# COMPUTATIONAL RESEARCH IN BOSTON AND BEYOND SEMINAR

**Friday, June 7, 2024**

**12:00 PM – 1:00 PM**

**https://mit.zoom.us/j/96155042770**

# Revealing the molecular origins of surface condition-dependent nanoparticle structure using classical molecular simulations


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## Abstract:

Nanoparticles have become crucial materials in pharmaceutical formulation, unlocking the oral bioavailability of hydrophobic drug molecules. Processing drug nanoparticles requires the use of additives like polymers and surfactants which can interact with nanoparticles in multiphase mixtures and dispersions and modulate nanoparticle structure, which is crucial to the performance and efficacy of the drug. However, while significant research has investigated how single additives modulate nanoparticle structure, there is little work exploring the mechanistic interactions of multiple additives with drug nanoparticles. Here, we use high-performance classical molecular dynamics (MD) simulations to explore how the structure of a drug nanoparticle changes as a result of competitive and cooperative interactions between additives on the surface of the nanocrystal. We observe that the degree of order on the drug surface increases with surfactant concentration, in agreement with previous empirical results. Our simulations reveal two dominant underlying molecular mechanisms: (1) surfactants screen the nanoparticle surface from de-stabilizing polymer interactions and (2) surfactants complex polymers far from the nanoparticle surface which de-localizes polymers from the surface. We also uncover a connection between accelerated dynamics in the bulk of the crystal and the experimentally measured extent of crystallinity. These simulations are the first to directly characterize structural changes in a drug nanocrystal as a function of additive composition and relate extent of crystallinity to molecular-level structure.


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