# Hexagonal-disk magnetic nanoparticles emphasize the secondary role of Brownian rotation to heating and allow switching between domains of actuation

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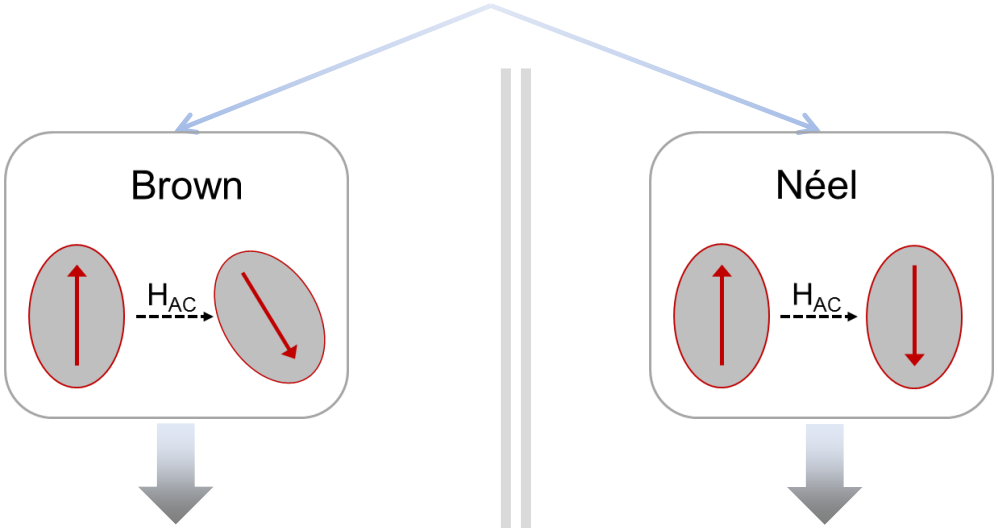
QUESTION:

...what is the contribution of Brownian rotation to heating in the magnetic hyperthermia regime, usually 0.1 – 1.0 MHz?

*Our computer simulations show that the contribution is rather small, but we show that it is possible to use the same particles and switch between hyperthermia and magnetomechanical domains of actuation – novel option for therapy?*

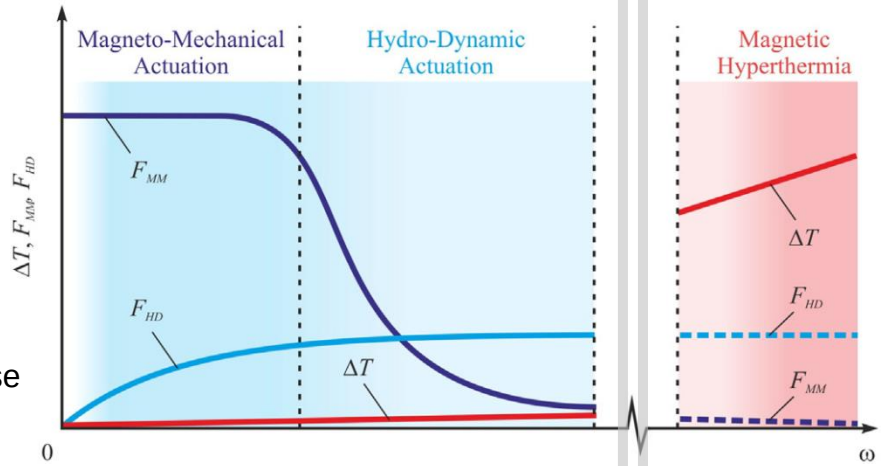
Context:

# MNPs in viscous environments under AC fields




Reorientation: **efficient at low-f**

Heating: **efficient at high-f**




J. Controlled Release 10, 43-60 (2015)

MMA and MFH usually considered as completely separated time domains

**M**agneto-**M**echanical **A**ctuation

**M**agnetic-**F**luid **H**yperthermia

Our approach: to study the heating role of Brownian rotation for hyperthermia, under optimum conditions

- ***Disk-shape, to enhance the viscous interaction with the environment***
- ***Infinite coupling of the magnetisation to the lattice (efficient torque)***

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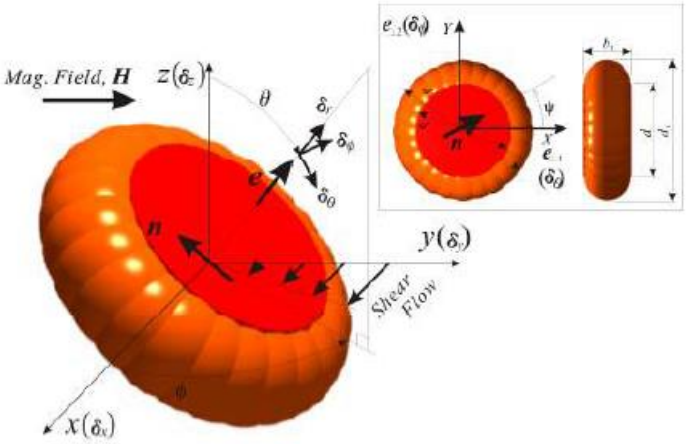
Theoretical model to ensure the fulfillment of the conditions




Colloids and Surfaces A: Physicochemical and Engineering Aspects

Volume 483, 20 October 2015, Pages 341–351

Brownian dynamics simulation of a dispersion composed of disk-like hematite particles regarding the orientational distribution and the magneto-rheological properties

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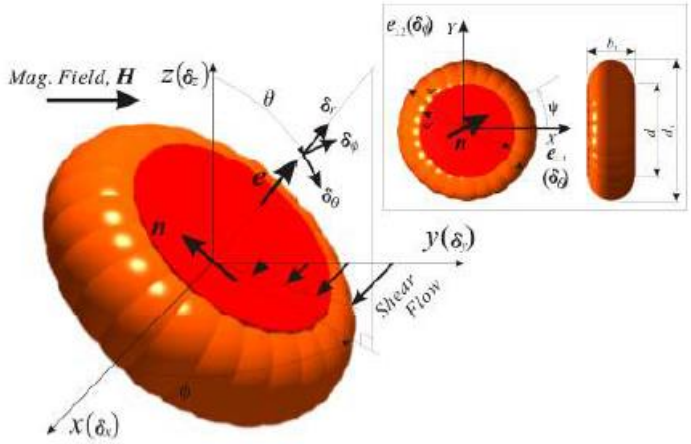
Brownian dynamics simulations

