Multiscale Modeling of Multicompartment Micelle Nanoreactors

Seung Soon Jang

Computational NanoBio Technology Laboratory, School of Materials Science and Engineering, Georgia Institute of Technology, 771 Ferst Drive NW, Atlanta, GA 30332-0245, USA
E-mail address: seungsoon.jang@mse.gatech.edu

In recent years, research in industrial applications of polymeric materials has begun to explore the field of immobilized catalysis. In particular, the idea of catalysts bound to a micelle backbone, creating a nanoscale molecular reactor (commonly referred to as nanoreactor), has become an area of great interest. From a computational perspective, investigating the potential of micelles as nanoreactors requires analyzing the miscibility of block copolymers, both on a fully atomistic and on a mesoscale basis. The model proposed by Flory and Huggins offers an interaction parameter χ which quantifies the favorability of mixing between two polymers. This interaction parameter depends on many process conditions, not least of which are the temperature and composition of a solution, in order to properly estimate the strength of the interaction between a given pair of polymer molecules. Extensive work has already been completed in this group to establish a robust method of estimating the χ-value for a given pair of molecules; this information is necessary for preparing coarse-grained modeling and simulations (e.g., micellization simulations). In our present work, we apply miscibility analyses to a relatively nascent technology in immobilized catalysis science, viz. the multicompartment micelle nanoreactor. This technology offers a way to harness both the enhanced reactivity of homogeneous catalysis *and* the ease of separation traditionally enjoyed by heterogeneous catalysis. Through the use of mesoscale calculations, we will study the feasibility of a three-compartment micelle nanoreactor. For this purpose, we have developed a systematic strategy to calculate χ parameters, which has been applied and validated through mesoscale simulations of micelle consisting of triblock copolymers. We hope to demonstrate that this triblock copolymer can form a micelle capable of reaction compartmentalization and tandem catalysis, two hugely promising capabilities for highly selective multistep-catalyzed reactions.