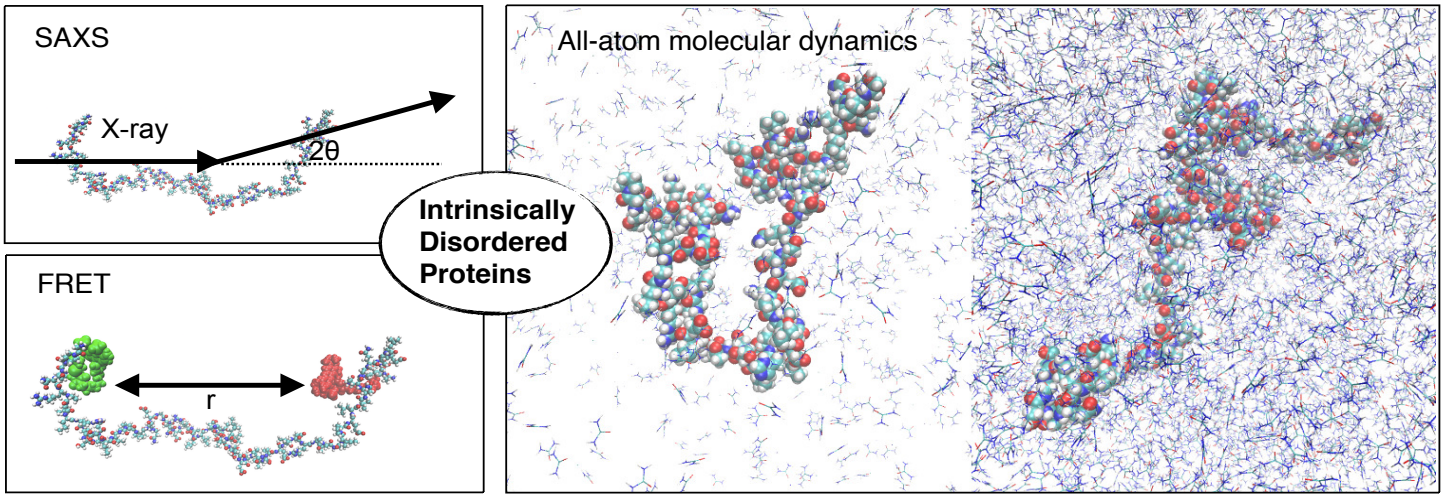
Structure and dynamics of intrinsically disordered proteins from simulations and experiments



Science & Mathematics Colloquium Series

Presentation by Wenwei Zheng

Postdoctoral Fellow, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK), NIH

Wed., March 15, 2017, 3 pm

Cooley Ballroom C, Student Union
ASU Polytechnic campus

The importance of disorder in protein structure and function is becoming increasingly evident. However, interpretation of experimental results becomes more challenging due to the averaging of observables over the very broad distribution of disordered protein conformations. For example, the two most commonly used experimental methods—Förster resonance energy transfer (FRET) and small-angle X-ray scattering (SAXS)— have yielded qualitatively different results for the effect of chemical denaturants on unfolded proteins. Molecular simulations can potentially fill this gap, but have not been applicable to disordered proteins due to shortcomings of the energy function used. We have recently improved all-atom simulation models to work with both folded and intrinsically disordered proteins. We then applied the model to resolving the decades-old controversy in the field, between the FRET and SAXS experiments on the unfolded proteins. We showed how the discrepancy arose from the way in which the experiments were analyzed and how that can be avoided. Finally, I will present my recent progress on the formation of membrane-less organelles through liquid-liquid phase separation of intrinsically disordered proteins, and my future plans for this work.

Wenwei Zheng is currently working on modeling intrinsically disordered proteins, including force field development, experimental data interpretation and liquid droplet formation.

Before entering the intrinsically disordered protein field, he focused on understanding protein folding mechanisms by developing advanced sampling and reaction coordinate methods.

To date, Zheng has published 21 papers and he has recently been awarded the Nancy Nossal fellowship award from NIDDK for excellence in postdoctoral research. He earned a BS in physics from Fudan University and a PhD in chemistry from Rice University.

Faculty and practitioners discuss their current research and field projects in the college's Science and Mathematics Colloquium Series, held throughout the academic year at the ASU Polytechnic campus. All seminars are free and open to the public.

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