Structure and dynamics of intrinsically disordered proteins from simulations and experiments

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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.

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