# Brownian dynamics simulations



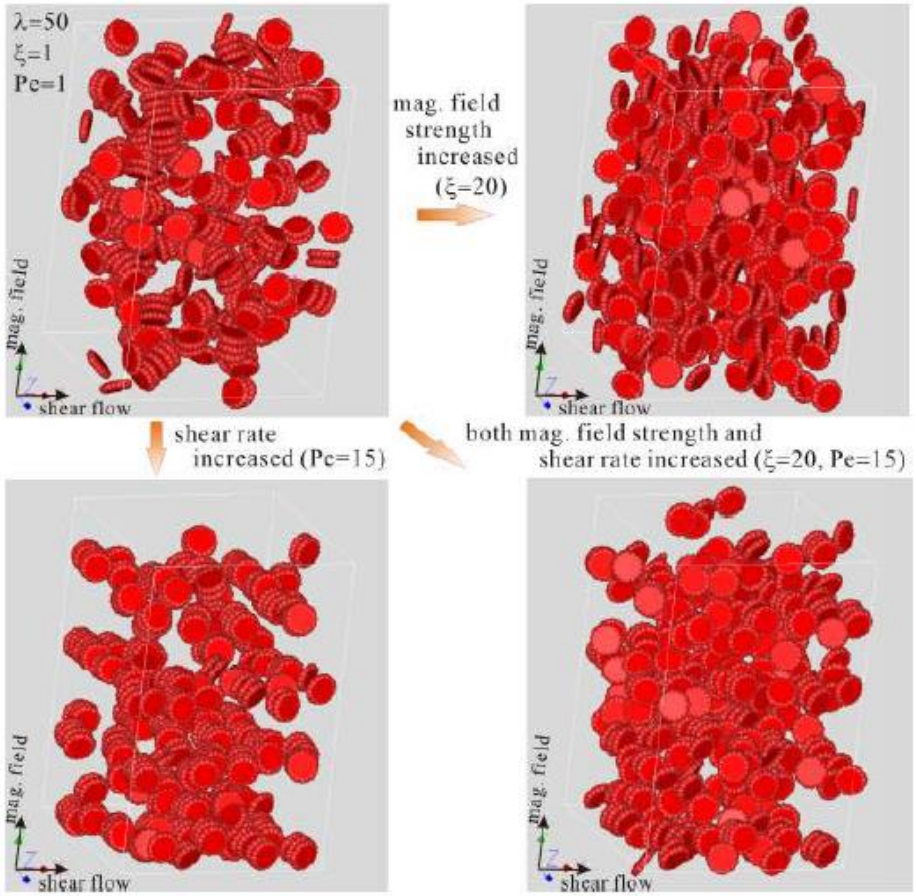

$$\boldsymbol{r}_{\parallel}(t+\Delta t) = \boldsymbol{r}_{\parallel}(t) + \boldsymbol{U}_{\parallel}\Delta t + \frac{1}{kT} D_{\parallel}^{T} \boldsymbol{F}_{\parallel}^{P}(t)\Delta t + \Delta r_{\parallel}^{B}\boldsymbol{e}(t)$$

$$\boldsymbol{r}_{\perp}(t+\Delta t) = \boldsymbol{r}_{\perp}(t) + \boldsymbol{U}_{\perp}\Delta t + \frac{1}{kT} D_{\perp}^{T} \boldsymbol{F}_{\perp}^{P}(t)\Delta t + \Delta r_{\perp 1}^{B}\boldsymbol{e}_{\perp 1}(t) + \Delta r_{\perp 2}^{B}\boldsymbol{e}_{\perp 2}(t)$$

$$\boldsymbol{e}(t+\Delta t) = \boldsymbol{e}(t) + \boldsymbol{\Omega}_{\perp} \times \boldsymbol{e}\Delta t + \frac{1}{kT} D_{\perp}^{R} \boldsymbol{T}_{\perp}^{P}(t) \times \boldsymbol{e}\Delta t - \frac{Y^{H}}{Y^{C}}\left((\boldsymbol{e}\cdot\boldsymbol{e}\boldsymbol{e}) : \boldsymbol{E}\right) \times \boldsymbol{e}\Delta t + \Delta\phi_{\perp 1}^{B}\boldsymbol{e}_{\perp 1} + \Delta\phi_{\perp 2}^{B}\boldsymbol{e}_{\perp 2}$$

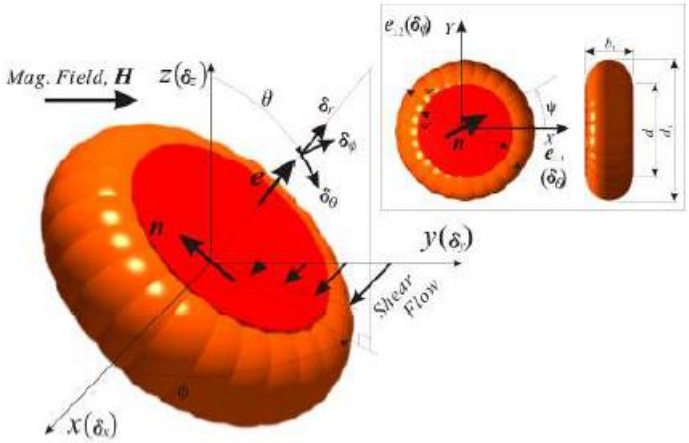
$$\boldsymbol{n}(t+\Delta t) = \boldsymbol{n}(t) + \boldsymbol{\Omega}_{\parallel} \times \boldsymbol{n}\Delta t + \frac{1}{kT} D_{\parallel}^{R} \boldsymbol{T}_{\parallel}^{P}(t) \times \boldsymbol{n}\Delta t + \Delta\phi_{\parallel}^{B}\,\boldsymbol{e} \times \boldsymbol{n}$$

DON'T LOOK




Displacement; rotation; shear flow; applied field

# Brownian dynamics simulations




$$\boldsymbol{r}_{\parallel}(t+\Delta t) = \boldsymbol{r}_{\parallel}(t) + \boldsymbol{U}_{\parallel}\Delta t + \frac{1}{kT} D_{\parallel}^{T} \boldsymbol{F}_{\parallel}^{P}(t)\Delta t + \Delta r_{\parallel}^{B} \boldsymbol{e}(t)$$

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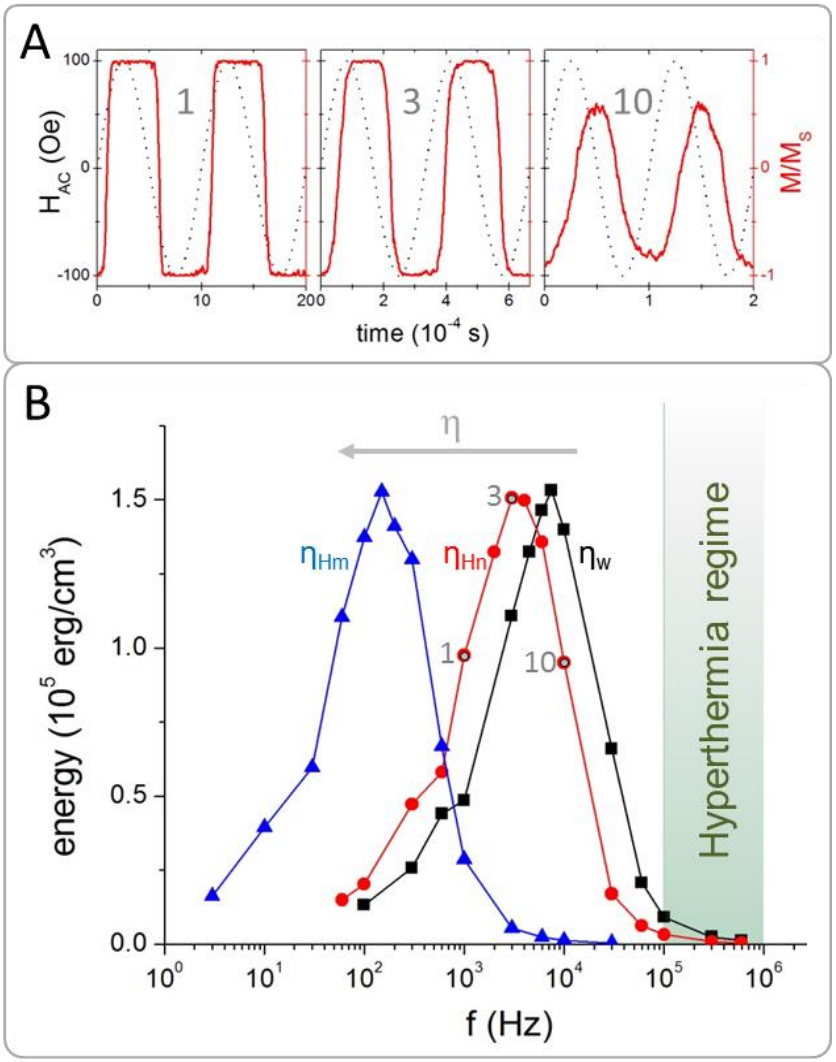
Focused on the pure Brownian rotation effect: isolated and non-interacting MNPs

