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Ionomer Self-assembly in Dilute Solution: a Coarse-grained Molecular Dynamics Study. MAHDI GHELICHI, KOUROSH MALEK, MICHAEL EIKERLING, Simon Fraser University — Self-assembly of semiflexible ionomer chains in dilute solution is studied by classical molecular dynamics (MD). Ionomer molecules consist of hydrophobic backbones, grafted with pendant side chains that are terminated by anionic headgroups. Coarse-grained MD simulations show the self-assembly of the semiflexible ionomer chains into cylindrical bundle-like aggregates. Bundles are comprised of a core of backbone chains surrounded by a surface layer of charged anionic headgroups and a diffuse halo of counterions. Parametric studies of bundle properties explored the role of backbone hydrophobicity, strength of electrostatic interactions between charged moieties, side chain content, and counterion valence. Expectedly, the size of bundles increases with backbone hydrophobicity. The aggregate size depends nonmonotonically on the value of the Bjerrum length. Increasing the grafting density of pendant side chains results in smaller bundles and the counterion valence exerts a strong effect on bundle size and counterion localization in the near-bundle area. Results are interpreted in terms of the interplay of the surface energy of hydrophobic chains and the electrostatic repulsion among the anionic headgroups. The findings are discussed within the context of experimental studies on the formation of rodlike structures in ionomer solution.

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