Title:	Patchy Particles for Modelling Biomolecular Condensates
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Abstract:	Biomolecular condensates are membraneless organelles essential for the biochemical functionality and spatiotemporal organization of cells. These organelles form through the liquid-liquid phase separation (LLPS) of their constituents with the cytosol, allowing for precisely tuned local concentrations and rapid assembly or dissociation in response to ex- ternal stimuli. Recent in vitro studies have demonstrated that even in minimal setups of a few proteins, complex behaviors can emerge, such as changes in concentration affecting the stability and structure of the condensate, or phosphorylation of specific sites on proteins leading to condensate dispersion. Although these behaviors are assumed to have signifi- cant functional implications, the interplay in complex assemblies of many proteins remains poorly understood. To study this behavior, we employ a coarse-grained approach using patchy particles, where proteins are modeled as repulsive spheres with localized bonding sites. This model facilitates the simulation of large system sizes while maintaining binding specificity and local bond structures. In my thesis, I begin with a thorough investigation of a model proposed by Espinosa et al., which exhibited glassy behavior, limiting fluid behavior to a narrow temperature range due to dramatically slowed dynamics at lower temperatures. We hypothesize that minor perturbations, such as adding a different type of patchy particle, could dramatically affect the system's fluidity, to an extent where systematic study becomes challenging. As we can attribute the glassy behaviour to the fully bonded character of the underlying network, we propose a modification to the patchy particle model: we add an attractive, isotropic potential to the core. This allows for weakening the individual bonds by lowering their patch strength by compensating the energetic loss using the core. We found that while weaker isotropic core interactions render the condensate more fluid, higher potential strengths modify the structure of the condensate, leading to new arrangements of particles and a non-monotonic behaviour in the dynamics of the system.
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