14th International Conference on the Physics and Chemistry of Ice (PCI-2018 in Zürich)

Contribution ID: **76** Type: **Talk**

Modeling Elementary Heterogeneous Atmospheric and Interstellar (Photo)chemical Processes on Ice and their Dynamics using Amorphous Solid Water

Thursday 11 January 2018 11:30 (20 minutes)

A thermodynamically reversible path was suggested to exist linking the low density forms of amorphous ice (LDA) and deeply supercooled liquid water (LDL), through the so-called no man's land and finally onto normal liquid water.(1) Furthermore, at temperatures below its calorimetric glass transition temperature (Tg ˜ 136K), transport kinetics are exceedingly slow in amorphous solid water (ASW). Therefore, it might provide a convenient model system to study elementary heterogeneous atmospheric and interstellar chemistry processes that occur on the quasi-liquid layer (QLL) that forms at the air-ice interface in the atmosphere at T<Tm. We will discuss how studying interfacial dynamics at cryogenic temperatures enables the decoupling of processes occurring onto the surface of ASW from those that take place within the bulk by strongly inhibiting the diffusive uptake kinetics. Using this strategy, we will show that ionic dissociation of simple acids [i.e., HF,(2) HCl,(3) HNO3(4)] remain facile down to temperatures as low as 20K at the surface of ASW. We will also demonstrate that heterogeneous nitrates photolysis can be enhanced up to 3-fold at the ASW surface hinting at a significant contribution from heterogeneous (photo)chemistry to the photochemical NOx fluxes that emanate from the sunlit snowpack to polar boundary layer.5

(1) O. Mishima and H.E. Stanley, Nature 396, 329–335 (1998).

(2) P. Ayotte, M. Hébert, and P. Marchand, J. Chem. Phys. 123 184501 (2005); R. Iftimie, V. Thomas, S. Plessis, P. Marchand, and P. Ayotte, J. Am. Chem. Soc. 130, 5901-5907 (2008); P. Ayotte, S. Plessis and P. Marchand, Phys. Chem. Chem. Phys. 10, 4785-4792 (2008); P. Ayotte, Z. Rafiei, F. Porzio, and P. Marchand, J. Chem. Phys. 131, 124517 (2009); G. Marcotte and P. Ayotte, J. Chem. Phys. 134, 114522 (2011).

(3) P. Ayotte, P. Marchand, J. L. Daschbach, R. S. Smith, and B. D. Kay, J. Phys. Chem. A 115, 6002-6014 (2011).

(4) P. Marchand, G. Marcotte, and P. Ayotte, J. Phys. Chem. A 116, 12112-12122 (2012); G. Marcotte, P. Ayotte, A. Bendounan, F. Sirotti, C. Laffon and P. Parent, J. Phys. Chem. Lett. 4, 2643-2648 (2013).

(5) Guillaume Marcotte, Patrick Marchand, Stéphanie Pronovost, Patrick Ayotte, Carine Laffon and Philippe Parent, J. Phys. Chem. A 119, 1996-2005 (2015).

Significance statement

Modeling of ice surface Chemistry using advanced spectroscopic tools and ASW allows slow interfacial dynamic processes to be studied with surface science approaches.

Author: Prof. AYOTTE, Patrick (Université de Sherbrooke)

Presenter: Prof. AYOTTE, Patrick (Université de Sherbrooke)

Track Classification: Chemistry