- Not shear flow
- No interactions (neither physical overlapping, nor magnetostatic coupling)
- Displacement not important

# Brownian dynamics simulations




$H_{AC}(t)=H_{max}\sin(2\pi f\cdot t)$

$\eta_w = 0.89 \times 10^{-3}$ Pa·s

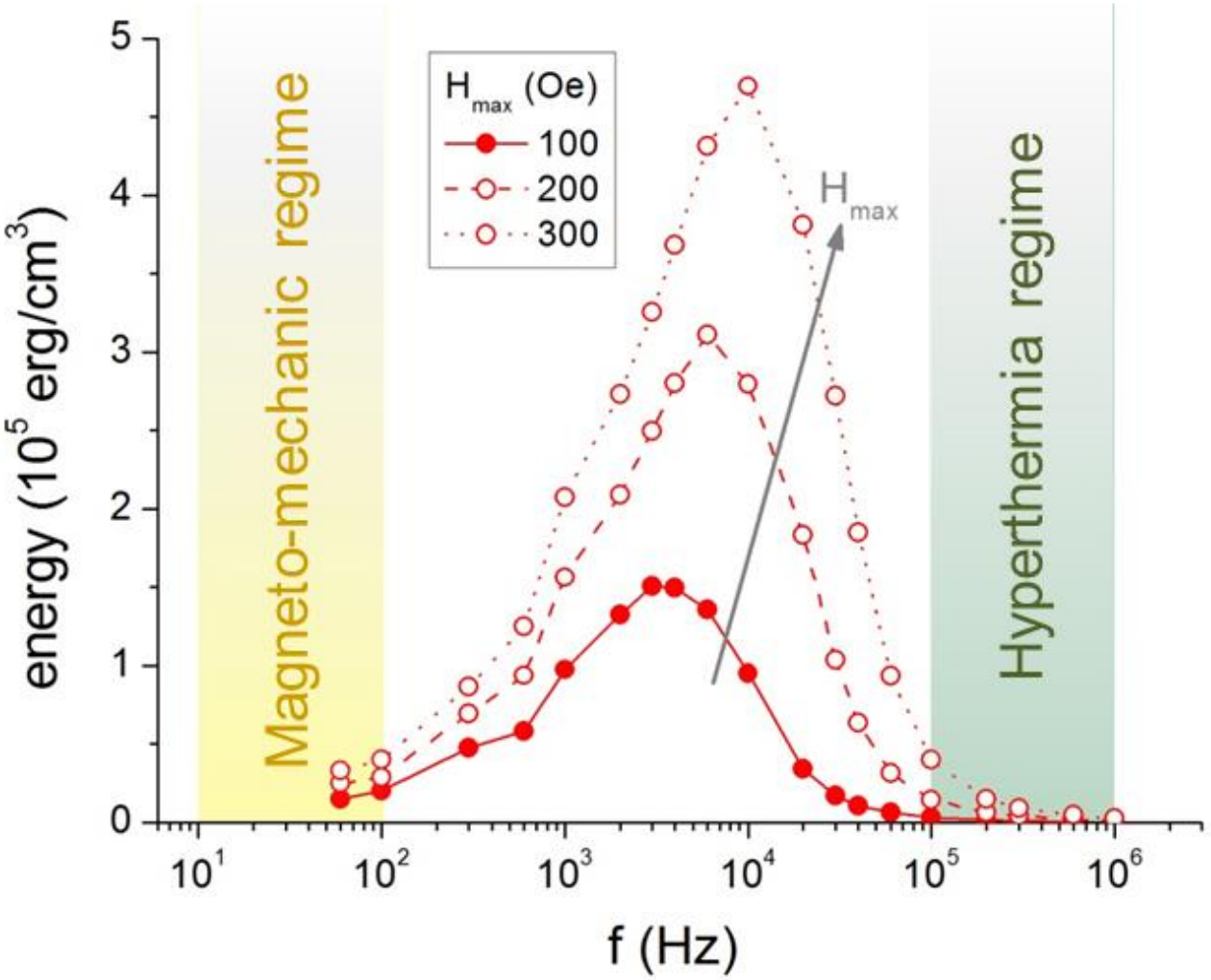
$\eta_{HeLa(nano)} = 2.0 \times 10^{-3}$ Pa·s

$\eta_{HeLa(macro)} = 4.4 \times 10^{-2}$ Pa·s

$H_{max} = 100$ Oe

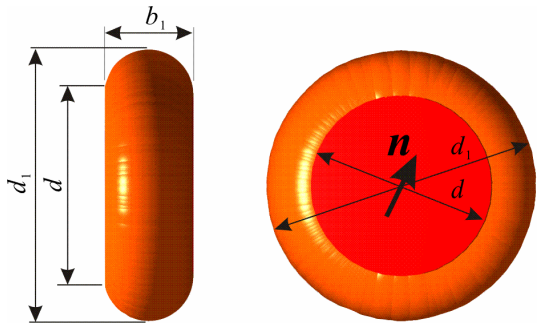
# Brownian dynamics simulations

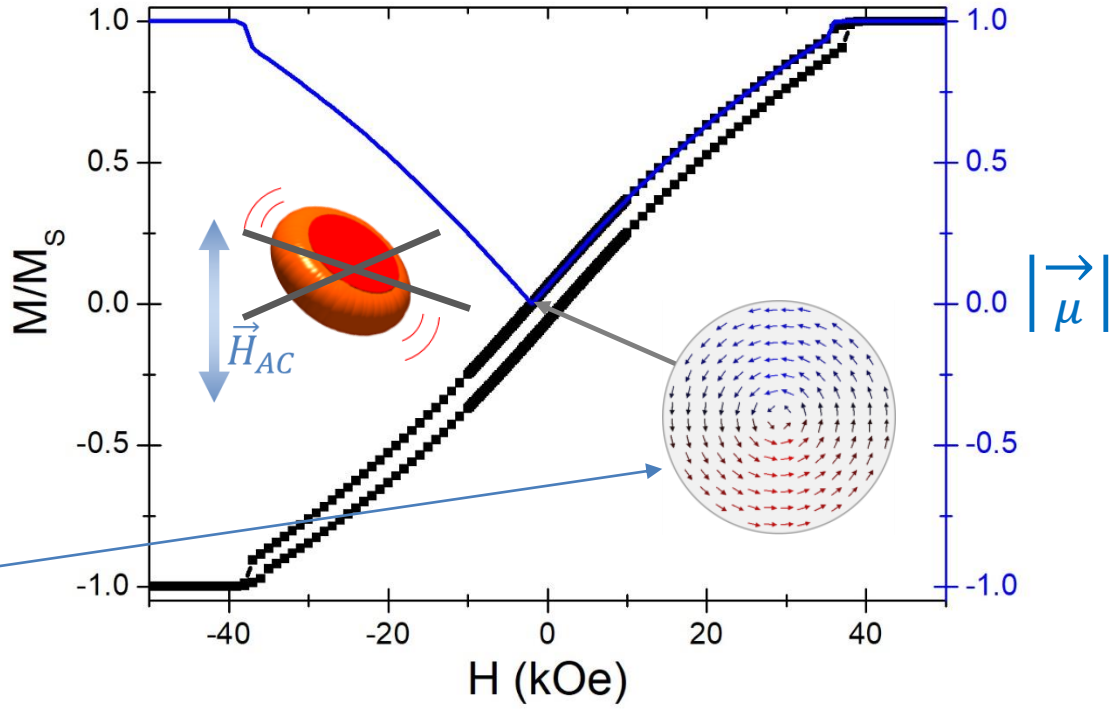
$\eta_{HeLa(nano)} = 2.0 \times 10^{-3}$ Pa·s



