Self-Assembly of Janus Colloids under Flow

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The self-assembly of amphiphilic Janus colloids under flow was studied using hybrid molecular dynamics simulations with fully resolved hydrodynamic interactions incorporated through the multi-particle collision dynamics algorithm. The simulations were conducted at a density and temperature range where the Janus colloids spontaneously self-assembled into spherical micelles to minimize the interface between the solvophobic caps and the surrounding solvent. Under strong shear flow, the micelles broke up into smaller fragments and isolated particles. Nonetheless, an intermediate shear rate regime was found where the balance between rearrangement and dissociation favored the growth of the aggregates. Additionally, the simulations revealed that clusters composed of either 6 or 13 particles were most stable towards shear flow due to the high geometric symmetry of these aggregates. When the system was exposed to Poiseuille flow, a highly non-uniform cluster size distribution was found between the channel walls, where the aggregation number decreased close to the walls. Furthermore, a sizable fraction of free particles and small clusters with three and four members was found at the walls when the microfluidic channel was made out of a comparably solvophobic material as the Janus colloids.