近畿大学理工学総合研究所コロキウム

第 318 回 平成 30 年 10 月 30 日 (火) 15:30~16:30 於 38 号館 2 階 多目的ホール

Directed assembly of structured nanoparticles
through rapid micromixing
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Tailored nanoparticles are increasingly sought after for many scientific and technological applications, such as optoelectronic devices and highly selective catalysts. However, both research and commercialization of these materials has been impeded by the lack of suitable fabrication techniques. One promising approach for overcoming this hurdle is flash nanoprecipitation, where (soft) nanoparticles are assembled through rapid micromixing of polymers in solution with a miscible poor solvent. This continuous process allows for high yields as well as precise control over particle size and morphology. We employed multiscale computer simulations of this process to understand its underlying mechanisms and to efficiently explore parameter space. We first performed explicit solvent molecular dynamics (MD) simulations of a bead-spring polymer model to study the microscopic properties of the fabrication process. Then, we fed the MD data into a kinetic Monte Carlo algorithm to reach macroscopic length- and timescales. We discovered that the nanoparticle size can be reliably tuned through the initial polymer concentration and the mixing rate. Further, we were able to fabricate a wide variety of structured colloids, such as Janus and core-shell particles, when polymer blends were used in the feed stream.

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