# Brownian dynamics simulations

- Néel contribution: simulations of M(H) loops of non-rotatable particles (at different angles)
- PROBLEM: **the shape assumed in the BD simulations is not magnetically robust** – not possible to deliver efficient torque



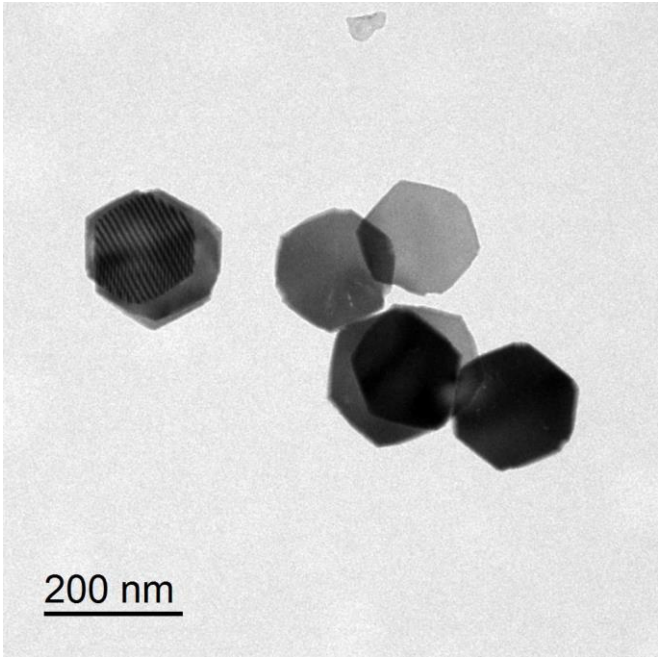




Magnetic vortex state

# Brownian dynamics simulations

- Systematic analysis of the “robustness” of different shapes of same aspect ratio (oblate elipsoid; section of a cylinder; etc.)

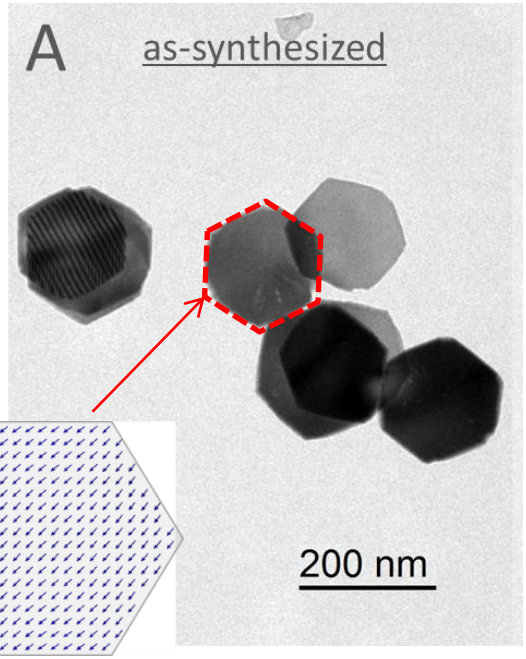
  ↳ SOLUTION: **hexagonal-shape disks**



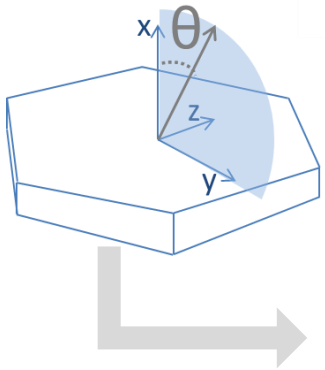

How shape and internal structure affect the magnetic properties of anisometric magnetite nanoparticles
H. Gavilan *et al*., Acta Mater. 125, 416 (2017)

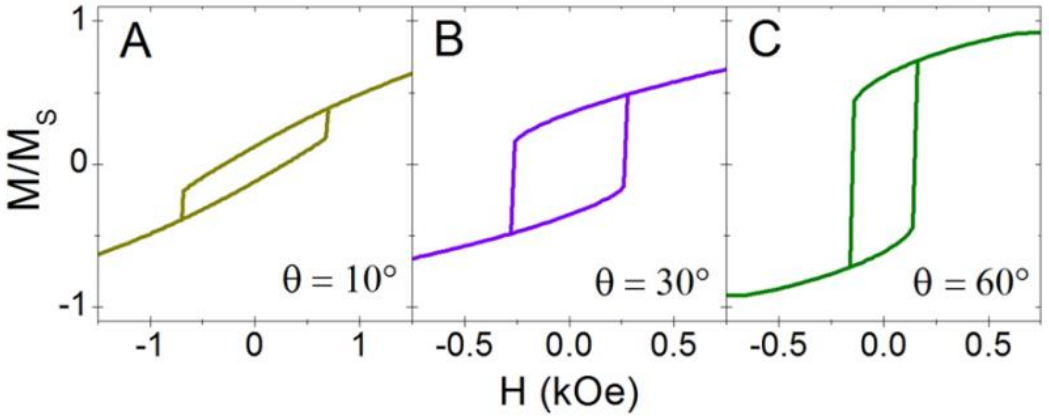
# Hexagonal-shape disks

Robust magnetic response:




