Chaining in Biomagnetic Nanoparticles

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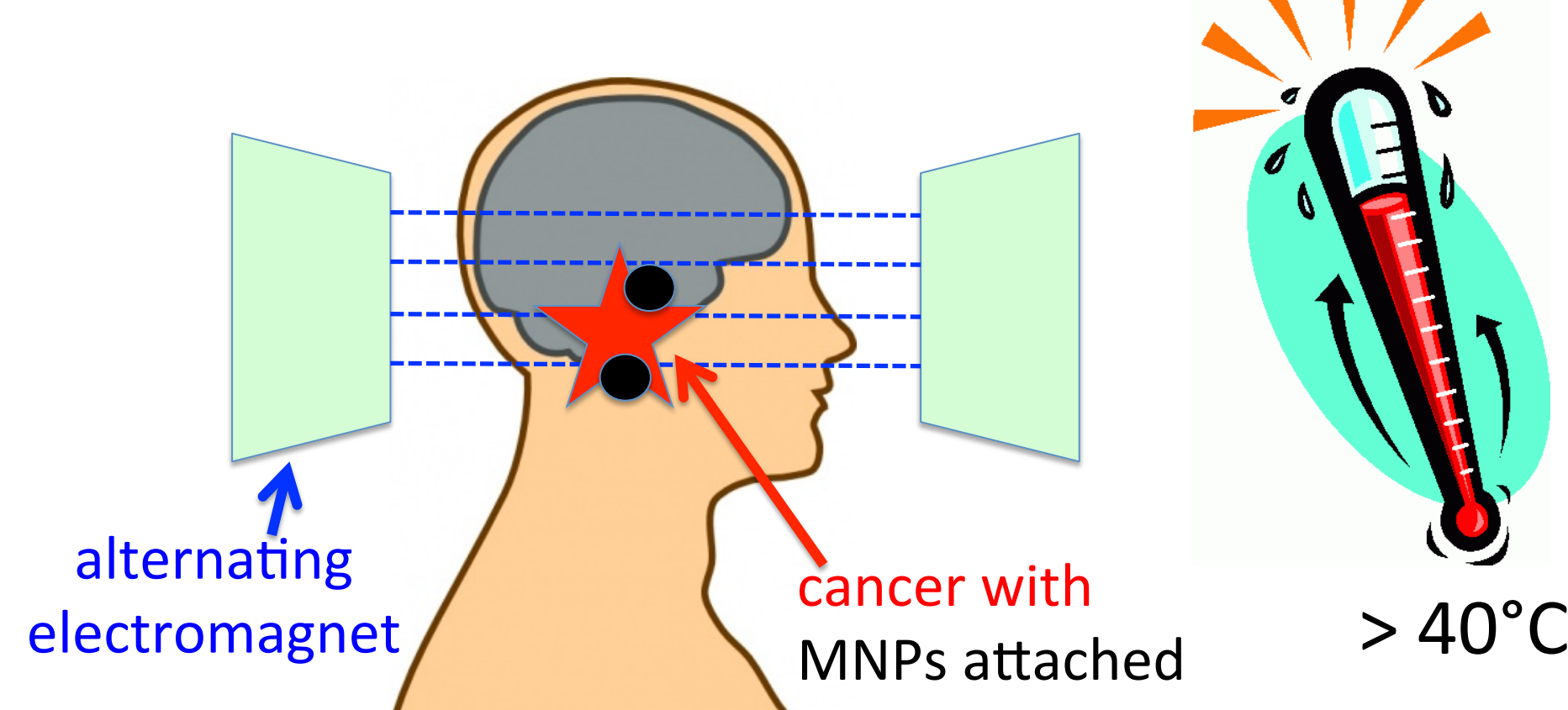
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1) Biomedical applications of magnetic nanoparticles (MNPs)

