

Thermodynamic and structural properties of water film adsorbed on MgO (100) ionic surface.

J.P. Coulomb,^{*,a} B. Demirdjian^a D. Ferry^a and M. Trabelsi,^b

^a C.I.N.A.M-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France

^b Faculté des Sciences de Bizerte, département de Physique, Bizerte, Tunisie

E-mail: coulomb@cinam.univ-mrs.fr

High homogeneous MgO (100) powder is a very suited substrate to investigate the influence of square symmetry surface on the properties of physisorbed rare gases (2D) films [1]. In addition, such a MgO (100) powder is of great interest to analyse the surface electric field E influence on polar adsorbed monolayer (as for instance, NO, CO or C_2H_2). In the present study, we describe the thermodynamic and structural properties of (2D) water film physisorbed on MgO (100) surface. Some interesting results concern also the H-binding formation within the water monolayer and between such a monolayer and the surface oxygen ions of the MgO substrate.

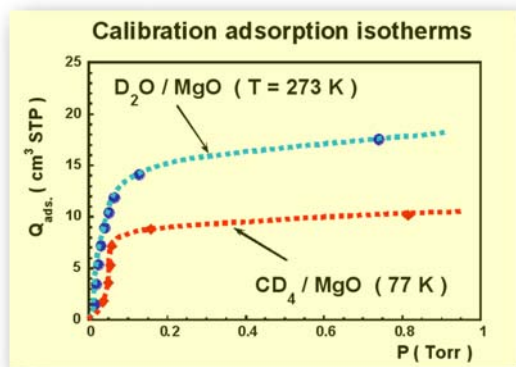


Figure 1 : Calibration adsorption isotherm of heavy water (D_2O) on MgO (100) powder measured at $T = 273$ K. By comparison, on the same MgO sample we have measured, a methane (CD_4) adsorption isotherm, at $T = 77.3$ K.

We have measured the neutron diffractograms of water (D_2O) phase adsorbed on MgO (100) surface at different film thicknesses (0.93 ; 1.5 ; 4.0 and 20 layers). The determination of the water monolayer structure from the analysis of the 0.93 layer diffractogram was not so easy. In a first time, we start our analysis by considering water (2D) structure similar to the densest plane of hexagonal ice (Ih) and cubic ice (Ic). The results were not at all significant. In a second time, we have conserved the high density ices (ices which exist in the high pressure range). We note that the main neutron diffraction peak of the cubic ice VII and the main peak of our 0.93 layer diffractogram are very close to each other. Surprisingly, the densest plane of ice VII (plane (100)) is very close to the $P(2 \times 3)$ commensurate structure that we have already conjectured for the water monolayer structure [2]. In the present paper, we confirm such a $P(2 \times 3)$ over-structure mesh and we have determined the position and orientation of the water molecules within the mesh. The principal characteristic of the (2D) water organization is that all the D_2O molecules are laying along the MgO (100) surface rows (as represented on **Figure 2**).

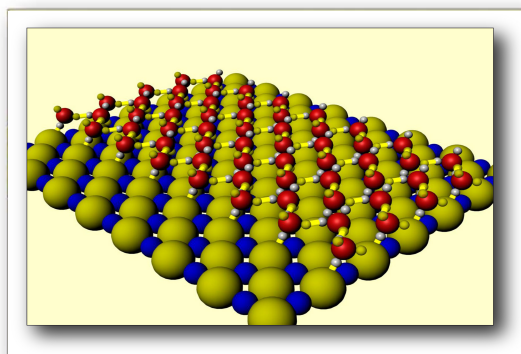


Figure 2 : Schematic representation of the commensurate $P(2 \times 3)$ (2D) structure of water monolayer adsorbed on the MgO (100) surface. We note that all the H_2O molecules are laying along the surface rows formed by the Mg^{2+} cations .

1. J.P. Coulomb, T.S. Sullivan and O.E. Vilches, Phys. Rev. **B 30** (1984) 4753.
2. B. Demirdjian, J. Suzanne, D. Ferry, J.P. Coulomb and L. Giordano, Surf. Science **462** (2000) L581.