Micromagnetic simulation shows uniform state for hexagon



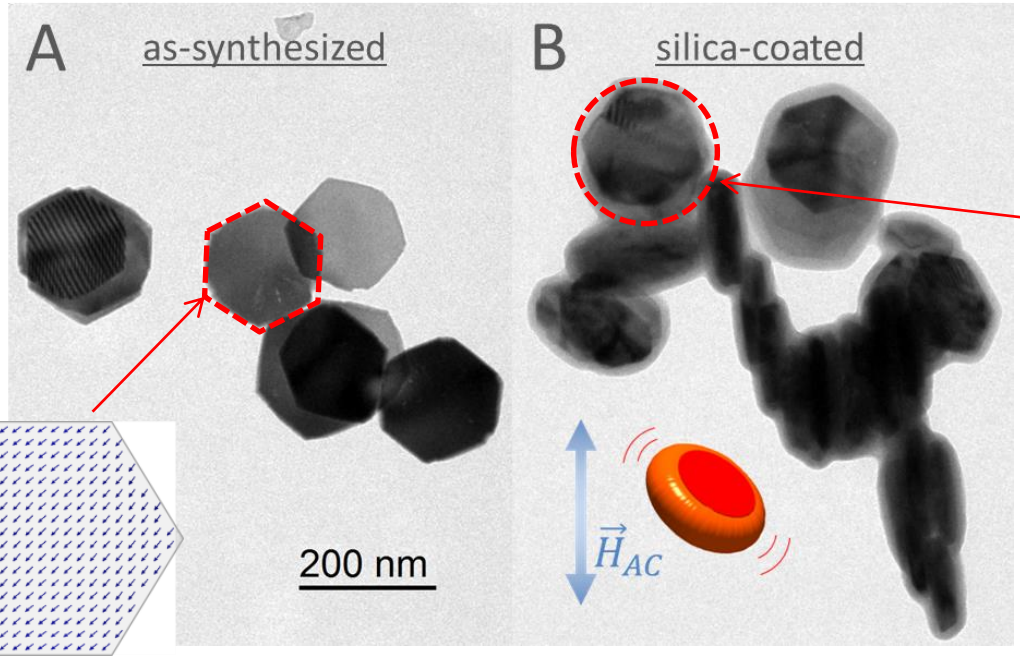




Coherent-like behaviour ✓

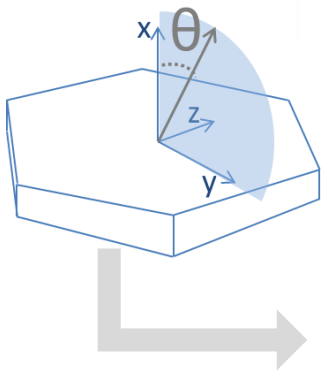
$$\frac{\Delta|\vec{\mu}|}{\Delta\theta, \Delta H} < 1\% \forall \theta$$

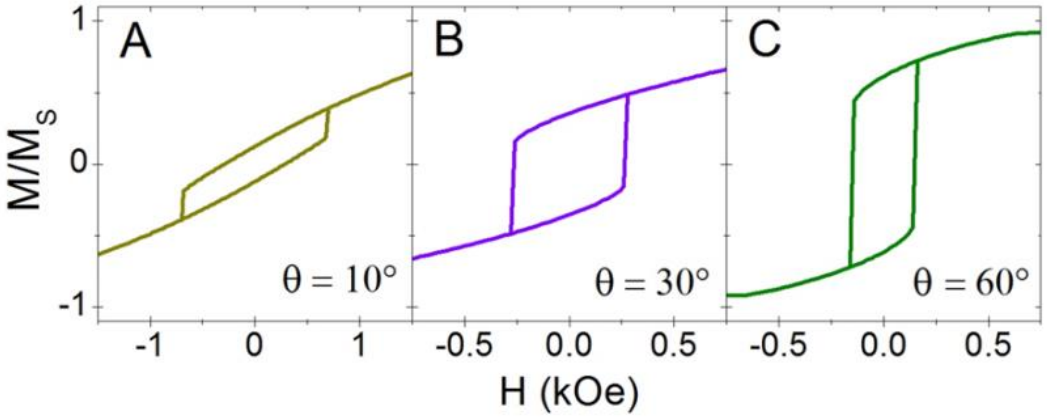
# Hexagonal-shape disks

Robust magnetic response:




Desired round shape for the rheological properties.

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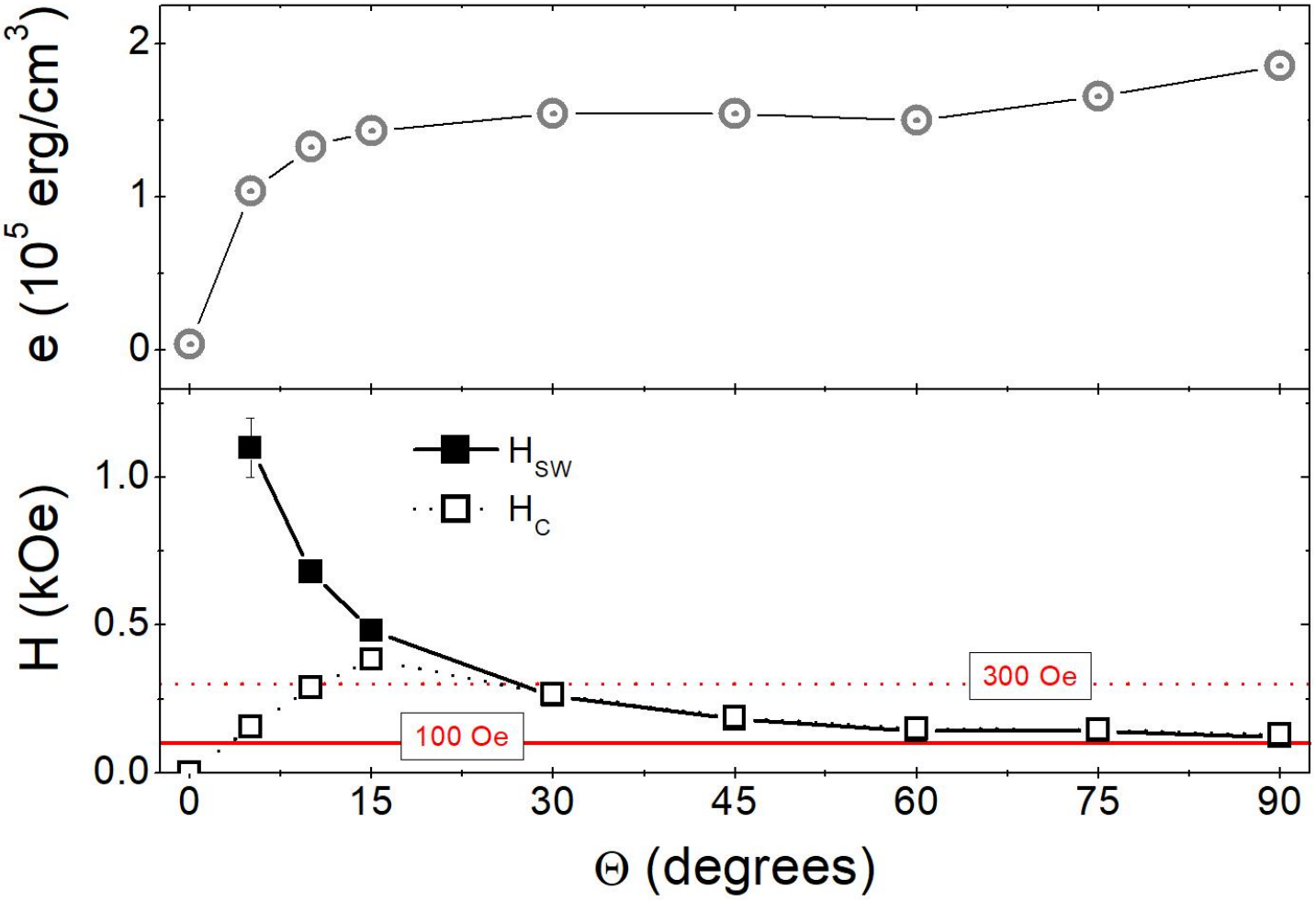
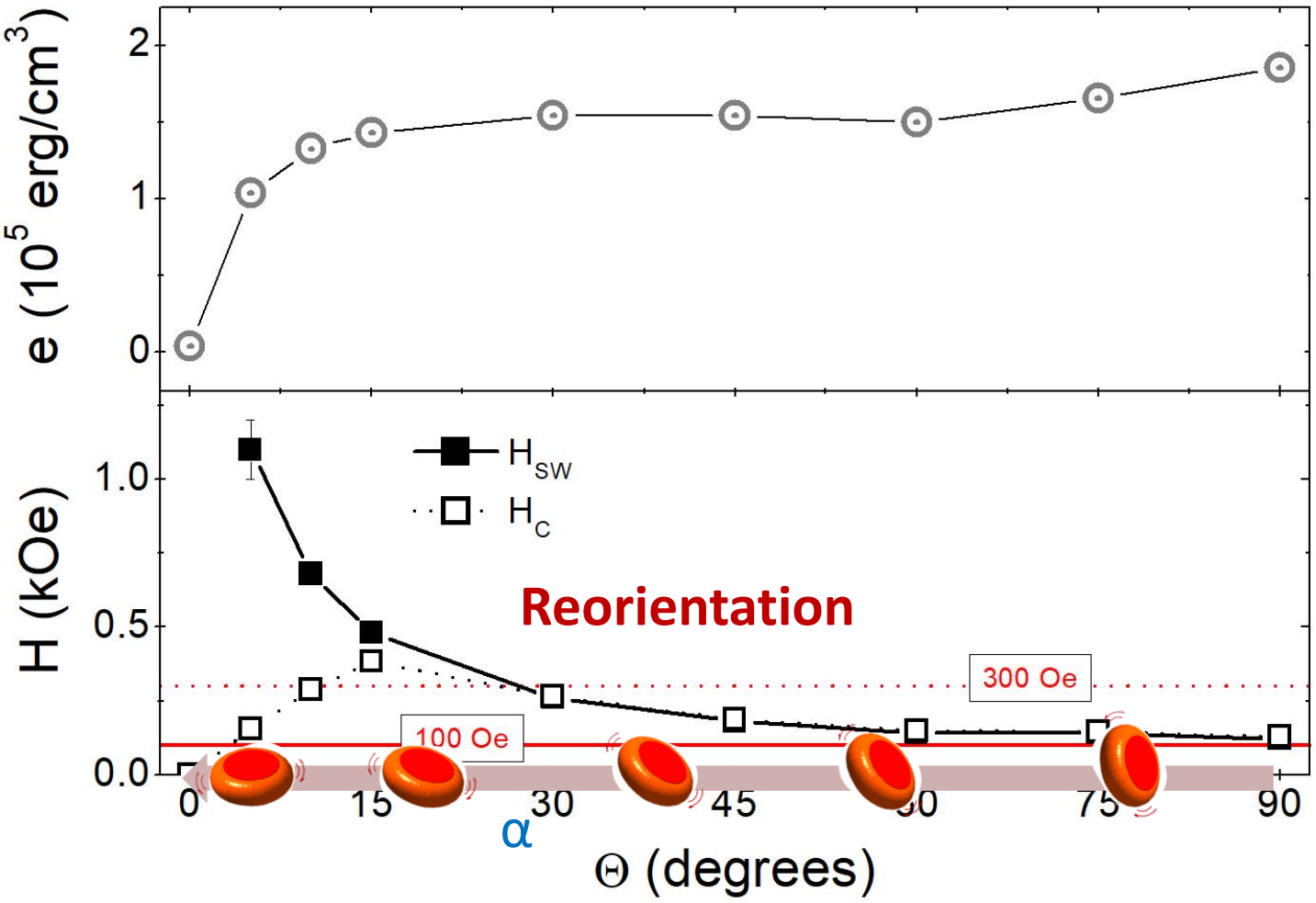
# Hexagonal-shape disks