Drug delivery

Fluorophore
Polymer Coating
Therapeutic Agent
MNP Core
Permeation Enhancer
Targeting Agent
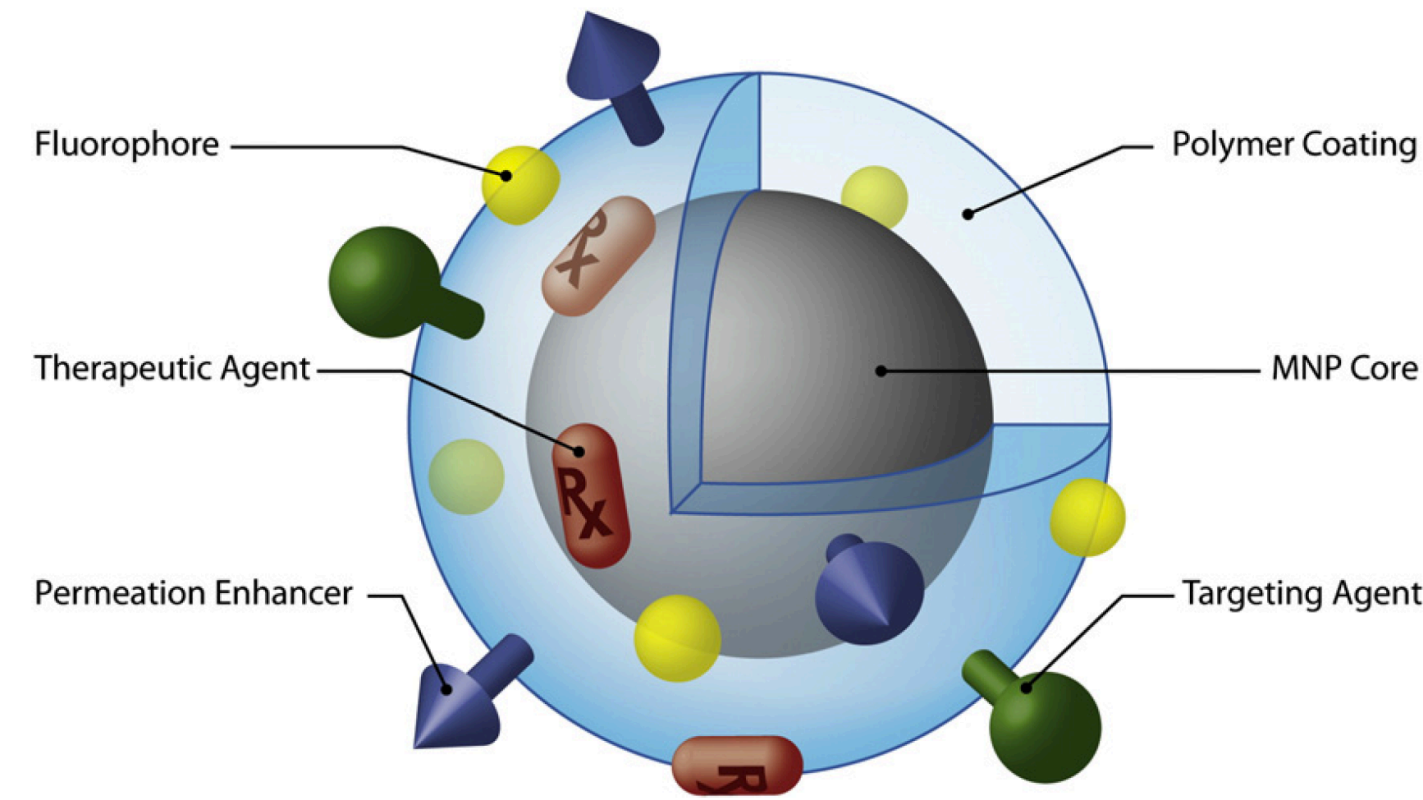
*Sun et al. Adv. Drug Deliv. Reviews **60**, 1252 (2008)*

