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Understanding the rotational excitation in scattering of D₂ from CH₃-Si(111)

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Synopsis We have studied the origin of the striking rotational excitation probability, found experimentally, for D₂ upon scattering from a organic-terminated Si(111) surface.

Organic-terminated Si surfaces are the subject of a great interest in surface science. Such surfaces exhibit improved oxidative and electrochemical stability, relative to hydrogen-terminated silicon, for practical applications such as biosensing electronics [1] or photoelectrodes in electrochemical cells [2]. Silicon surfaces functionalized with methyl termination have emerged as the best alternative to hydrogen termination [3], giving suppression of surface reconstruction and resistance to oxidation.

This system has been investigated with a range of experimental techniques. Recent experimental results show [4] a noticeable rotational excitation for D₂ (see Fig.), which is not observed in the diffraction spectra measured for H₂. In order to understand the origin of this behavior, we have simulated these experimental spectra to determine the mechanism that explain this difference. In a first step we have construct a suitable potential energy surface (PES), using a Modified Shepard interpolation method [5]. In a second step we have tested the accuracy of our PES by means of classical dynamics simulations.

First dynamical results already show that our six-dimensional PES reproduces accurately the anisotropy of the system. Our classical dynamics calculations show rotational excitation probabilities of the order of 22% for D₂ and of 8% for H₂, always within the incidence energy experimental range. Finally, quantum calculations have been used to further assess the appropriateness of the

classical analysis [6]

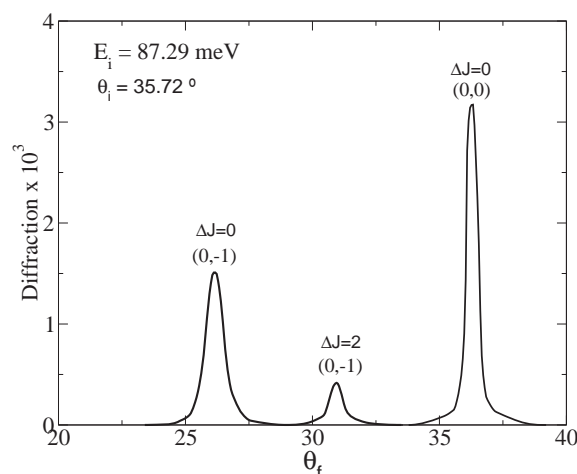


Figure 1. Experimental diffraction spectrum of D₂ scattered from CH₃-Si(111), along the incidence direction ΓM . Incidence energy 87.29 meV, polar angle 35.72 deg.

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