

Drug loading and release in stimuli-responsive microgels: insights from coarse-grained simulations

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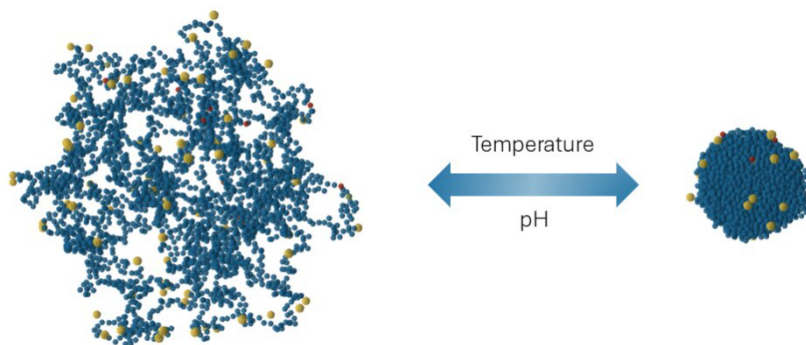
Stimuli-responsive microgels are promising platforms for controlled drug delivery, combining structural tunability with sensitivity to external stimuli such as temperature and pH. In this work, coarse-grained simulations were used to investigate the physicochemical parameters governing drug loading and release in temperature- and pH-responsive microgels. Thermoresponsiveness is modelled using a monomer–monomer hydrophobic interaction potential, while pH-sensitivity is introduced by incorporating charged monomers into the polymer network, mimicking the ionization of chemical groups at different pH conditions.

First, we characterized the structural and electrostatic properties of the microgels in the absence of drug molecules, analysing how particle size, net charge, and surface potential change depending on both the number of charged monomers and the hydrophobic interaction strength. Then, drug loading and temperature-triggered release were studied by modelling drug molecules as nanoparticles with tunable hydrophobicity, varied through a monomer–nanoparticle interaction potential. The effects of drug concentration, drug–polymer affinity, and the degree of microgel collapse on drug loading and release are explored.

These findings contribute to the understanding of the key parameters governing drug uptake and release in stimuli-responsive microgels, providing guidelines for the rational design of microgels as drug delivery systems.

Keywords:

Microgels, coarse-grained, simulations, drug delivery, stimuli-responsiveness



Snapshots of a drug-loaded microgel in the swollen (left) and collapsed (right) states, illustrating the structural response to temperature and pH. Blue and orange spheres represent neutral and charged monomers, respectively; yellow spheres represent drug nanoparticles.

References:

[1] María del Mar Ramos-Tejada, Alberto Martín-Molina, Daniel Montesinos, Luis Pérez-Mas and Manuel Quesada-Pérez. *Coarse-Grained Simulations of Thermosensitive Polymer Nanocomposites*. *Macromolecules* 59, 2360-2370 (2026). <https://doi.org/10.1021/acs.macromol.5c02656>

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