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Dissipative Particle Dynamics Method on PH-Responsive Polymeric Drug Delivery System YINGYING GUO, City University of HongKong — The self-assembled morphologies formed by polymer in selective solvent could be potentially used as drug-delivery vehicles and has attracted great attention recently. In our work, the drug release mechanism of polymeric delivery vehicle (polymeric microsphere) is investigated with Dissipative particle dynamics simulation. Poly (Lactic Acid)-b-polyethylene glycol (PLA-b-PEG) diblock copolymer is the carrier while IBU is selected as the model drug. A core-shell spherical micelle with drug encapsulated in the core is obtained in our simulation. By changing the medium from neutral to acid, the drugs release via a diffuse mechanism. Both the formation mechanism of the encapsulant and the release mechanism for the drugs are studied in our work. For the formation process, it can be ascribed as the coalesce of the small clusters and the disperse of the drugs; while for the drug release behavior, the process can be divided for three stages: (1) swell of the polymeric carrier, (2) drug diffuse in the carrier and some acid molecules disperse into the carrier, (3) drug release towards the acid medium. Our results might provide a mesoscopic methodology for the evaluation and prediction for polymeric self-assemblies as a carrier for pharmaceutical interest.

Yingying Guo
City University of HongKong

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