Water in confined spaces

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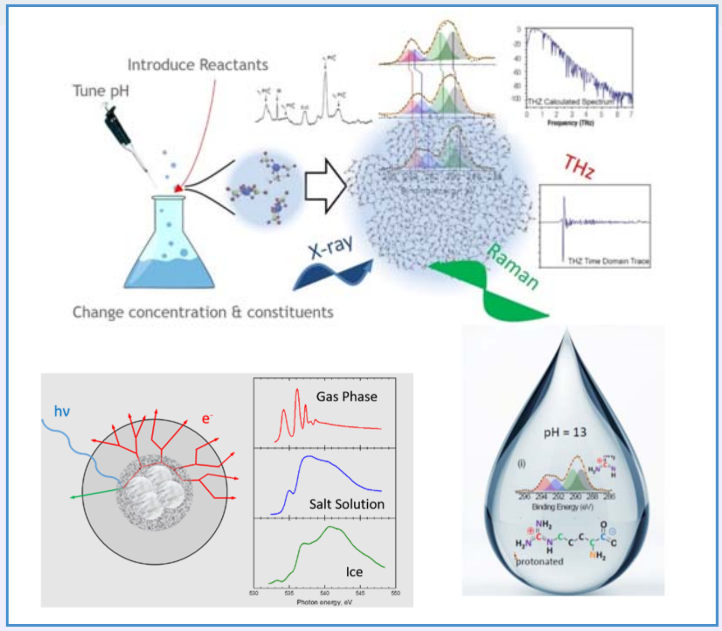
Motivation

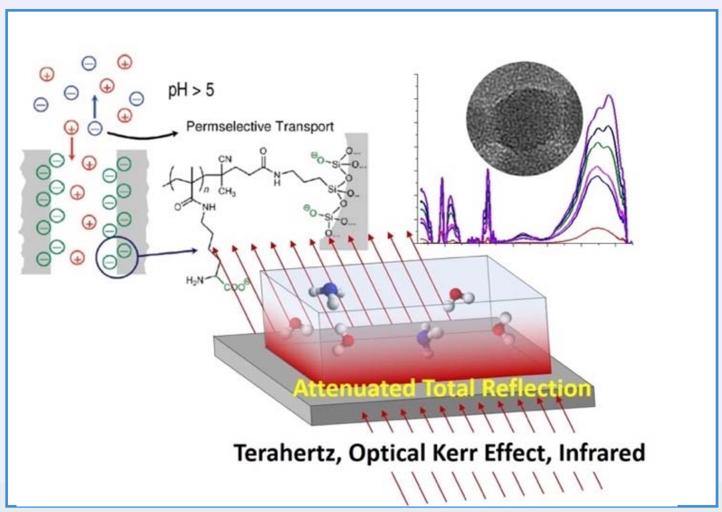
Desalination, removal of salts and minerals, is required to make water from the oceans, and brackish sources accessible for use in industry, agriculture and delivered to our homes. Experimental data and theory models seem to indicate that water confined by solid walls to spaces smaller than a few tens of nanometers is strikingly different from those of bulk water. This can influence function and operation of biological systems (cells, membranes, water pockets in proteins), geological structures (percolation, ion adsorption and mineral dissolution) and human devices (polyelectrolyte membranes, ion-exchange resins, xerogels, nanotubes etc.).Here we propose to study the properties of water in these confining conditions, to prepare the groundwork for technologies that would be transformative in desalination and other separation techniques.



Top- Probing aqueous nanoparticles with X-Ray, Raman & Terahertz Spectroscopy. Bottom- Left – Phase changes of water in nanoparticles (Kostko, JCP 2017), right- pH dependent photoelectron spectra of arginine nanoparticles (Xu, CPC 2017)

Research

To probe this requires novel tools and strategies that allows chemical sensitivity and access to kinetics and dynamics within these spaces. We propose to visualize the hydrogen bond network dynamics of water in a variety of confining geometries (squeezed water) that become accessible in carbon nanotubes, mesoporous silica shells, gels and membranes. A key component of the proposal is to develop Infrared/terahertz (IR/THz) spectroscopy, and X-Ray spectroscopies to access the structure and dynamics of water in some of the world's smallest test tubes. The results obtained can be directly tested against theoretical predictions and will guide implementation into technology.



In-situ Attenuated Total Reflection silicon chip based system with confining thin film (polymer brush, adapted from Calvo et al. 10.1021/ja9031067). Fourier Transform Infrared Spectra of water uptake on 2 nm mesoporous silica (unpublished results).

References:

O. Kostko, B. Xu, M.I. Jacobs, M. Ahmed, "*Soft X-ray spectroscopy of nanoparticles by velocity map imaging,*" 10.1063/1.4982822

B. Xu, M.I. Jacobs, O. Kostko, M. Ahmed, "*Guanidinium group is protonated in a strongly basic arginine solution,*" 10.1002/cphc.201700197

Acknowledgements