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Asymmetrical collapse of charged heterogeneous macromolecules
NATALIA DENESYUK, JOHN WEEKS, Institute for Physical Science and Technology, University of Maryland, College Park — We propose a new method based on local molecular field (LMF) theory to treat Coulomb interactions in simulations of ionic fluids. This method has been tested in Langevin dynamics simulations of a model protein, which consists of a random sequence of charged hydrophilic and neutral hydrophobic monomers, in salt solution. The concentration of salt ions in the simulation box is maintained by grand canonical Monte Carlo. Our general strategy is to perform averages over an ensemble of sequences in order to identify those general properties that are sequence independent. We find that, independently of their random sequence, heterogeneous polyelectrolytes undergo the asymmetrical collapse in which one of their quadruple moments vanishes.

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