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Contribution ID: **4331** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Fully three-dimensional dynamical self-consistent field theory for dendritic phytoglycogen nanoparticles

Monday, May 27, 2024 2:45 PM (15 minutes)

Phytoglycogen (PG) is a glucose-based polymer with a dendritic architecture that is extracted from sweet corn as a soft, compact, monodisperse, 22 nm radius nanoparticle. Our recent model for a PG particle in solvent (water), based on dynamical self-consistent field theory (dSCFT), was successful in producing a dendrimer with a core-chain morphology, radius, and hydration, in close agreement with observations [1]. However, this model assumed, for simplicity, that the solvent distribution around the particle was spherically symmetric. This prevented us from studying heterogeneous structures on the particle surface. In this talk, we extend our dSCFT model, and consider a fully three-dimensional solvent distribution. We compare the new predictions for the morphology, radius, and hydration of PG to our earlier results. Motivated by experimental investigations of chemically modified versions of PG, we discuss preliminary results for the surface structures produced by the association of small, hydrophobic molecules with PG.

[1]: Morling, B.; Luyben, S.; Dutcher, J. R.; Wickham, R. A. Efficient modeling of high-generation dendrimers in solution using dynamical self-consistent field theory (submitted).

Keyword-1

Polymer physics

Keyword-2

Phytoglycogen nanoparticles

Keyword-3

Dendrimers

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