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Abstract for an Invited Paper
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Mesosopic Dynamics of Biopolymers and Protein Molecular Machines¹

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The dynamics of biopolymers in solution and in crowded molecular environments, which mimic some features of the interior of a biochemical cell, will be discussed. In particular, the dynamics of protein machines that utilize chemical energy to effect cyclic conformational changes to carry out their catalytic functions will be described. The investigation of the dynamics of such complex systems requires knowledge of the time evolution on physically relevant long distance and time scales. This often necessitates a coarse grained or mesoscopic treatment of the dynamics. A hybrid particle-based mesoscopic dynamical method, which combines molecular dynamics for a coarse-grain model of the proteins with multiparticle collision dynamics for the solvent, will be described and utilized to study the dynamics of such systems. See, C. Echeverria, Y. Togashi, A. S. Mikhailov, and R. Kapral, *Phys. Chem. Chem. Phys.* 13, 10527 (2011); C. Echeverria and R. Kapral, *Phys. Chem. Chem. Phys.*, 14, 6755 (2012); J. M. Schofield, P. Inder and R. Kapral, *J. Chem. Phys.* 136, 205101 (2012).

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