

Modulation of the mechanical response of biomolecular complexes by the dynamics of applied tension

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Biomechanical functions of protein assemblies such as microtubules (MTs), which exhibit unusual physico-chemical properties such as viscoelasticity and spontaneous shape-changing, are important in cytoskeletal support and cell motility. Tandems of titin govern elasticity within muscular contractile units and the titin-telethonin complex is anchoring titin repeats in the Z-disc of the sarcomere. Understanding the microscopic origin of these unique properties and elucidating the molecular mechanisms of the response of biological assemblies to the dynamics of mechanical inputs constitute major areas of research in biophysics. Although state-of-the-art single-molecule experiments have become available to explore these properties, due to their high complexity and large size, these experiments yield results that are nearly impossible to interpret accurately without input from theoretical modeling. Consequently, linking the submolecular transitions to observed changes in structural and dynamic properties at the macroscopic level has emerged as one of the main challenges of the day. The Self Organized Polymer (SOP) model, implemented on Graphics Processing Units, provides a simplified yet accurate topology-based description of the polypeptide chain of proteins that allows for a full investigation into the effect of tension propagation on the mechanical response of large biomolecules. Application of this methodology to follow the micromechanics of the titin-telethonin complex and MTs reveals that these large molecules are so finely tuned to the force load regime that minimal changes in the magnitude of the load can change drastically their mechanical response. Importantly, these findings provide a molecular basis for interpretation of the results from a number of experimental investigations.

Biography

Ruxandra Dima has completed her Ph.D in Physics from The Pennsylvania State University and postdoctoral studies in Physical Chemistry from the Institute for Physical Science and Technology at the University of Maryland. Since 2006, she is an Assistant Professor in the Department of Chemistry at the University of Cincinnati. She has published more than 25 papers in reputed journals. She has a multi-disciplinary background in biophysics and physical chemistry, with special emphasis on computer simulation and modeling.

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