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A backbone based protein model with explicit solvent SUMIT SHARMA, Princeton University, SERGEY BULDYREV, Yeshiva University, PETER J. ROSSKY, University of Texas Austin, H. EUGENE STANLEY, Boston University, PABLO G. DEBENEDETTI, Princeton University, C. AUSTEN ANGELL, Arizona State University, SANAT K. KUMAR, Columbia University —
The computational expense of folding atomistically detailed protein models is prohibitive. Hence minimalist models of proteins are a popular choice. The minimalist models developed so far have excluded water, and treated the hydrophobic effect as an effective attraction between hydrophobic monomers. This simplified treatment does not capture the temperature-dependent variations in entropy and enthalpy of water molecules. Proteins have a predominantly water-screened hydrophobic core and water-exposed polar groups. This structural feature should alter the dynamics of proteins and surrounding water from that of a hydrophobic homopolymer in water. To include these features in a minimalist model, we designed heteropolymers of polar and hydrophobic monomers in explicit water-like medium. The polar monomers and water molecules were modeled with the Jagla potential, which has been shown to reproduce many water-like thermodynamic properties, and the hydrophobic monomers as hard spheres. We discuss a methodology for optimizing the sequence of these heteropolymers and how the hydrophobic collapse of these heteropolymers differs from that of a random heteropolymer.

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