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A Model for the Thermally Induced Polymer Coil-to-Globule Transition DAVID SIMMONS, Univ. of Texas, ISAAC SANCHEZ, Univ. of Texas — A quantitative mean-field model for the thermally-induced (heating-induced) polymer coil-to-globule transition (HCGT) is developed with no adjustable parameters. The transition temperature Θ is given for a long chain by the equation $\Theta = 2T_p^* \left[1 - \tilde{\rho}\left(\Theta\right)\right]$ where T_p^* is the characteristic temperature of the polymer for the lattice fluid model and $\tilde{\rho}\left(\Theta\right)$ is the reduced solvent density at the transition temperature Θ. Calculated HCGT temperatures show good agreement with experimental LCSTs. The physics of the HCGT transition is shown to be consistent with the physics of the LCST transition. The predicted globular state is characterized by the dominance of attractive polymer self interactions over excluded volume interactions. This model can be easily generalized to treat cross-linked gels and their contraction-expansion characteristics.

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