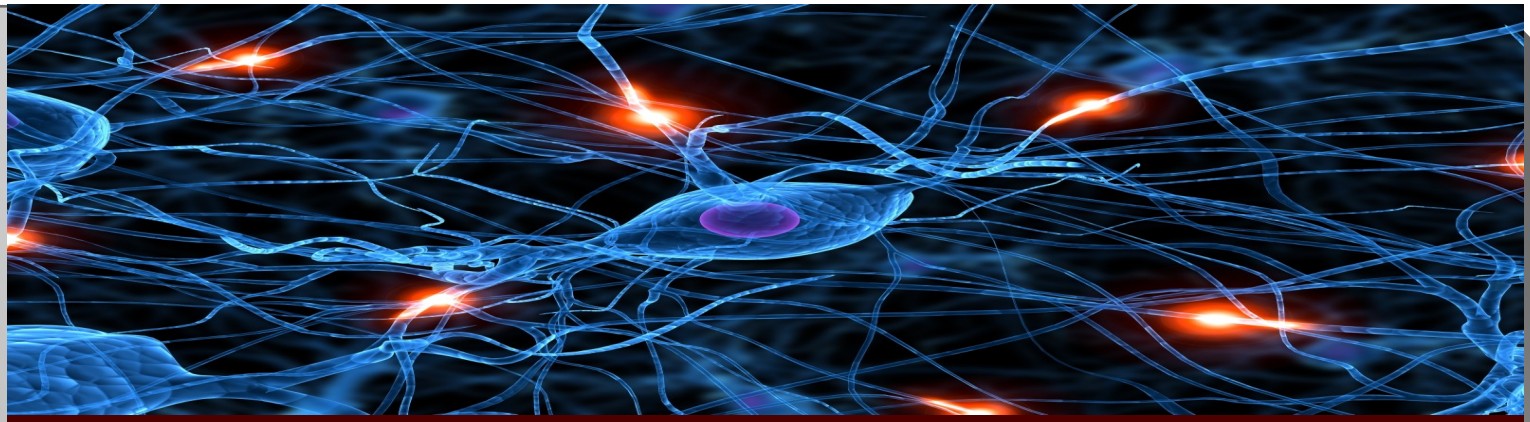
# Bioengineering Seminar

**Friday, April 20th, 2012**
**12:30pm-1:30pm, Room 3507 Nguyen Engineering Building**



## Silvina Matysiak Ph.D.

*Assistant Professor at Fischell Department of Bioengineering at the University of Maryland College Park*

### Direct characterization of hydrophobic Hydration during cold and pressure denaturation

Many computational approaches for large biomolecular systems renormalize the role of the solvent into the definition of effective inter-residue interactions by coarse-grained models to access biologically relevant time-scales. However, the discrete nature of water and its effects on protein structure, dynamics and function cannot be explored in a predictive way with models that implicitly describe the solvent.

We present here a new off-lattice coarse-grained protein model where individual water molecules are explicitly accounted for in order to accurately describe the protein structure and molecular interactions. The water model includes tetrahedral interactions and correctly describes the phase diagram of water. The protein model exhibits pressure, cold and thermal denaturation. It also allows the formation of secondary structure elements such as □-helices and □-sheets.

We will present the methodology and the results of how the length of a protein and sequence of hydrophobic and hydrophilic monomers affects protein stability.

## Biography

**Silvina Matysiak is an assistant professor in the Fischell Department of Bioengineering at the University of Maryland, College Park. Matysiak was awarded a diploma in chemical engineering from the Instituto Tecnologico de Buenos Aires, Argentina in 2001, and received her Ph.D. in chemistry from Rice University in 2007.**

**Before joining the University of Maryland, she was a postdoctoral fellow at the University of Texas at Austin in the department of Chemistry and Biochemistry and at the Institute of Computational Sciences and Engineering. She serves as a reviewer for a variety of journals including Physical Review Letters, was a fellow at the Institute for Pure and Applied Mathematics at UCLA, and has been a visiting scientist at the Max-Planck Institute for Polymer Research and the Manufacturing Research Center at the Georgia Institute of Technology.**

**Matysiak's primary area of interest is in the characterization of protein dynamics and function at the molecular level. Her work includes using computer simulations to study the mechanisms of protein folding and misfolding associated with Alzheimer's and Parkinson's diseases, protein assembly in biomedically relevant systems, and how solvent organization affects cooperative transitions in biomolecular systems. Her work has appeared in the Proceedings of the National Academy of Sciences.**

**For any questions, please contact Claudia Borke at cborke@gmu.edu**

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