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Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING
and the
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

November 30, 2001, 2:15 pm - Concordia University H-1070

Molecular Dynamics Studies of Pollutant Adsorption on Ice Surfaces

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In the very rich field of atmospheric chemistry, our knowledge is rather poor about the global role of the ice surface formed in Polar Stratospheric Clouds (PSCs) and the relative influence of various pollutant species in the reaction mechanisms in the troposphere and stratosphere (ozone depletion, acid rain, greenhouse effect…). In order to gain a better understanding of these processes at the molecular level, we simulated with classical Molecular Dynamics techniques the diffusion of a pollutant through an ice film. The dynamics of the pollutant / ice interface is described theoretically in terms of structure, thermodynamics, residence times and bond lifetimes. The adsorption and incorporation properties are compared for various pollutants (HF, HCl, CH_3COOH, HCOOH…) at typical stratospheric temperatures. Ice surface melting is thought to play a key role in atmospheric chemistry, even though this is still a controversial issue. The structural and dynamical properties of the ice surface were thus analysed over the temperature range 190-270 K for bulk ice and for a MgO-supported ice film, which has been investigated by Quasi-Elastic Neutron Scattering experiments for direct comparison. Further developments will be discussed.

Dr. Céline Toubin obtained a Doctorat in Chemical Physics in 2001 from the Université de Besancon (France), where she worked under the supervision of Dr. Sylvain Picaud in the Laboratoire de Physique Moléculaire. She was part of a theory group specialized in computer simulations of surface and interfacial molecular processes. She also worked on atmospheric problems such as the adsorption of hydracids on ice surfaces in collaboration with Dr. James T. Hynes (Ecole Normale Supérieure, Paris), until she joined the research group of Dr. Gilles H. Peslherbe at Concordia University as a Postdoctoral Fellow. Her current work aims at combining both quantum chemistry and classical molecular dynamics techniques in order to study the reactivity of biologically relevant molecules, both under physiological conditions and in the interstellar medium. This work involves multiple collaborations with Profs. Ann M. English and James T. Hynes.