understand the image of scanning tunneling microscopy (STM) observed during hydrogen adsorption on palladium. We use numerical simulation techniques based on the first principles density functional theory (DFT) to support our quantum delocalization arguments. As observed in a recent experiment [Nature 422, 705 (2003)] two vacances of hydrogen on palladium surface appears three loped triangle in experimental STM image and dissociative hydrogen adsorption on palladium requires aggregates of three or more vacancies. Our STM simulation and total energe calculation based on DFT using quantum delocalization model explain consistently the above experimental results.

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