

## *Dr. Maria Sushko*

*Pacific Northwest National Laboratory in Richland, WA*

*Friday, March 27<sup>th</sup>, 2015*

*BB 3.04.18*

*3:00 PM*

### **Electrolyte solutions – active medium for biomolecular and inter-particle interactions.**

Microscopic interactions in electrolyte solutions and electrolyte/solid interfaces play central role in many chemical and biological processes including nucleation, particle mediated crystal growth, self-assembly, recognition reactions and freezing transitions. The challenge for theoretical treatment of microscopic interactions in heterogeneous condensed phase systems is in accurate description of many-body interactions that is valid for a wide concentration range from dilute solutions to the solid state. Empirical potential force-fields that use the concept of pair-wise atom-atom interactions are usually fitted to reproduce either the properties of dilute solutions or the properties of solid state, but are not suitable for the intermediate concentration range or for the description of freezing transitions, except in some very rare cases. Mesoscopic theories of electrolyte solutions, on the other hand, treat many-body interactions from first principles, but lack the essential microscopic detail. One breakthrough in the theory of heterogeneous condensed matter systems came with the development of the Fundamental Measure Theory (FMT), which linked the theory of many-body interactions and molecular detail. Coupled with a first principles treatment of first and second order electrostatics, FMT became the basis for classical Density Functional Theory (cDFT). In this talk a minimum parameter-free cDFT model for electrolyte solutions will be discussed through the prism of its application to revealing the details of ionic atmosphere around biomolecules, and understanding the physics of nanomechanical biosensing and particle mediated crystal growth.



#### **Department Contact Information**

Dr. Marcelo Marucho [marcelo.marucho@utsa.edu](mailto:marcelo.marucho@utsa.edu)

Christella Robledo [Christella.Robledo@utsa.edu](mailto:Christella.Robledo@utsa.edu)

<http://physics.utsa.edu>

