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Modeling controlled release from responsive microgel capsules[1]

ALEXANDER ALEXEEV, HASSAN MASOUD, Georgia Institute of Technology, George W. Woodruff School of Mechanical Engineering — We introduce a coarse-grained computational method that explicitly captures the release of nanoparticles and macromolecules from responsive microgel capsules. The model is based on the dissipative particle dynamics. Our simulations reveal that not only swelling, but also deswelling of hollow microcapsules can be harnessed for controlled release. We show that the release from swollen capsules is diffusion driven, whereas the release from deswelling gel capsules occurs due to the flow of encapsulated solvent that is expelled from the shrinking capsule interior. The latter hydrodynamic release is burst-like and continues only during capsule deswelling. We find that deformable polymer chains that can easily penetrate thorough membrane pores are released in larger amounts from deswelling capsules, than nanoparticles that are filtered out by shrinking membrane pores. Our simulations further demonstrate that the inclusion of rigid microrods inside deswelling capsules mitigates the membrane pore closing, and, in this fashion, provides an effective method for regulating the rate of hydrodynamic release of nanoparticles.

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