

The quantum dynamics of the diffusion of H on Pd (111) surface

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Dissociative chemisorption on metal surfaces requires a detailed understanding about how molecules diffuse and their reactivity. There are not many experimental techniques capable of unravelling the mechanism of the lateral diffusion of atoms and molecules on a surface. In this work we show that the quantum diffusion of H is related to a strong coupling between states of the same symmetry localized at the adsorption sites "fcc" and "hcp" (see Fig.1) . The formation of a bandwidth with decreasing degree of coverage of the substrate is responsible for a further diffusion by delocalization. These purely quantum mechanically effects are expected to happen, but have never been rationalized so far.

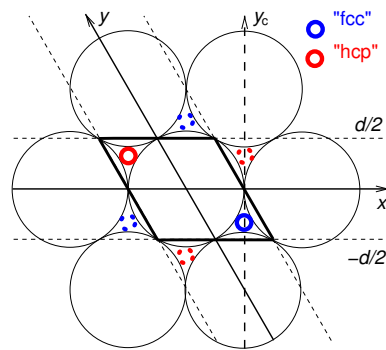


FIG. 1 – The elementary cell chosen to describe the diffusion.