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What drives hydrophobic polymer collapse and re-entry transitions in miscible good solvents?¹ FRANCISCO RODRIGUEZ ROPERO, TIMIR HAJARI, NICO F. A. VAN DER VEGT, Tech Univ Darmstadt — Herein, we study co-nonsolvency of poly(N-isopropylacrylamide) (PNiPAM) in methanol aqueous solutions. Our results show that both the coil-to-globule transition at low methanol concentrations and the globule-to-coil re-entrance at high methanol concentrations are entropy driven. At low alcohol content, methanol preferentially binds to the PNiPAM globule and drives polymer collapse. Rather than being driven by electrostatic, hydrogen bonding or bridging-type interactions with the globule, preferential methanol binding is found to result from a significant increase of the chain configurational entropy, stabilizing methanol-enriched globular structures over wet globular structures in neat water. The globule-to-coil re-entrance at high methanol concentrations is instead driven by changes in solvent-excluded volume of the coil and globular states imparted by a decrease in solvent density with increasing methanol content of the solution. The co-nonsolvency mechanism proposed in this contribution provides a new angle on how to develop Coarse Grained simulation models for responsive soft matter systems. Moreover, several of the solvation effects described in this contribution can be incorporated in theories for cosolvent-induced conformational transitions in dilute polymer solutions.

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