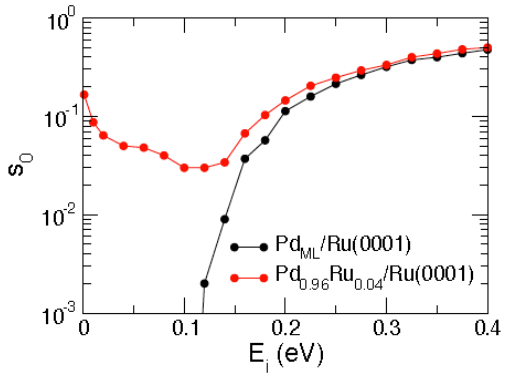
Reactivity of bimetallic surface alloys: H_2 adsorption on Pd_xRu_{1-x}/Ru(0001)

M. Ramos[1], C. Díaz[2], F. Martín[2,3], A. E. Martínez[1], H. F. Busnengo[1]

[1]*Instituto de Física de Rosario and Univ. Nacional de Rosario, 2000 Rosario, Argentina*
[2]*Dept de Química, Univ. Autónoma de Madrid, 28049 Madrid, Spain*
[3]*Inst. Madrileño de Estudios Avanzados en Nanociencia, Cantoblanco, 28049 Madrid, Spain*
cristina.diaz@uam.es

During the last few years, bimetallic surface alloys have attracted surface scientists attention due to its great flexibility to design interfaces with specific properties [1-4]. From a experimental point of view, the used of physical vapour deposition (PVD) and adequate annealing conditions, it make possible to control both the amount of adatoms deposited on the host surface and theirs locations and surroundings.

In the case of Pd_xRu_{1-x}/Ru(0001) surface, temperature programmed desorption (TPD) experiments have shown that the atomic hydrogen binding energy decreases when the amount of Pd atoms increases. But, on the other hand, sticking experimental measurements shown a constant initial reactive sticking coefficient (s_0) within a wide range of Pd concentrations, and a suddenly decreases when a Pd monolayer if formed.



Aiming to unravel these puzzling experimental results, we have performed a detailed theoretical analysis. Our classical dynamics simulations, based on accurate DFT (density functional theory) potential energy surfaces (PES), show a totally different behaviour of S_0 for H_2/Pd/Ru(0001) and H_2/$Pd_{0.94}Ru_{0.04}$/Ru(0001) at low incidence energy. As shown in the figure, whereas in the case of a monolayer of Pd on Ru(0001) S_0 is zero at low energy, when the concentration of Pd is 96% S_0 increases when the incidence energy decreases. Thus, only 4% of reactive Ru atoms are enough to induce an indirect dissociation mechanism. On the other hand, when the concentration of Pd is small, it should be taken into account that the Ru atoms close to a Pd atom become more reactive. Thus, increasing the Pd concentration increases the fraction of less reactive sites, but also the number of Ru atoms more reactive increases, thank to the presence of a near Pd atom. These combined phenomena explain the constant x-dependence, observed experimentally, of s_0 for Pd_xRu_{1-x}/Ru(0001) at low energy [5].

References:
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