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Understanding the rotational excitation in scattering of D_2 from CH_3-Si(111)

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Synopsis We have studied the origin of the striking rotational excitation probability, found experimentally, for D_2 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 D_2 (see Fig.), which is not observed in the diffraction spectra measured for H_2. 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 D_2 and of 8% for H_2, always within the incidence energy experimental range. Finally, quantum calculations have been used to further assess the appropriateness of the classical analysis [6]

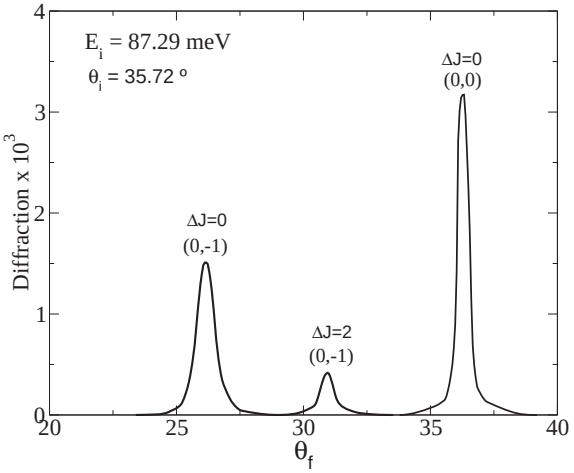

Figure 1. Experimental diffraction spectrum of D_2 scattered from CH_3-Si(111), along the incidence direction ΓM. Incidence energy 87.29 meV, polar angle 35.72 deg.

References

[1] T. L. Lasseter *et al* 2004 *J. Am. Chem. Soc.* **126**, 10220.
[2] X. Shen *et al* 2010 *ACS Nano* **4**, 5869.
[3] R. D. Brown *et al* 2013 *Phys. Rev. Lett.* **110**, 156102.
[4] Z. M. Hund *et al* to be published
[5] T. J. Frankcome *et al* 2012 *J. Chem. Phys.* **137**, 144701.
[6] D. Farías *et al* 2004 *Phys. Rev. Lett.* **93**, 246104.

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