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Effective interactions and aggregation of rodlike polyelectrolytes[1]

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Rodlike polyelectrolytes are known to exhibit various aggregation phenomena, assembling into structures that range from bundles to rafts. Such self-assembly is important in numerous biological and synthetic applications. Here, I provide an overview of various important aspects of such phenomena. In particular, I will highlight computational work on the free-energy landscape of various rod configurations. Furthermore, the role of many-body effects will be discussed. First, ionic excluded-volume effects lead to correlations, which can become particularly important in the dense environment within an aggregate. Second, induced polarization charges arise from the dielectric mismatch between the polyelectrolyte and the surrounding solvent. The latter are rarely taken into account, owing to the computational complexity of solving the bound charges, but can significantly alter the electrostatic interactions that are responsible for aggregation in the first place. New, efficient techniques now make it possible to incorporate these effects in standard molecular dynamics or Monte Carlo simulations. Using these techniques, I examine the role of both types of many-body effects on bundle configuration and stability.

[1]Work performed in collaboration with Kipton Barros and Daniel Sinkovits.