Poster Session

[PO-03] Structure and dynamics of amphiphilic patchy cubes in slit-like confinement

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Structure and dynamics of amphiphilic patchy cubes in slit-like confinement

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1   Introduction

Self-assembly is a ubiquitous phenomenon in colloidal suspensions and offers a way to create novel materials with specific functionalities. Since the self-assembled morphologies strongly influence emergent macroscopic transport properties, such as viscosity and thermal conductivity, the precise control and prediction of the self-assembly process are essential for prospective applications including the cosmetics, food industry, and industrial lubrication.

A promising approach for manipulating self-assembly is the anisotropic modification of individual particle surfaces, so-called "patches". By introducing the interaction *via* surface patches, a diverse self-assembly of highly ordered structures has been observed, including the chains [1], micelles [2], and network structures [3]. In addition to surface anisotropy, particle shape also plays a critical role in the acquisition of rich self-assembled structures. The combination of surface and shape anisotropies offers a wider range of possibilities to control the self-assembly and the resulting transport properties.

Recent research on amphiphilic nanocubes, employing molecular dynamics (MD) and Monte Carlo simulations [4], has unveiled various finite-sized aggregates ranging from rods to fractal objects. Amphiphilic cubes emerge as particularly intriguing materials due to their simple geometry, space-filling properties, and multi-directional interaction anisotropy. Previous simulations of amphiphilic nanocubes in suspension have recently shown the various finite-sized aggregates ranging from rods to fractal objects [4]. A more recent study [5] using kinetic Monte Carlo calculations explored the self-assembly behaviors under shear, revealing shear-induced growth and breakup of these self-assembled clusters. We further investigate the structure formation and the rheological properties of amphiphilic cubes in bulk solutions in equilibrium and under shear [6].

Previous studies have extensively explored the structural dynamics of self-assembly in bulk systems, but there is a notable lack of attention to the impact of wall interactions. Some studies have demonstrated the distinctive self-assembled structures and morphologies of amphiphilic nanoparticles confined in narrow slit-like or tube geometries [7]. The self-assembly of amphiphilic cubes in confined geometries might exhibit increased complexity, showing behaviors not observed in bulk conditions, primarily due to wall-colloid interactions. Since many experiments and natural phenomena occur in confined geometries, this study has the potential to provide valuable insights into understanding the structural morphologies and resulting transport properties of nanocubes in more realistic environments.

In this study, we investigate the structure and dynamics of amphiphilic nanocubes confined in nanoslit geometry, incorporating both repulsive and attractive interactions with the walls at rest and under shear. To take into account hydrodynamic interactions, we employ a combination of multi-particle collision dynamics (MPCD) and conventional MD [8]. we aim to elucidate the structural transformations of amphiphilic nanocubes under different types of wall interactions, patch locations, and flow rates.

2   Problem Statement

The system used in this study is composed of point particles, considered as a coarse-grained model of atoms. For the nanocubes, we use a discrete particle model [9], composed of a set of point particles connected to nearest neighbors and diametrically opposite ones by a harmonic potential. We modeled the amphiphilic nanocubes to have one or two attractive surfaces (colored yellow in Fig.1 (I)) with two arrangements (type I and II) and other repulsive surfaces (purple). We introduce the Lennard-Jonnes potential for attractive interactions between solvophobic particles and the Week-Chandler-Andersen potential for repulsive interactions between other particles. These nanocubes are confined in a slit-like channel and experience attractive or repulsive interactions with the walls. The coordinate system was chosen so that the principal axes coincide with the flow (x), vorticity (y), and wall directions (z). The

channel dimensions are set to ($L_x = L_y = 80\,a$) and ($L_z = 40\,a$). We simulated binary mixtures of one- and two-patch nanocubes at a volume fraction ($\phi = 0.005$). All simulations are performed by HOOMD-blue [10, 11] (ver. 2.9.6).

3 Results

In the equilibrium state, we observed the self-assembled structures such as rod-like and fractal objects due to the patch arrangements, which are qualitatively similar to our previous simulations of bulk suspensions. The rod-like clusters are limited in growth due to the presence of walls, resulting in shorter lengths compared to bulk conditions. This structural formation in the equilibrium is greatly changed when the fluid flow is applied. Long clusters in the system are broken up and decomposed into smaller clusters or isolated particles. We plan to quantitatively analyze the structure and flow properties of these mixtures, and will also investigate the correlation between shear-induced structural formation and viscosity changes.
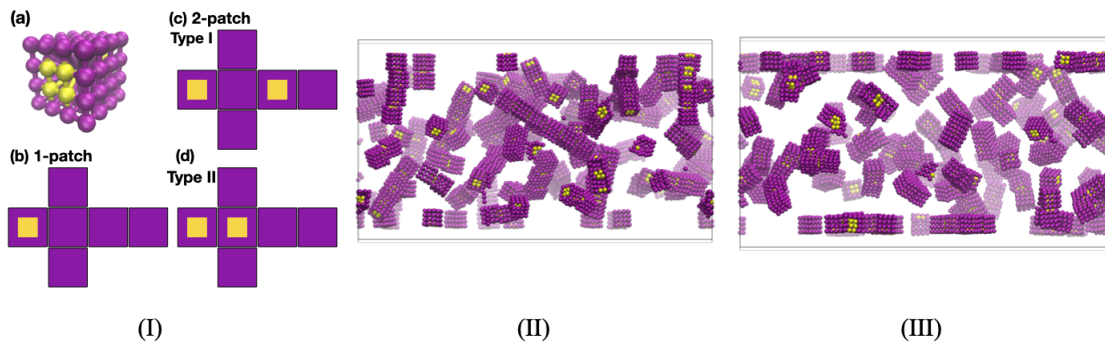

Figure 1: (I) Unfolded representation of a nanocube. (II), (III) Representative snapshots of amphiphilic patchy nanocubes of type I and type II, respectively.

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