Tunneling dynamics of H/Pd(111) and its effect on the quantum mechanical evaluation of the ISF

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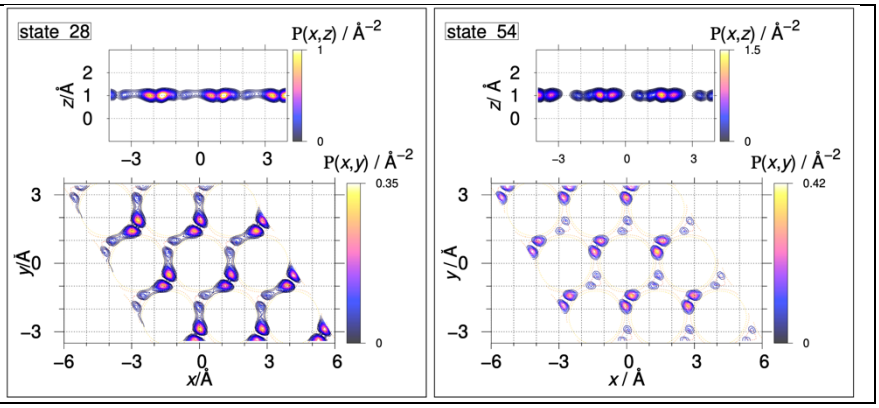
Understanding the properties and interactions of atoms and molecules on the surfaces of solids is crucial for many technological applications involving surface reactions such as the corrosion of metallic objects or heterogeneous catalysis. It is now well-established that many chemical processes are impacted by strong quantum effects involving the nuclei.

The topography of the multidimensional potential energy surface describing the interaction of atoms or molecules with the absorbing surfaces is rich of multiple adsorption wells and barriers that influence the diffusion of the adsorbates along the substrate. The resulting structure can be tackled either within the framework of a time-independent picture, i.e. by the calculation of the stationary states, or by studying the time evolution of the system starting from specific initial conditions. In this contribution, we adopt both approaches and relate the findings to observable quantities from HREELS [1] and ^{3}He-spin echo experiments [2], such as the intermediate scattering function (ISF).

The figure shows reduced probability densities (RPD) of two tunneling components related to the fcc and hcp equilibrium sites of H adsorbed on a 3x3 Pd(111) elementary cell.

Top: reduction over y. Bottom: reduction over z. RPD are superimposed on equipotentials ranging from 0 to 300 meV represented by dashed yellow lines (z = 90 pm).



Keywords: quantum dynamics, surface science, quantum diffusion, spin-echo experiments, intermediate scattering function

[1] H. Conrad et al., *Surface Science* 178 (1986) 578
[2] A. Jardine et al. , *Progress in Surface Science* 84 (2009) 323