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Quantum Nature of Hydrogen on Metals: Dissociative Adsorption SEONG-GON KIM, SUNGHO KIM, Mississippi State University, STEVEN C. ERWIN, Naval Research Laboratory — When hydrogen is adsorbed on a Pd(111) surface, very simple vacancy defects – which form quite commonly – exhibit fundamentally quantum wavelike behavior. We show that a full quantum treatment of the hydrogen nuclear motion, in addition to electron motion, predicts that the dissociative adsorption of H2 will be strongly suppressed at divacancies—in violation of the standard description from classical Langmuir adsorption kinetics—but will easily occur at trivacancies. Recent experiments confirm that aggregates of three or more hydrogen vacancies are required for efficient H2 dissociation, while divacancies are inactive [Mitsui et al, Nature 422, 705 (2003)]. Our findings indicate that traditional classical explanations for such observations require revisiting, and suggestthat the quantum nature of hydrogen may play a surprisingly prominent role in future hydrogen technologies.

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