Crowding in the cellular context: Tales of Clusters and Dynamics

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Abstract

Biological macromolecules are highly concentrated in biological environments giving rise to crowding effects that impact structure, dynamics, and ultimately function. It is increasingly becoming clear that weakly attractive non-specific interactions may be a significant factor in crowding effects. Such interactions can lead to the dynamic formation of clusters which impacts diffusive properties and may lead to the formation of phase-separated states. Recent results from molecular dynamics computer simulations of cellular systems at different scales are presented that relate biomolecular interactions to cluster formation and altered diffusive behavior. Models of concentrated protein solutions, bacterial cytoplasms, with and without the presence of membrane surfaces are discussed. The models range from fully atomistic systems to coarse-grained models derived from the atomistic systems in order to expand to larger spatiotemporal scales. Where possible, the results from the simulations are related to experimental data.

Keywords: crowding, molecular dynamics, coarse, grain models

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