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Six-dimensional theoretical study of H_2 scattering from LiF(001): From thermal to high incidence energies

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Synopsis We have computed an accurate potential energy surface (PES) describing the electronic structure of the system H2/LiF(001). Based on this PES, we have performed an analysis of the dynamics of the system trying to understand recent experimental results obtained at fast grazing incidence conditions.

Interaction of molecules with insulating surfaces has received little attention in surface science, mainly due to the fact that surface scientists have been very much focused on systems and phenomena relative to heterogeneous catalysis. However, recent experiments showing diffraction of atoms and light molecules under fast (100 eV-1 keV) grazing incidence (0.5°-2°) conditions upon scattering from insulating surfaces [1], have renewed the interest on this kind of surfaces.

We have focused on molecular projectiles because diffraction patterns are expected to be richer, due to the internal degree of freedom. In this case, theory is called to pay a key role in understanding experimental results. And therefore, accurate 6D PES describing the electronic structure, and accurate dynamics methods describing the dynamics of the system are required.

Here, we present, to our knowledge, the first 6D PES describing the electronic interaction between a diatomic molecule and an insulating surface (H_2(D_2)/LiF(001)), based on density functional theory calculations [2]. In order to test the accuracy of our PES, we have carried out dynamics calculations of elastic and inelastic scattering at low incidence energy (< 1 eV), and we have compared our results with previous experimental and theoretical ones [3, 4]. From the excellent agreement obtained, we have concluded that our PES is accurate enough to perform a complete analysis of the dynamics of the system, from very low to very high incidence energy. In fact, our first results at fast grazing incidence already show that the tools we have used are able to reproduce experimental results at these extreme conditions (see Fig.)
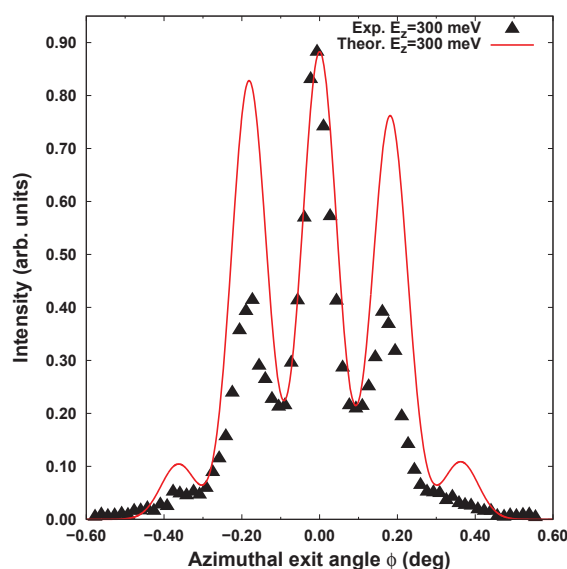
Figure 1. Experimental and simulated diffraction spectrum of H_2 scattered from LiF(001), along the incidence direction [100]. Experimental data from [5].

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