# From Theoretical Limits to Nanofabricated Designed Particles for Hyperthermia

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**Abstract:**

Magnetic nanoparticle-based hyperthermia offers a compelling strategy for localized cancer treatment, but the effectiveness of clinically approved superparamagnetic iron oxide nanoparticles (SPIONs) is constrained by intrinsic material limitations, such as low saturation magnetization and small hysteresis losses. In this talk, we review our multiscale modeling and experimental efforts to overcome these limits and move toward nanoparticles that approach the theoretical maximum in heat dissipation.

We begin by discussing the fundamental physical limits of heat generation using superparamagnetic particles under alternating magnetic fields, addressing the interplay of Neel and Brownian relaxation mechanisms [1]. We then present a self-consistent simulation framework that couples magnetization dynamics with mechanical Langevin dynamics, implemented within the ESPResSo molecular dynamics engine [2]. The stochastic Landau-Lifshitz-Gilbert equation is solved simultaneously with the translational and rotational equations of motion for each particle, capturing both magnetic and viscous dissipation channels. The two dominant loss mechanisms — internal magnetization flipping and surface friction — can be cleanly separated, and their dependence on field strength, frequency, and particle size is mapped across the full parameter space. The model reproduces key analytical benchmarks including the Stoner-Wohlfarth hysteresis, Larmor precession frequency, Langevin equilibrium magnetization, and thermal switching rates. For interacting ensembles, dipole-dipole coupling leads to transient agglomeration that shifts friction losses toward lower frequencies, with the dynamic susceptibility revealing the competition between Brownian and Neel relaxation across all anisotropy regimes.

Finally, we present results from micromagnetic modeling and the fabrication of synthetic antiferromagnetic particles that exhibit maximal hysteresis losses. Characterization using Magnetic Force Microscopy reveals the switching pathways at the single-particle level, validating the predictive power of our simulation approach. While all preceding simulations treat each particle as a single magnetic domain, we have recently coupled molecular dynamics with full micromagnetics, resolving the spatially varying magnetization within every particle of the ensemble. A prerequisite for this is an extremely fast micromagnetic solver; very recently we have developed jaxmag, a JAX-based GPU-accelerated framework that scales to over 4 billion computational cells. This integrated strategy paves the way for hyperthermia agents optimized to operate near the fundamental limits of magnetic energy dissipation.ss

**References:**

[1] S. Helbig et al., "Self-consistent solution of magnetic and friction energy losses of a magnetic nanoparticle," Phys. Rev. B 107, 054416 (2023).

[2] S. Helbig et al., "Heating efficiency of suspended magnetic nanoparticles," submitted (2026).