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First-Principles Modeling of Nanoparticle Magnetization, Chaining, and Motion

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Abstract : The ability to effectively design and test magnetic nanoparticles for controlled movement has been an elusive goal in the design of these particles. Magnetic nanoparticles of various characteristics have been created for use towards therapeutic effects, however the challenge of designing for controlled movement remains unmet. A step towards design in this aspect is a first principles model that captures and predicts the behaviors of particles in a magnetic field. The model is governed by four forces acting on the particles, the magnetic gradient, the dipole-dipole forces, the steric forces, and the viscous drag force. The particles are multi-core or single core, and incorporate a preferred magnetization axis. Particles exhibit behaviors, such as chaining, in simulations that are similar to those witnessed through experimentation. Currently, experimental results are being compared to the modeling results for verification of the model, through the analysis of chaining behaviors. This modeling system will be used in designing magnetic nanoparticles for specific chaining and movement behaviors.

Keywords : controlled movement, modeling, magnetic nanoparticles, nanoparticle design
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