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Can Martini coarse-grained models capture antifouling behavior of polyzwitterionic brush coatings?

Biofouling has widespread implications for everyday materials, including biomedical devices, personal protective equipment, and marine coatings, leading to performance degradation and high costs. Polyzwitterionic brush coatings are known to exhibit antifouling behavior due largely to a strongly coupled hydration layer, yet the detailed mechanism is not fully understood. Moreover, only a handful of polymer chemistries have thus far been identified as highly antifouling.

Molecular dynamics (MD) simulations are a vital tool for studying polymer-protein interactions at angstrom-scale resolution, enabling both screening of polymer chemistries for antifouling properties, and interpreting experimental results indicating antifouling behavior. Coarse-grained (CG) simulations, in which atoms are grouped into effective interaction sites, lead to substantial gains in computational efficiency and allow for accessing microsecond timescales in large polymer systems.

In this work we present new Martini CG models for a series of polyelectrolyte and polyzwitterion chemistries compatible with Martini 2 polarizable water. CG brush models are validated by comparing density profiles and pair correlation functions against all-atom systems. Finally, adsorption free energies of lysozyme into the brushes are computed via metadynamics. We assess whether the models can capture the expected effects of brush chemistry and salt on antifouling behavior.

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Topical Area

Soft matter: polymers, and complex fluids

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