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A Coarse-Grained Model for Thermoresponsive Poly(*N*-isopropylacrylamide) LAUREN J ABBOTT, MARK J STEVENS, Sandia National Laboratories — Poly(*N*-isopropylacrylamide) (PNIPAM) is a thermoresponsive polymer that undergoes a phase transition at its lower critical solution temperature (LCST). Although atomistic simulations have been effective to study PNIPAM single chains in solution, they are limited in reaching longer length- and time-scales. In this work, a coarse-grained (CG) model is developed for PNIPAM that captures its thermoresponsive behavior. Nonbonded parameters are fit to experimental thermodynamic data, with minor adjustments to provide better agreement with radial distribution functions from atomistic simulations. Bonded parameters are fit to probability distributions from atomistic simulations using multi-centered Gaussian-based potentials. The temperature-dependent potentials derived for the CG model in this work properly capture the coil-globule transition of PNIPAM single chains and yield a chain-length dependence consistent with atomistic simulations and experiment. The self-assembly of PNIPAM surfactants is also explored. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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