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Controlling solubility of pNIPAM in aqueous solutions using hydrophobic and photoresponsive molecular units RAHUL SINGH, Iowa State University, SANKET DESHMUKH, SUBRAMANIAN SANKARANARAYANAN, Argonne National Laboratory, GANESH BALASUBRAMANIAN, Iowa State University — The structural properties of pNIPAM (poly-N-isopropylacrylamide), which is a thermally sensitive polymer, are investigated by copolymerizing it with molecular units that are either (1) hydrophobic (polystyrene) or (2) photoresponsive (spiropyran-merocyanine pair). We employ molecular dynamics (MD) simulations to examine aqueous solutions of pNIPAM (modified with these molecules) across a temperature range below and above the LCST of pure pNIPAM to understand the fundamental physics underlying the coil-to-globule transition in pNIPAM and the contribution of the attached constituents on the LCST. The LCST can be tuned by copolymerizing pNIPAM with polystyrene (PS), a hydrophobic molecule. We prepare a number of copolymers with different chain lengths of the hydrophobic units (PS) and observe the lowering of the LCST of the modified pNIPAM by computing the radius of gyration and end-to-end distances across the temperature range. Also, the aqueous solubility of pNIPAM can be controlled by functionalizing it with a photoresponsive moiety as this new copolymer exhibits a shifted LCST phase transition. Thus, the temperature sensitive behavior of pNIPAM can be tuned by copolymerizing it with varying molecular lengths of hydrophobic block units or attaching reversibly switchable photoresponsive moieties. Our work demonstrates the controllability of pNIPAM solubility aqueous solutions and recommends strategies to design complex programmable polymers that have wide-ranging applications in several biomedical and industrial processes.

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