

O 97: Poster Session VII: Poster to Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces II

Time: Thursday 10:30–12:30

Location: P

O 97.1 Thu 10:30 P

Interfacial Water Ordering Is Insufficient to Explain Ice-Nucleating Protein Activity — ●MAX LUKAS¹, RALPH SCHWIDETZKY¹, ANNA T. KUNERT², ELLEN H.G. BACKUS^{1,3}, ULRICH PÖSCHL², JANINE FRÖHLICH-NOWOISKY², MISCHA BONN¹, and KONRAD MEISTER^{1,4} — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Max Planck Institute for Chemistry, Mainz, Germany — ³University of Vienna, Vienna, Austria — ⁴University of Alaska Southeast, Juneau, United States

Bacterial ice nucleation proteins (INPs) are the known to be the most efficient ice nucleators known. Here we study the solution structure of INPs from *Pseudomonas syringae* and find that there is no significant conformational change upon cooling. In contrast, upon heating on temperature exceeding ~ 55 °C the structure changes irreversibly, accompanied by a complete loss of ice nucleation activity. Structural ordering of interfacial water as it is observed by nonlinear sum-frequency generation (SFG) spectroscopy upon cooling is similar for active and heat-inactivated protein solutions. Our results demonstrate that the INPs' outstanding ice nucleation efficiency can not sufficiently be explained with increased water ordering at low temperatures and that the intact 3D protein structure is crucial for the underlying mechanism - taken altogether pointing to the importance of supramolecular interactions.

O 97.2 Thu 10:30 P

Photon impact induced luminescence spectroscopy of a liquid microjet — ●DANA BLOSS¹, ANDREAS HANS¹, CHRISTIAN OZGA¹, PHILIPP SCHMIDT¹, XAVER HOLZAPFEL¹, ARNO EHRESMANN¹, PETR SLAVÍČEK², BERND WINTER³, and ANDRÉ KNIE¹ — ¹Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ²Department of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, 16628 Prague, Czech Republic — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Methods for Material Development, Albert-Einstein-Straße 15, 12489 Berlin, Germany

Liquids and especially liquid water have been subject to intense research for a long time due to their role in many chemical and biological systems. However, the investigation of liquid targets with fundamental methods of atomic and molecular physics, such as soft X-ray induced fluorescence spectroscopy, were a big challenge due to the required vacuum conditions. With the development of the liquid microjet technique the investigation of pure liquids or solutions after irradiation with synchrotron radiation became possible, which allows the exploration of the electronic structure of such complex systems. Here we present our results of dispersed luminescence from liquid water and demonstrate the possibilities of this detection method using this prototype system. One of the observed emission could be assigned to gas phase excited by Auger electrons escaping the liquid-vapor interface.

O 97.3 Thu 10:30 P

Structure of Aqueous Solutions via X-ray spectroscopies based on non-local Auger processes — ●EVA MUCHOVA and PETR SLAVÍČEK — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

Novel Auger-type X-ray spectroscopies are bringing new insights in the structure and electronic properties of aqueous solutions. It allows studying the chemical environment in solutions, e.g. the mutual effects of ions and solvent on each other, as well as ultrafast processes following ionization. The spectroscopy is also depth-sensitive and can reveal structural changes in interfaces. Sensitivity to ion pairing is achieved mainly by analysis of secondary electron spectroscopies, especially when newly identified non-local electron decay processes. The experiments, however, require a complex theoretical interpretation. In the contribution, we can show for a series of Na⁺, Mg²⁺ and Al³⁺ ions how the non-local Auger spectroscopy (mainly intermolecular Coulomb decay process, ICD) can provide details of speciation, e.g. show different type of interaction between ions and between ions and solvent. We can further discuss recent development of theoretical toolkit for non-local processes which we combine with multiscale methods like QM/MM or QM:QM in order to realistically model the environment.

O 97.4 Thu 10:30 P

Kinetics of Nano-Droplet Halide Emission from Salty Interfaces — ●PHILIP LOCHE¹, DOUWE J. BONTHUIS², and ROLAND R. NETZ¹ — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — ²Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

Ozone is one of many atmospheric trace gases whose presence is crucial for sustaining life on earth. Most of the ozone is located in the stratosphere (12 km - 55 km) where it absorbs short-wave radiation from the Sun and thus protects living organisms from potentially fatal genetic damage. Ozone depletion especially in the arctic can lead to temperature changes and influence the Southern Hemisphere mid-latitude circulation. The ozone concentration in the lower atmosphere is correlated with the halide concentration which is emitted from seawater.

Here, we use molecular simulations to study the kinetics of Cl⁻ by the evaporation from the air-water interface. We show that the emission of ions is a 2-state process. First hydrated ions are emitted, forming water fingers with the surface up to a distance of ~ 2 nm from the Gibbs dividing surface. If ions overcome this distance, they lose their hydration shell after ~ 20 nanoseconds and distances of several μm . From the determined reaction rate coefficient of evaporation we obtain the total flux of chloride ions per year from the earth's ocean and estimate that it would take roughly 90 years until the current chloride concentration in the lower atmosphere is reached.