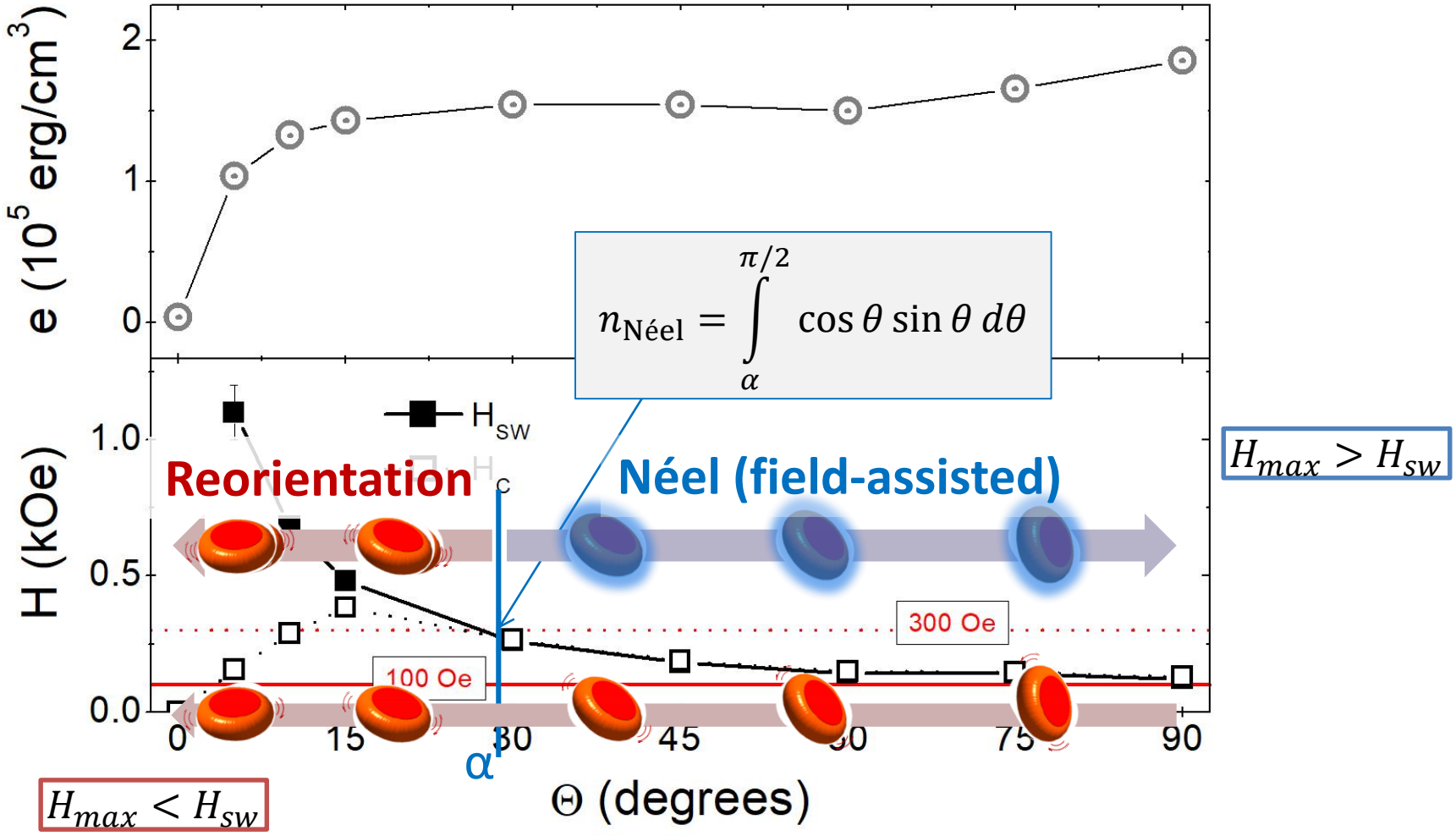


# Hexagonal-shape disks



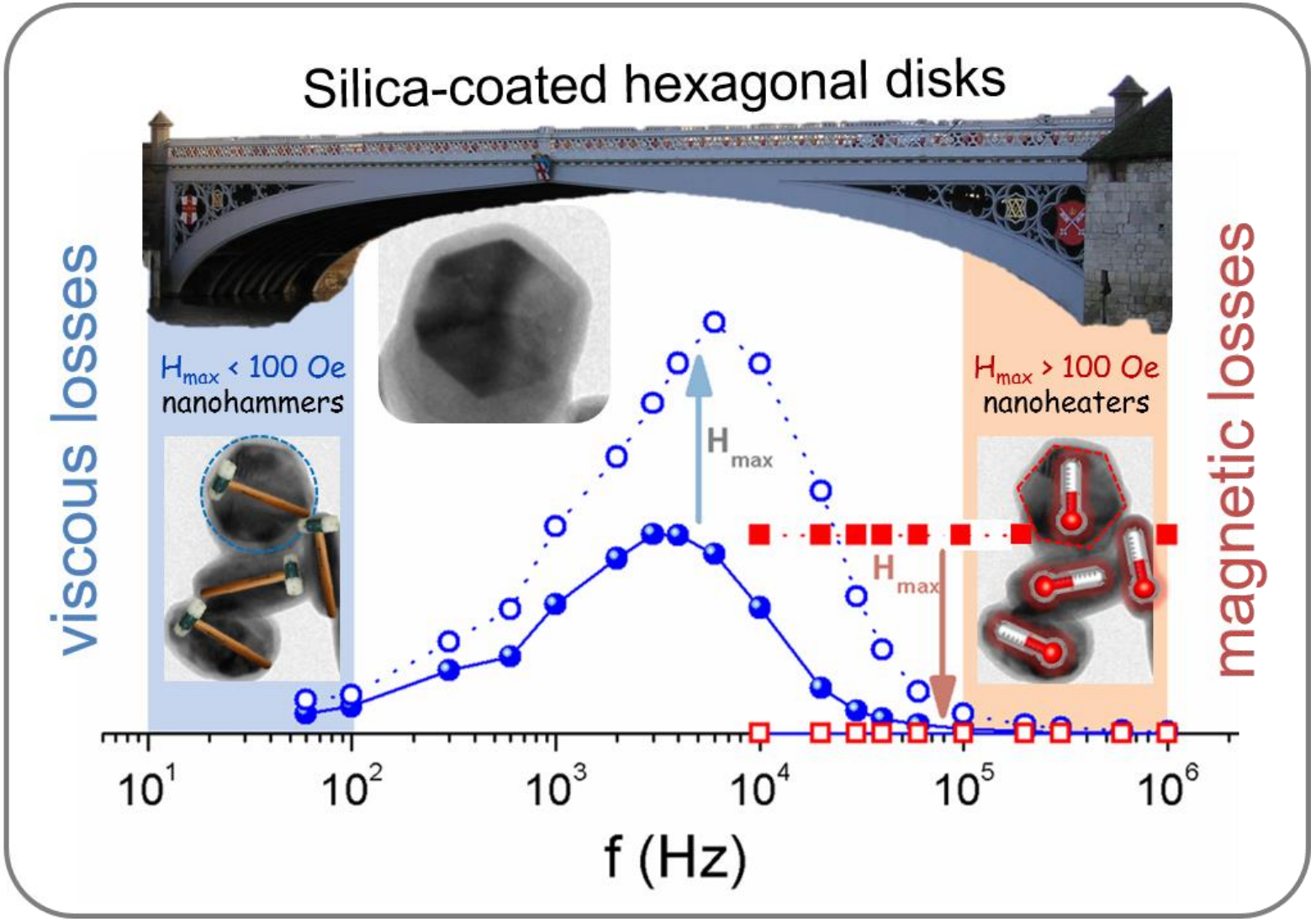

$H_{max} > H_{sw}$

# Hexagonal-shape disks

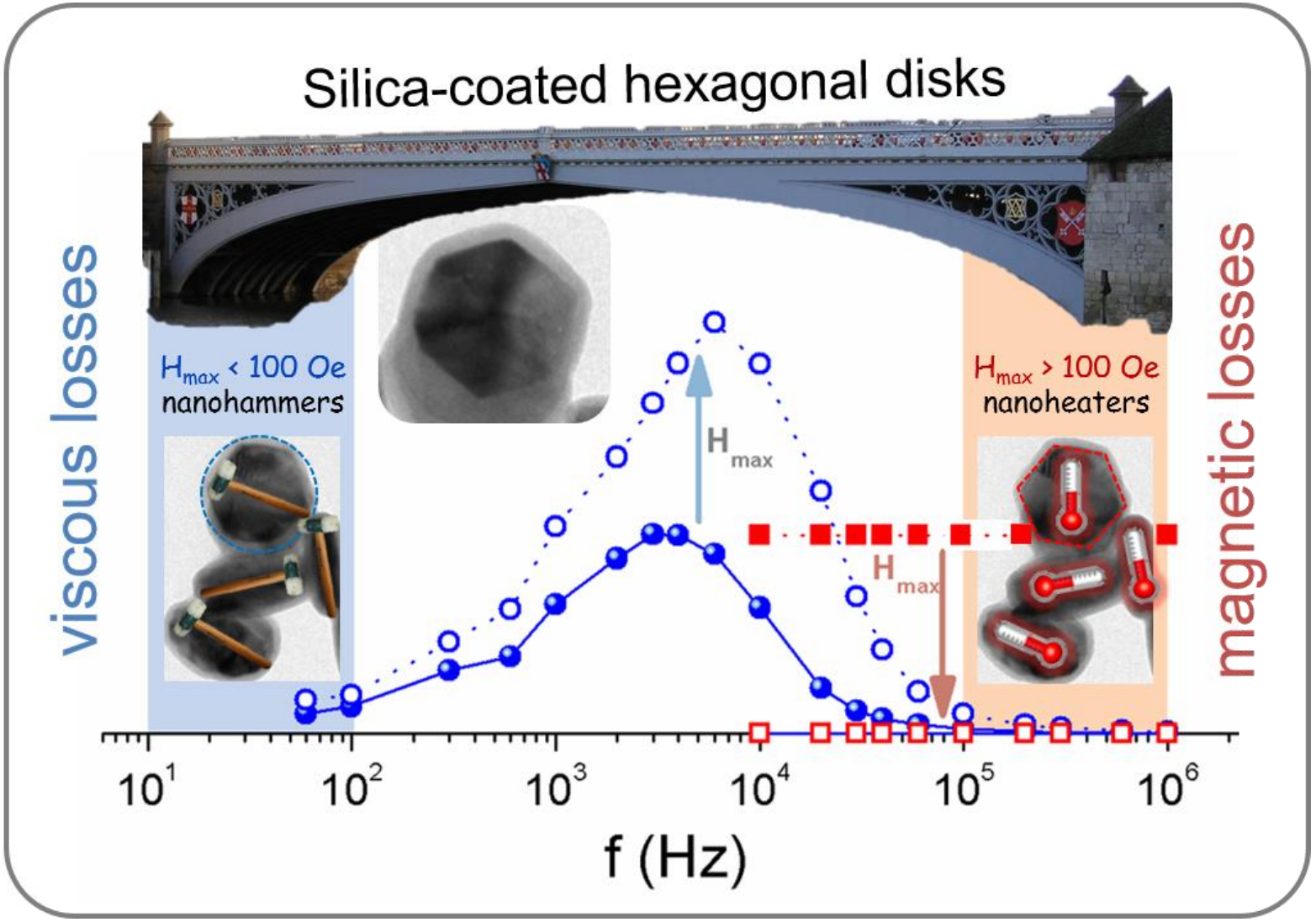


# Conclusions

- Even under the more favorable conditions (large aspect ratio particles, efficient magnetic torque) Brown conribution to heating is negligible in comparison with Néel type.
- OUR GUESS: **Negligible heating ≠ not playing a role**
- Reorientation: much longer timescale (further investigation needed!)
- Disk-shape particles allow complete disentangling between reorientation and field-induced swithing, with significant heating
- Possible double functionality for magneto-mechanical actuation at low-f, and heating at high-f. Easy alternation between both modalities just by changing the amplitude and frequency of the AC field.