Hyperthermia

alternating electromagnet
cancer with MNPs attached
> 40°C

MRI contrast agents

Without contrast   With contrast agents
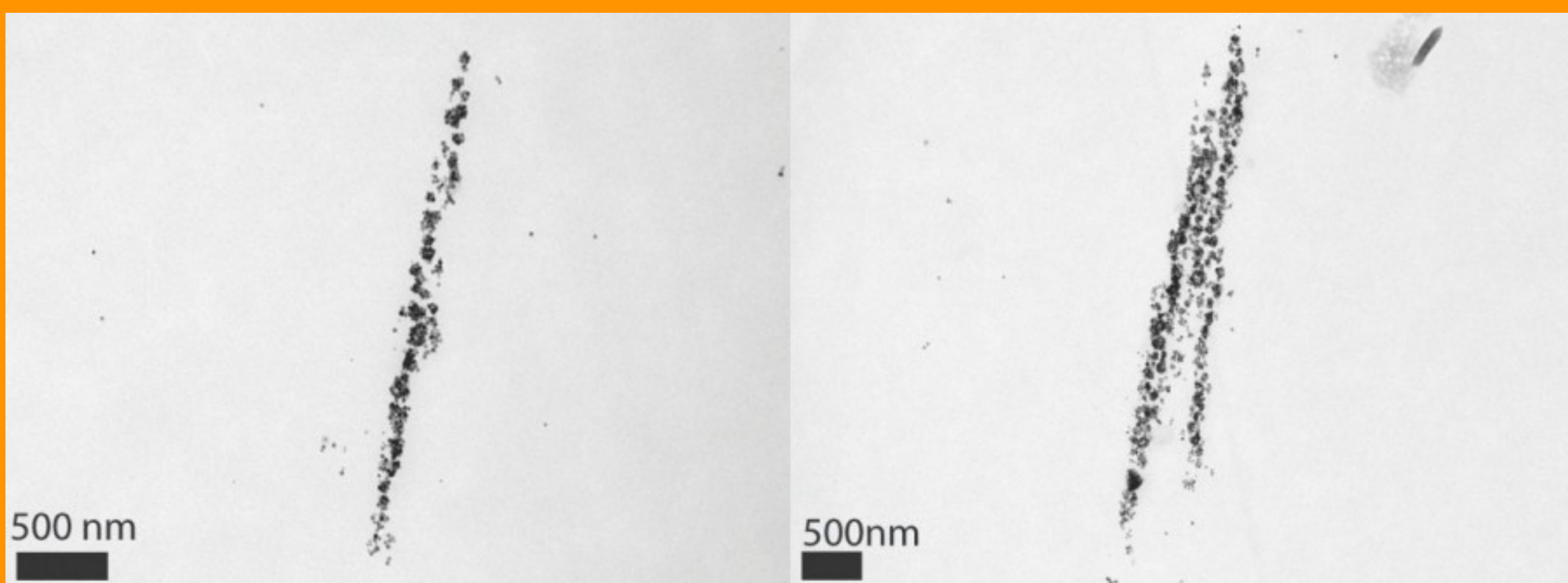
MNPs are negative contrast T2 agents
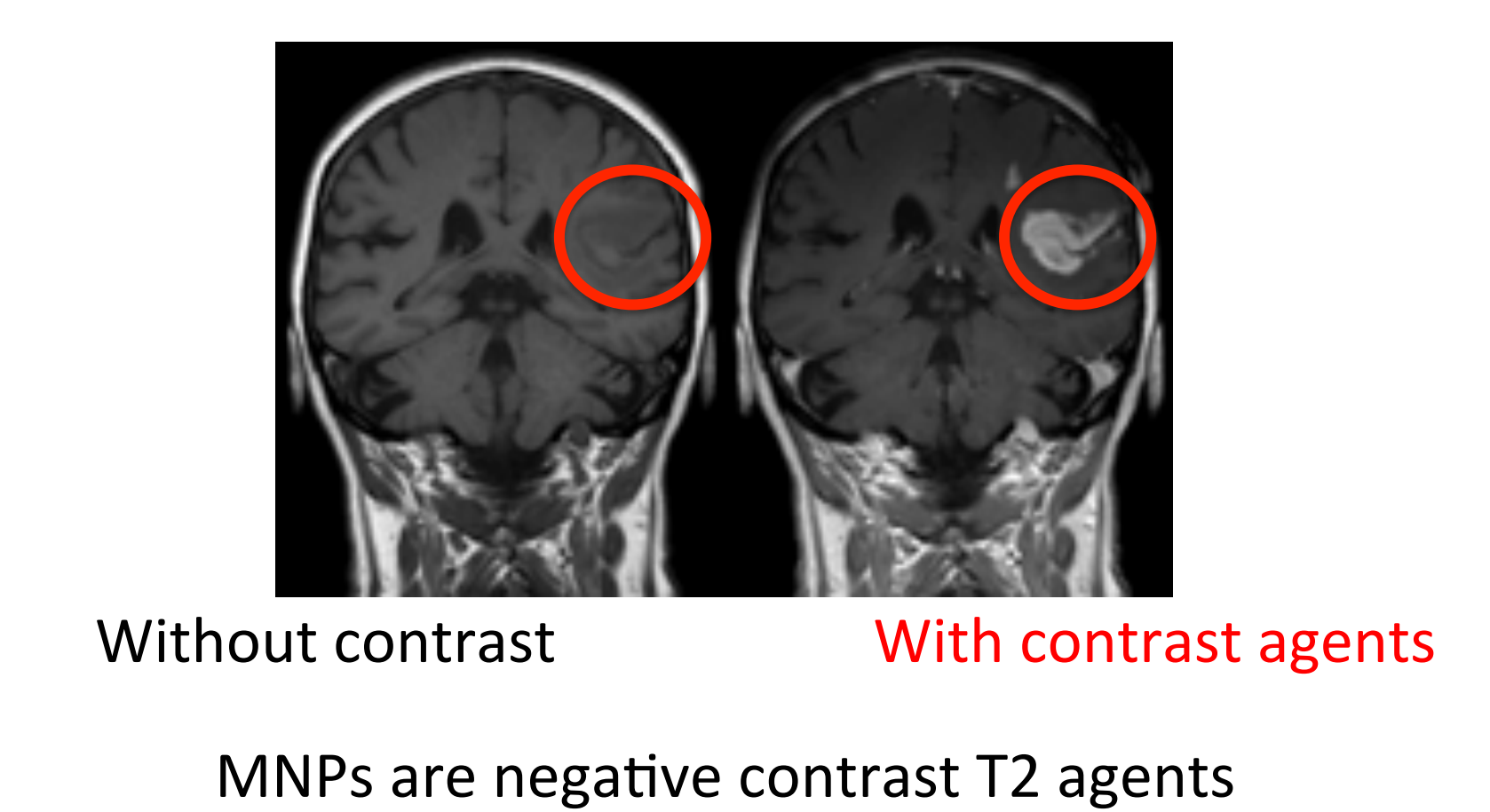
2) Magnetic properties change due to chaining

