Multiscale molecular dynamics of disordered proteins and their complexes

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For decades, it has been assumed that function of a protein stems from its specific spatial structure. However, around 2000, it has been recognized that many proteins are intrinsically disordered as they lack well defined structures and yet they play many important functional roles in the cell. The main objective of the proposed research is to study interesting examples of such proteins through the molecular-dynamics simulations: all-atom and coarse-grained. The possible examples relate to the memory consolidation, degradation of cellulose into simple sugers, neurodegeneration, and issues of food science.