*Thank you for your attention!*

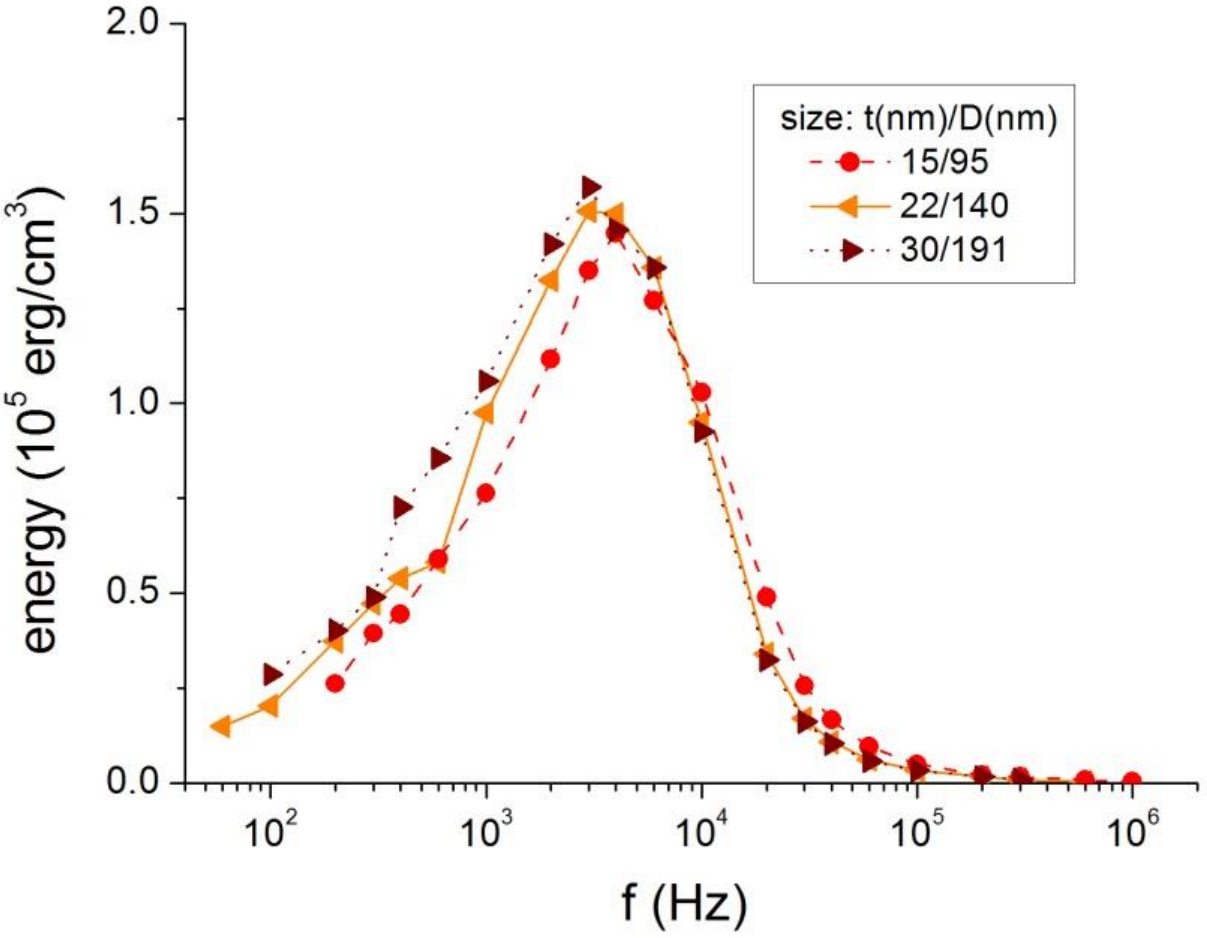



Funding acknowledgements:

THE ROYAL SOCIETY

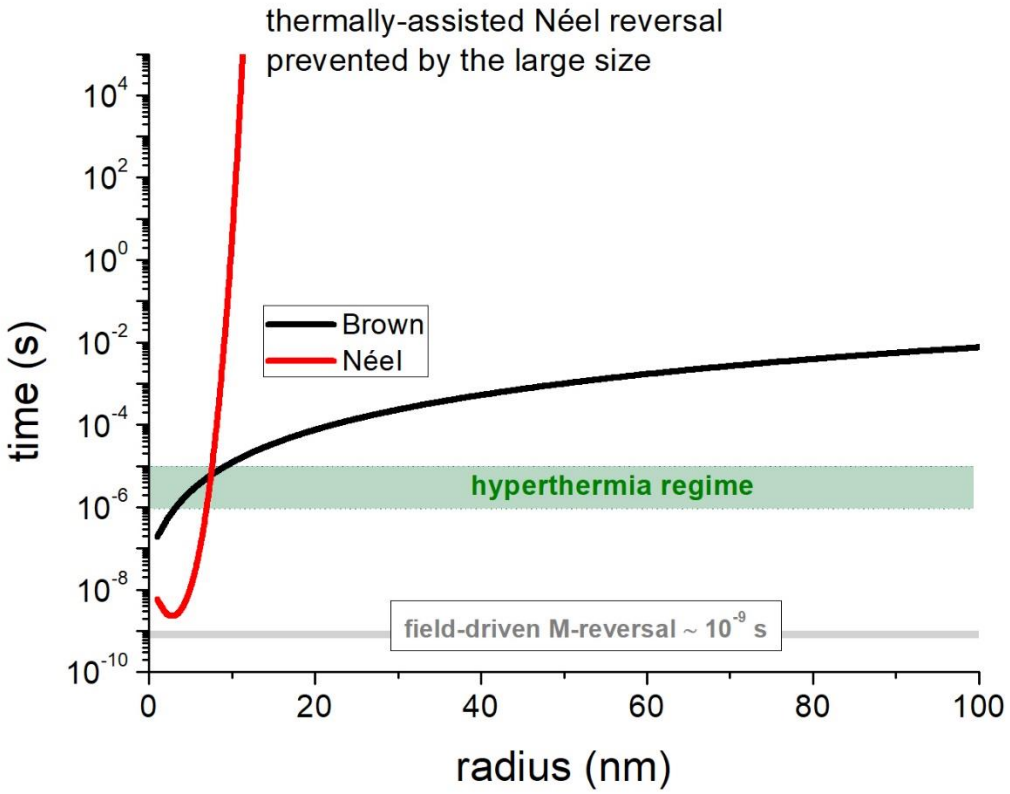
Investigación Innovación Crecemento I²=C

# Size-dependent Brownian-performance dependence



# Brownian dynamics simulations

- Prevalence of either reversal mechanism would usually be the less energetically consty, IF within the timescale of the experiment
- BD assumption of infinite coupling between magnetization and lattice requires very large anisotropy




- Néel reversal can only occur if field-induced
- $H_{max}$-thresshold to induce magnetization reversal