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Measuring Viscoelastic Properties of Magnetic Gels with Dissipative Particle Dynamics

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Magnetic gels are liquid swollen polymer networks embedded with *magnetic nanoparticles* (MNPs). These materials can be stimulated by external magnetic fields to alter their shape, mechanical properties, or generate heat, making them promising candidates for applications in soft robotics for actuation, targeted drug delivery, and medical therapies to treat hypothermia.
Quantifying the viscoelastic behaviour of magnetic gels is key to designing materials with targeted properties. Two primary approaches exist to characterize the viscoelastic properties of magnetic gels: (i) direct mechanical measurements, where an applied strain yields bulk or macroscopic material properties, and (ii) measuring magnetic susceptibility to obtain local material properties in the surroundings of the MNP via the Gemant-DiMarzio-Bishop theory.
In this work, we use the ESPResSo molecular dynamics simulation package to characterize the viscoelastic response of magnetic gels at both macro- and nanoscale levels, and to establish a correlation between these scales. The polymer network is modeled via a coarse-grained bead-spring representation immersed in a momentum-conserving dissipative particle dynamics (DPD) solvent. Direct rheology measurements are conducted using periodic Lees-Edwards shear boundary conditions. Starting from a minimal model, we validate and parameterize the system to reproduce typical hydrogel properties.
We are currently extending the model to incorporate MNPs, which are represented as Raspberry particles with multiple interaction sites coupling to both the DPD solvent and the polymer network. This approach enables us to systematically study the influence of embedded nanoparticles on local deformation mechanisms as well as the global viscoelastic response of the gel.

Type:

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