COMPOSITION AND STRUCTURE OF Si(001)/CaF_2 INTERFACES

Henry P. Pinto[1], Franco Chiaravalloti[2], Damien Riedel[2], Adam S. Foster[1] and Gérald Dujardin[2]

[1]Laboratory of Physics, Helsinki University of Technology, P.O.Box 1100, FI-02015 TKK, Finland
[2]Laboratoire de Photophysique Moléculaire, Université Paris-Sud 91405 Orsay, France
hpp@fyslab.hut.fi, franco.chiaravalloti@u-psud.fr

The development of practical molecular electronics relies on the identification of molecule-surface combinations where the molecule is bound to the surface without being electronically coupled. A possible approach is to consider molecules on insulating thin films on conducting substrates. This film is meant to isolate the molecule, while allowing controlled contact to the conducting substrate if wanted. Demonstrating the potential of such a setup requires complete characterization of both the atomic structure of the molecule-surface interface and the its electronic structure.

Calcium fluoride has always been considered as an interesting and prototypical insulating material to be grown epitaxially on silicon single-crystal surfaces. Due to the small lattice mismatch between the two materials 0.6% at room temperature, CaF_2 films of good crystal quality can be grown by molecular beam epitaxy MBE on silicon. CaF_2 has very good insulating properties and optical transmission in the range of infrared and visible radiation. Stimulated by the number of potential applications, extensive studies of the growth of CaF_2 on silicon have been mainly carried out on Si (111) [1]. Only a few attempts have been undertaken up to now to investigate the initial stages of CaF_2 growth on the technologically important Si(001) surface [2], and detailed studies in high resolution remain absent.

In this study, we use an ultra thin film of CaF_2 grown on the top of a Si(001) substrate as a prototype substrate for molecular adsorption. The film is grown using molecular beam epitaxy in ultra high vacuum at a substrate temperature of about 750 K. The films were characterized at several stages of their growth via low temperature scanning tunneling microscopy (LT-STM) and spectroscopy measurements. Using a plane-wave density functional theory, we compute the electronic and energetic properties of several structural candidates, and calculate the Gibbs free energy to determinate the most stable structures of the Si(001)/Ca_xF_y interface in thermodynamic equilibrium with a CaF_2 gas environment. We perform multiple scattering theory STM simulations on the most stable interface structures, and resolve the actual structure of the interface by comparison of theoretical and experimental linescans. Finally, the electronic and structural properties of the interface are discussed in the light of the experimental molecular adsorption results.

[1] E. Rotenberg, J. D. Denlinger, M. Leskovar, U. Hessinger, and M. A. Olmstead, Phys. Rev. B **50**, 11052 (1994).
[2] L. Pasquali, S. M. Suturin, V. P. Ulin, N. S. Sokolov, G. Selvaggi, A. Giglia, N. Mahne, M. Pedio, and S. Nannarone, Phys. Rev. B **72**, 045448 (2005)

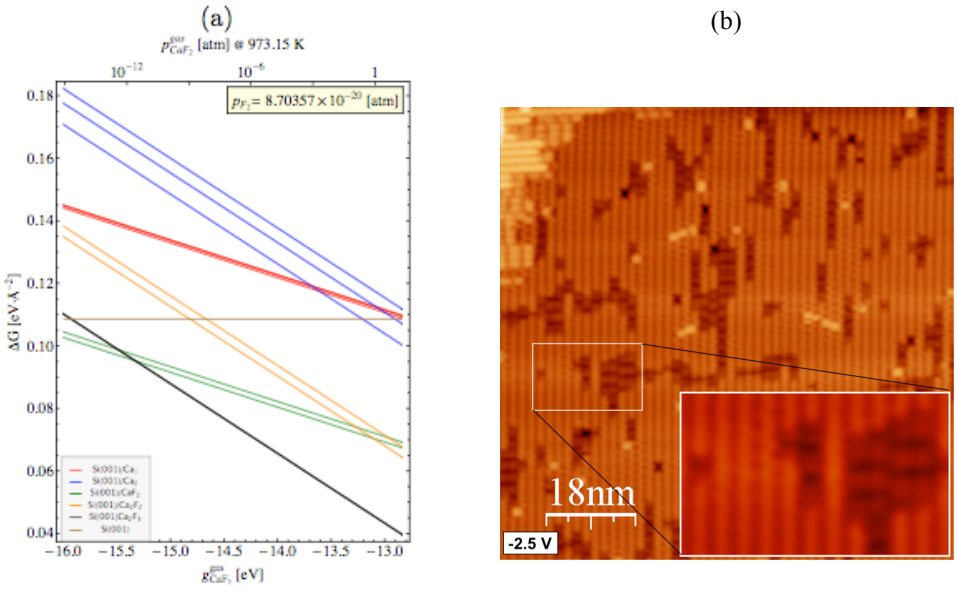

Figure 1: (a) Interfacial energy for various structures as a function of the free energy of the CaF_2 source. (b) STM image of the CaF_2 wetting layer on Si(001)

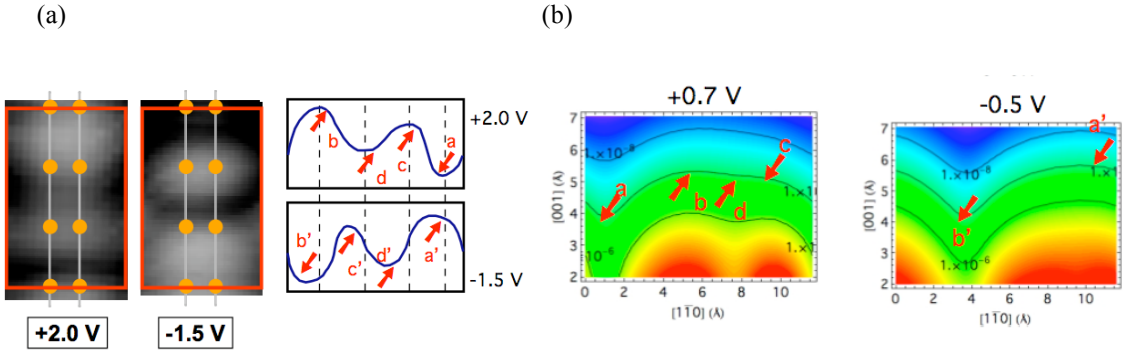

Figure 2: (a) Experimental images and scanlines, and (b) simulated STM scanlines of the interface at different bias voltages.