Simulating the dynamic susceptibility of magnetic colloidal polymers / Simulacija dinamičke susceptibilnosti magnetnih koloidnih polimera

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Naučna oblast: Physics

Opis teme

Magnetic Colloidal Polymers (MCPs) are polymer-like mesostructures composed of permanently crosslinked magnetic nanoparticles (MNPs), encompassing systems with varied magnetic content, solvent affinity, and composition profiles. Similarly to chemical polymers, their self-assembly into superstructures can be controlled through solvent selectivity and backbone composition. The interplay of solvophilic, solvophobic, and magnetic interactions gives rise to complex self-assembly behaviour that can be manipulated with external magnetic fields, offering dynamic control and high spatial resolution [1].

Studying dynamic susceptibility in MCP-based fluids requires advances in both simulation methodology and large-scale modelling. Dynamic susceptibility is a collective property of MCP-based fluids that characterises their dynamics, i.e. characteristic magnetic relaxation times, and is a key measurable quantity for the development of MCP-based magnetic fluids for applications such as magnetic hyperthermia [2].

Zadaci i ciljevi

Depending on their profile, a prospective student could contribute to:

- implementing physics-based heuristics in particle-mesh (P3M) methods;
- implementing load balancing in molecular dynamics simulations with hardware-accelerated mesh actors, to enable the use of realistic potentials of mean force that introduce chemically specific interactions into large-scale colloidal simulations of MCPs;

• simulating and calculating the dynamic susceptibilities of MCP-based fluid designs with explicit magnetodynamics, to understand the relationship between MCP design and the corresponding theoretical heat production.

Lista referenci

[1] Mostarac, D., Novak, E. V., & Kantorovich, S. S. (2023). Physical Review E, 108(5), 054601. DOI: 10.1103/PhysRevE.108.054601

[2] Khelfallah, M., Novak, E. V., Kuznetsov, A. A., Mostarac, D., Daffé, N., Sikora, M., ... & Kantorovich, S. S. (2026). Nanoscale. DOI: 10.1039/D5NR05218A

Tražene vještine od studenata

Must: excellent Python knowledge; statistical physics. Nice to have: molecular dynamics simulations experience; excellent C++ knowledge for the technical tasks.