

Abstract Submitted
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Evaporation of Solutions Containing Charged Polymers: A Molecular Dynamics Study CHENGYUAN WEN, SHENGFENG CHENG, Department of Physics, Virginia Polytechnic Institute and State University — Electrostatic interactions lead to rich behavior of solutions containing charged polymers different from that of neutral counterparts. The evaporation of the solvent from a polymer solution composed of a polar solvent, charged polymer chains, counterions, and salts is studied via large-scale molecular dynamics simulations. In our computational scheme, polymers are modeled as bead-spring chains containing neutral and charged beads. The solvent consists of dimers of oppositely charged beads connected by chemical bonds. Counterions are explicitly included as mobile single beads to make the whole system neutral. The morphology of the charged polymer chains at different volume fractions before evaporation and the structure of the resulting film after evaporation are compared and the effects of evaporation rate are clarified. We also add salts to the solution and study their influence on the polymer morphological evolution during evaporation.

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