Liquid structure of flexible polyelectrolyte solutions

JAMES DONLEY, The Boeing Company, DAVID HEINE, Sandia National Laboratories — MD simulations and the recently developed RORPA theory are used to examine the liquid structure of flexible polyelectrolyte solutions. Quantitative comparison is made with experiments that show an invariance of the structure factor peak height and wavevector with chain charge fraction f. This invariance has important implications for the design of polyelectrolyte-based materials. Previous theoretical results for rod polymers show that proper inclusion of polymer-polymer density correlations is sufficient to yield this invariance. However, for flexible polyelectrolytes other aspects such as counterion condensation or an explicit solvent seem to be at least partially necessary to produce the experimental trends. Possible causes of the anomalously large low wavevector scattering, i.e., slow mode, seen in many experiments will also be discussed.

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