500 nm   500nm

Eg. Linear aggregates have reduced transverse proton relaxation rates

*S. L. Saville et al. Nanoscale **5**, 2152 (2013)*

3) Monte Carlo calculation

Choose random magnetization directions **M** for each nanoparticle

1. Choose a particle, change **M**, calculate the energy change:

$$\Delta E = -(M_{new} - M_{old}) \cdot H_{total}$$

Applied field plus **dipole fields** from all the other particles

2. Metropolis algorithm accept change with probability that depends on temperature:

$$\min(1, e^{(-\Delta E/kT)})$$

Repeat steps 1 & 2

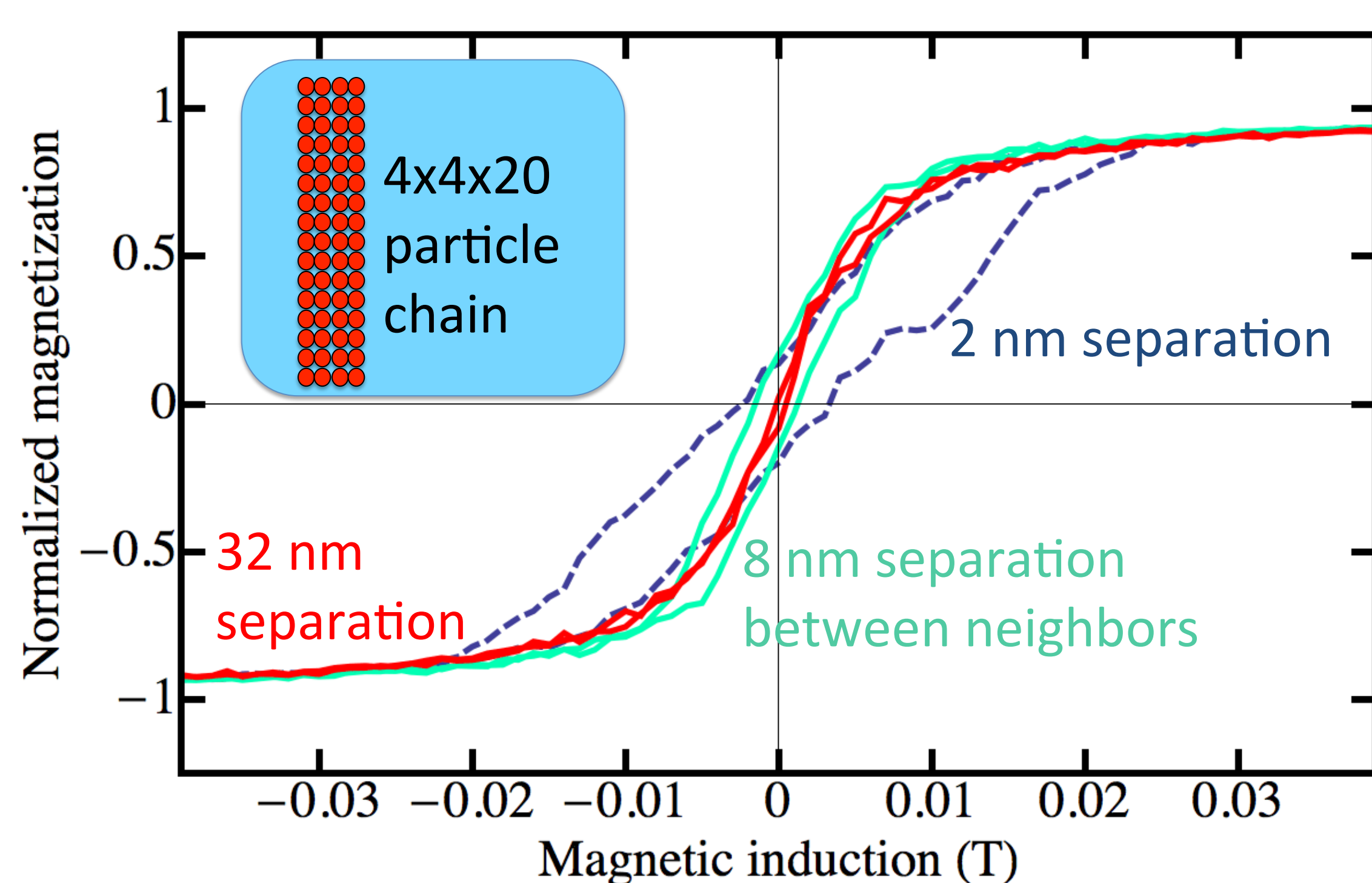## 4) Results   20 nm Fe_3O_4 particles

- Mean **separation** changes magnetization

4x4x20 particle chain

2 nm separation

32 nm separation

8 nm separation between neighbors

Normalized magnetization

Magnetic induction (T)

Increasing separation ➔ decreasing coercive field

Future work: Comparison to experiments
Field cooled simulations
Influence of disorder
How do chains form?

