Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **3312** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Dynamical self-consistent field theory simulation of dendritic phytoglycogen nanoparticles

Wednesday, 8 June 2022 16:15 (15 minutes)

Phytoglycogen (PG) is a naturally occurring, highly branched, glucose dendrimer that is extracted from sweet corn as soft, compact nanoparticles [1]. We use dynamical self-consistent field theory (dSCFT) to simulate the dynamical evolution of a PG nanoparticle solubilized in water. We evolve the 11-generation dendrimer using an efficient, stable operator decomposition of the dendrimer into its branches. By varying the strength of the interactions between the PG nanoparticle and water, we are able to tune the size and the degree of hydration of the nanoparticle to be in agreement with the values measured using small angle neutron scattering (SANS) [1]. We show that our model is capable of reproducing the 'hairy' morphology of PG nanoparticles as inferred from rheology, SANS, and atomic force microscopy measurements.

[1] J. Simmons et al. *Biomacromolecules* **2020**, 21, 4053-4062.

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Session Classification: W3-8 Soft Condensed Matter II (DCMMP) | Matière condensée molle II (DPMCM)

Track Classification: Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)