

Nonequilibrium dynamics of biofilaments and motor proteins

Wonmuk Hwang, Texas A&M University

At the core of all physiological functions and chemical activities of biomolecules are biophysical processes mediated by a cohort of intra- and inter-molecular forces. While bulk studies have led to staggering developments in biochemistry, nanomechanics of biomolecules and their assemblies have only begun to be explored as relevant experimental and computational tools became available in recent years. Due to the complex nature of these systems, it is essential to use computer simulations for developing atomistic insights. In this talk, I will present an overview of research projects in my lab, which are mainly on the dynamics of biofilaments (alpha-helix, amyloid, and collagen) and motor proteins (kinesin). They are major mechanical elements of the cell and elucidating their operational principles is important for a broad range of problems in biology, medicine, and bioengineering. Furthermore, they provide grounds on which a rich variety of fundamental questions are jointly addressed, including the dynamics of water, polymer mechanics, protein folding, macromolecular assemblies, and the physics at the bio-nano interface.