- **Aspect ratio** of the chain is important

All 2 nm separation

single particle

10x10x10

1x1x10

Normalized magnetization

Magnetic induction (T)
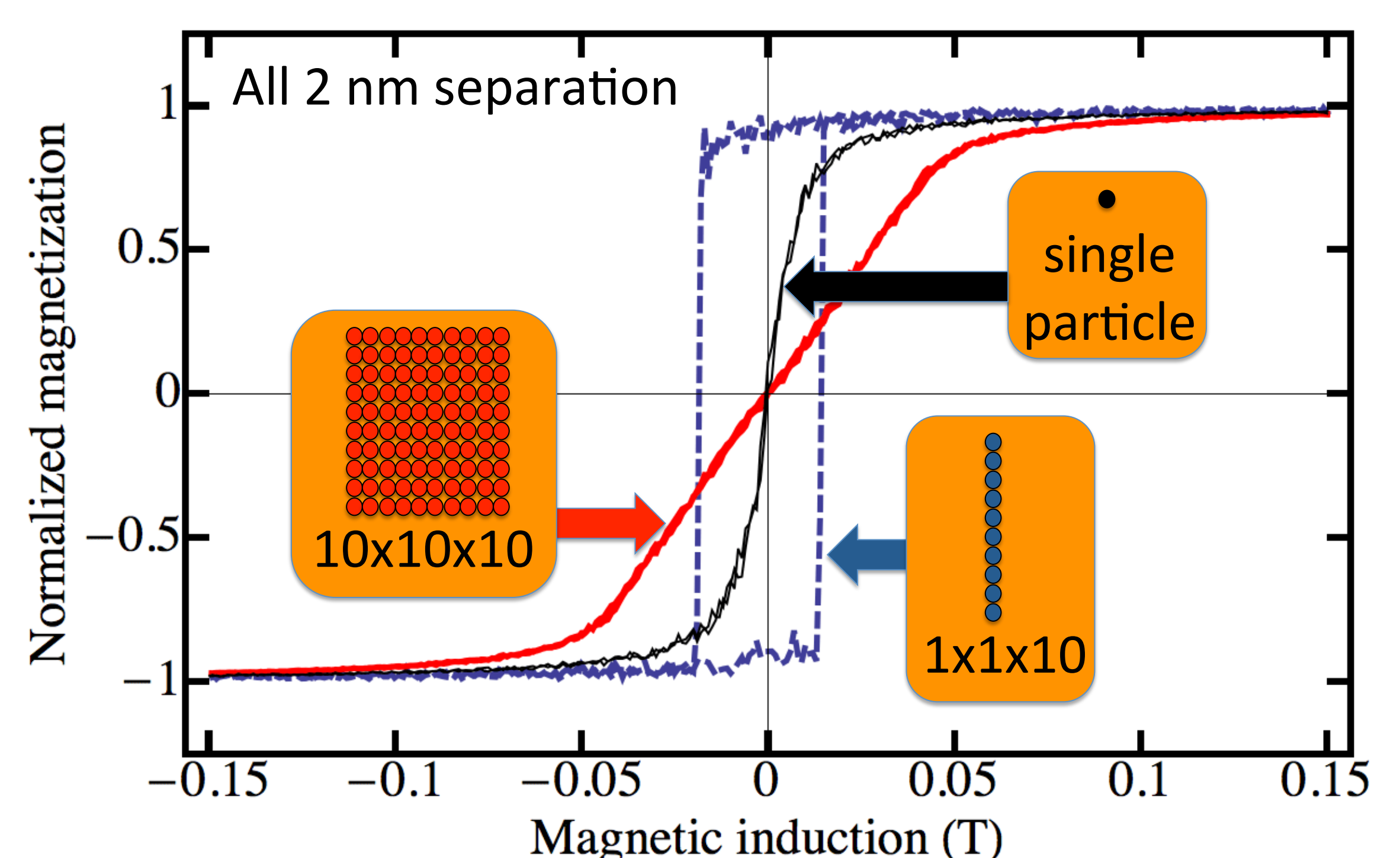
Superparamagnetic behavior can be lost due to interparticle dipole-dipole interactions

- **Multiple chains** have the same behavior as single chains, provided they are separated by roughly 100 nm