MAR09-2009-020401

Abstract for an Invited Paper for the MAR09 Meeting of the American Physical Society

Multi-resolution protein modeling by combining theory and experiment CECILIA CLEMENTI, Rice University

The detailed characterization of the overall free energy landscape associated with the folding process of a protein is the ultimate goal in protein folding studies. Modern experimental techniques provide accurate thermodynamic and kinetic measurements on restricted regions of a protein landscape. Although simplified protein models can access larger regions of the landscape, they are oftentimes built on assumptions and approximations that affect the accuracy of the results. We present new methodologies that allows to combine the complementary strengths of theory and experiment for a more complete characterization of a protein folding landscape at multiple resolutions. Recent results and possible applications will be discussed.