DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

SPRING 2017 SEMINAR SERIES

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WEDNESDAY, APRIL 12, 2017 **TIERNAN HALL**
2:30 PM **ROOM 373**

GUEST SPEAKER

Dr. Wenwei Zheng
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TOPIC

All-atom models for unfolded protein structure and dynamics using experiments and simulations

ABSTRACT

The importance of disorder in protein structure and function is becoming increasingly evident. However, until recently, disordered regions were poorly modeled by all-atom molecular simulations, whereas the two commonly used experimental methods—Förster resonance energy transfer (FRET) and small-angle X-ray scattering (SAXS)—generate qualitatively different results for the unfolded proteins with increasing denaturant concentration. We have recently improved the all-atom simulation models by correcting the protein-water and protein-denaturant interactions. We have then applied the model to resolving the decade-old controversies in the interpretation of FRET and SAXS experiments on the unfolded proteins. Finally, I will present the recent progress on understanding liquid-liquid phase separation of intrinsically disordered proteins.

BIOGRAPHY

Wenwei Zheng is currently a postdoctoral fellow at the Laboratory of Chemical Physics of NIDDK, NIH. He got his PhD in Chemistry from Rice University in 2013. He current research focuses on modeling intrinsically disordered proteins including force field development, experimental data interpretation and the liquid droplet formation. Before getting into the intrinsically disordered protein field, he worked on understanding protein folding mechanism by developing advanced sampling and reaction coordinate methods.

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