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Explicit-ion Effects in the Coil-Globule Transition of Weak Polyelectrolytes BENJAMIN J. SIKORA, JONATHAN K. WHITMER, University of Notre Dame — The first-order coil-globule transition in weak (annealed) polyelectrolytes involves a subtle balance of pH, charge strength, and solvation forces. In this work, we utilize a coarse-grain hybrid grand-canonical Monte Carlo and Molecular Dynamics approach to explore the free energetic topography of a model hydrophobic polybase [representing poly(2-vinylpyridine) (P2VP)] and explore the role of salt concentration/valency in influencing polyelectrolyte conformations using both an implicit Debye-Hckel and explicit salt approach. Our simulations reproduce the experimentally measured behavior for dilute annealed polyelectrolytes, and present a solid foundation for understanding pH responsive polyelectrolyte materials.

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