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**Ground-state structure of the hydrogen double vacancy on Pd(111)** SUNGHO KIM, SEONG-GON KIM, Mississippi State University, STEVEN ERWIN, Naval Research Laboratory — We determine the ground-state structure of a double vacancy in a hydrogen monolayer on the Pd(111) surface. We represent the double vacancy as a triple vacancy containing one additional hydrogen atom. The potential-energy surface for a hydrogen atom moving in the triple vacancy is obtained by density-functional theory, and the wave function of the fully quantum hydrogen atom is obtained by solving the Schrödinger equation. We find that an H atom in a divacancy defect experiences significant quantum effects, and that the ground-state wave function is centered at the hcp site rather than the fcc site normally occupied by H atoms on Pd(111). Our results agree well with scanning tunneling microscopy images.

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