Correlation Analysis of Biological Macromolecules

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Time: 2:30 – 3:30pm (*Discussions will follow)
Venue: WLB205, Shaw Campus

ABSTRACT

Within proteins, residues form highly correlated networks through hydrogen bonds and hydrophobic interactions, enabling proteins to effectively resist external environmental influences and maintain stable structures. And the folding processes of many proteins can be interpreted as first-order transitions. On the other hand, understanding about possible correlations of the structural components within intrinsically disordered proteins and DNA/RNA is very limited. We used molecular dynamics simulations, as well as statistical mechanics methods and theories, to study the aforementioned systems. We found magnesium ions can enhance the degree of correlation in the three-way junction pRNA in DNA assembly motors, endowing pRNA with high structural rigidity; identified the significant spatial correlation between DOPA and positively charged residues in the intrinsically disordered mussel adhesive protein, providing the protein with strong adsorption capabilities. We also revealed the correlation between the conformation fluctuations of RGG domains and their dynamic interaction.

BIOGRAPHY

Professor Jingyuan Li received his Bachelor (2002) and Ph.D. degree (2007) from Zhejiang University. After completing postdoctoral research at Columbia University, he joined the Institute of High Energy Physics, CAS as a professor in the multi-disciplinary research division (2011). In 2017, he joined Zhejiang University as a professor in the Department of Physics. He was selected for the "Hundred Talents Program" of CAS and received funding from NSFC's "Excellent Youth Science Fund". His research focuses on computational live matter physics with emphasis on the intrinsically disordered protein, i.e. to characterize, understand and predict IDP conformation and interaction.