Zeitschrift für Physikalische Chemie, Bd. 181, S. 305–312 (1993)
© by R. Oldenbourg Verlag, München 1993 – 0942-9352/93 $ 3.00 + 0.00

Electronic Structure of a Hydrogen Impurity Near a Pd (111) Surface*

By H. Ezzehar, L. Stauffer

Laboratoire de Physique et de Spectroscopie Électronique, U. R. A. 1435, F. S. T., 4 rue des Frères Lumière, F-68093 Mulhouse Cédex, France

and H. Dreyssé

Laboratoire de Physique du Solide, University of Nancy, B. P. 239, F-54506 Vandoeuvre les Nancy, France

H *impurity adsorption* / *Electronic structure* / Pd (111) *surface*

We study the electronic structure of a hydrogen impurity near a Pd (111) surface, in a tight-binding model using the generalized phase shift and recursion method. The surface and subsurface tetrahedral and octahedral adsorption positions are considered. Relaxation perpendicular to the surface is assumed for the impurity. The surface tetrahedral position is found to be the stablest one, in agreement with experimental results. Local densities of states and electronic occupations for these positions are presented and discussed.

1. Introduction

Surface and subsurface chemisorption of H on metals is the object of much experimental and theoretical research. The transition from adsorption at a surface site to a bulk site in the metal is, indeed, important for the understanding of the mechanism of hydride formation. A lot of studies have been devoted to the chemisorption of hydrogen in palladium. Behm *et al.* [1] by L.E.E.D. and thermal desorption spectroscopy (T.D.S.), Rieder *et al.* [2] by He-scattering and T.D.S. measurements found subsurface chemisorption of H in the case of Pd (110). On the other hand, no subsurface chemisorption has been observed for the H/Pd (001) system, in agreement with theoretical calculations [3, 4].

* Presented at the International Symposium on Metal–Hydrogen Systems, Fundamentals and Applications, Uppsala, Sweden, June 8–12, 1992.