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Quantum Nature of Hydrogen on Metals: Ground-State Geometry of Vacancies SUNGHO KIM, SEONG-GON 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. Conventional wisdom has it that the quantum nature of hydrogen and other light atoms is only rarely manifested, typically in specially designed experimental protocols. A great many studies have proceeded under the assumption that, for most purposes, as long as the electronic motion is handled quantum mechanically, the nuclear motion of hydrogen can be treated classically. We show that this approximation fails badly in a very simple system. Moreover, by treating the problem fully quantum mechanically, several recent experimental finding [Mitsui et al, Nature 422, 705 (2003)] can be plausibly interpreted as having a fundamentally quantum origin. In particular, we present new ground-state geometry of hydrogen vacancies on Pd(111) surface that are obtained from a full quantum treatment of the hydrogen nuclear motion. This new structures enable us to predict that all vacancy defects to have an unexpected triangular appearance in scanning tunneling microscopy; recent experiments have found precisely this behavior.

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