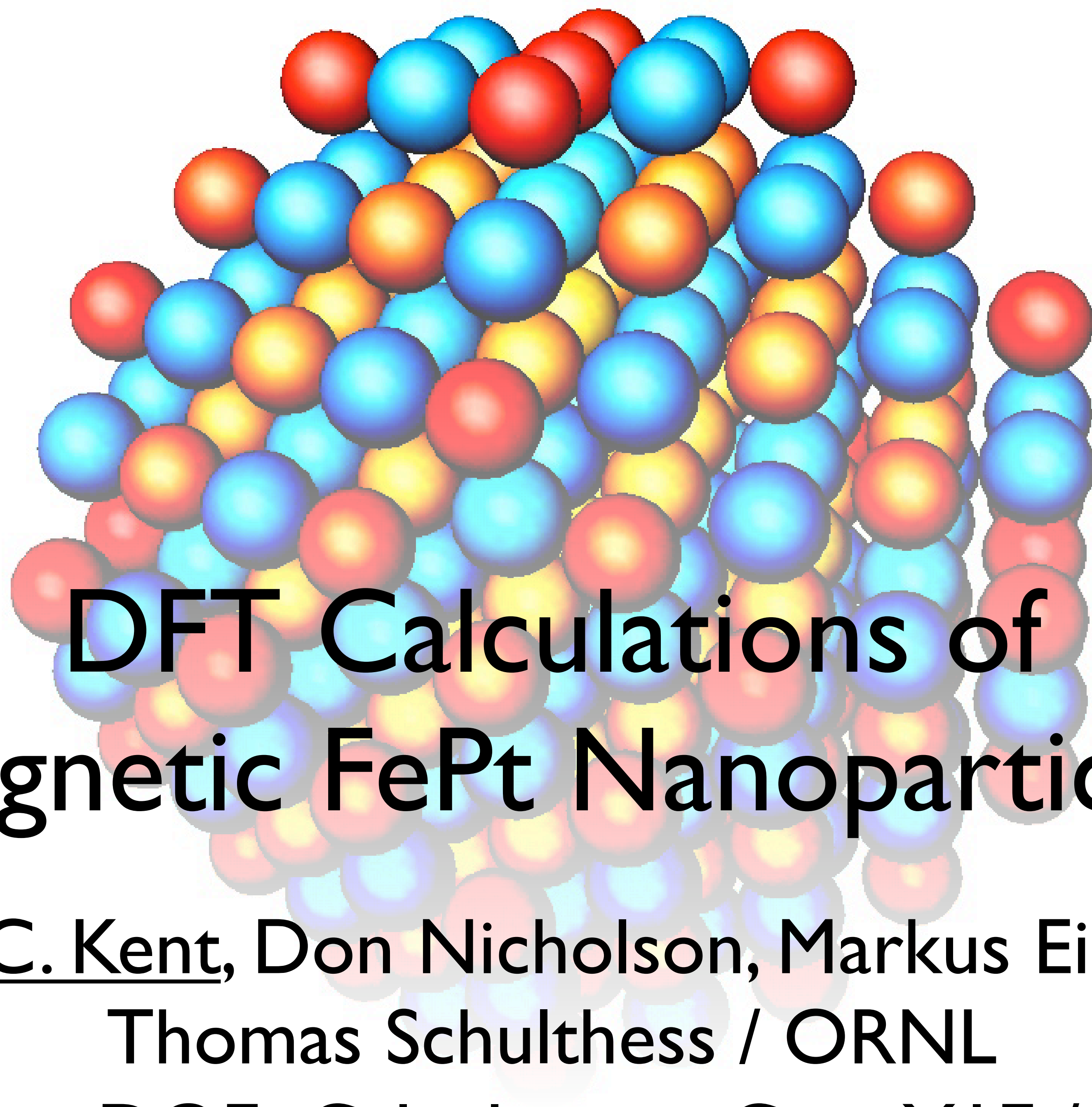

DFT Calculations of Magnetic FePt Nanoparticles

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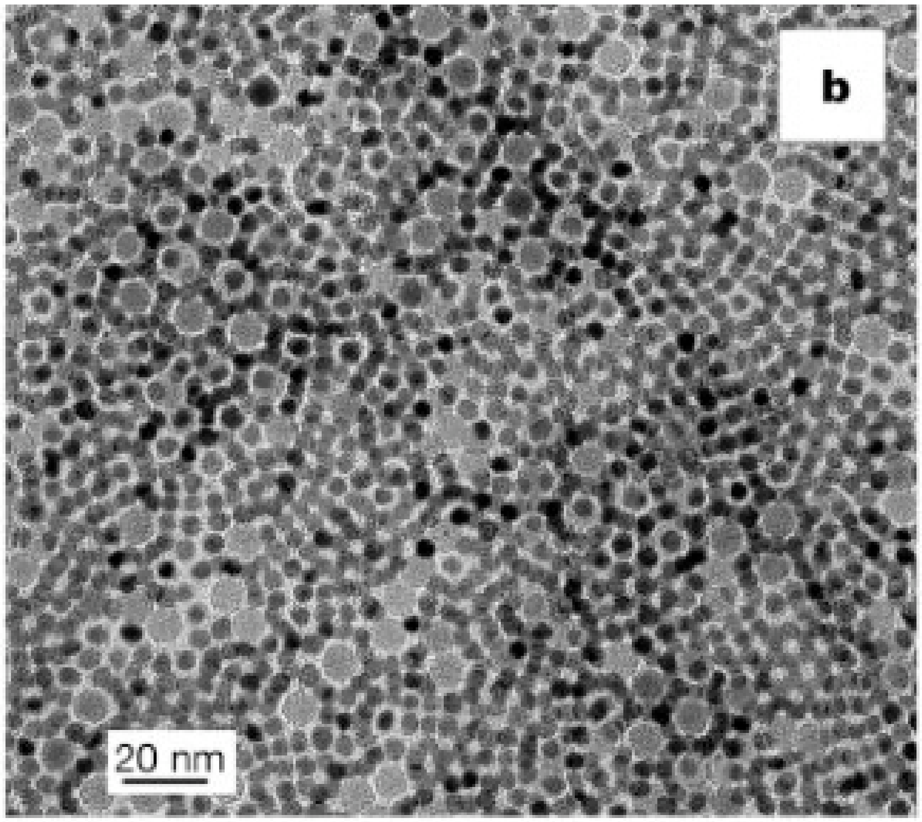
Motivation

Nanostructured FePt has potential applications in magnetic storage. (Session Z22 Friday)

Zeng et al. Nature 420 395 (2002)



Fe_3O_4 (8nm)/$Fe_{58}Pt_{42}$ (4nm). TEM.

1. Large magnetic anisotropy of $L1_0$ ordered f.c.t. FePt

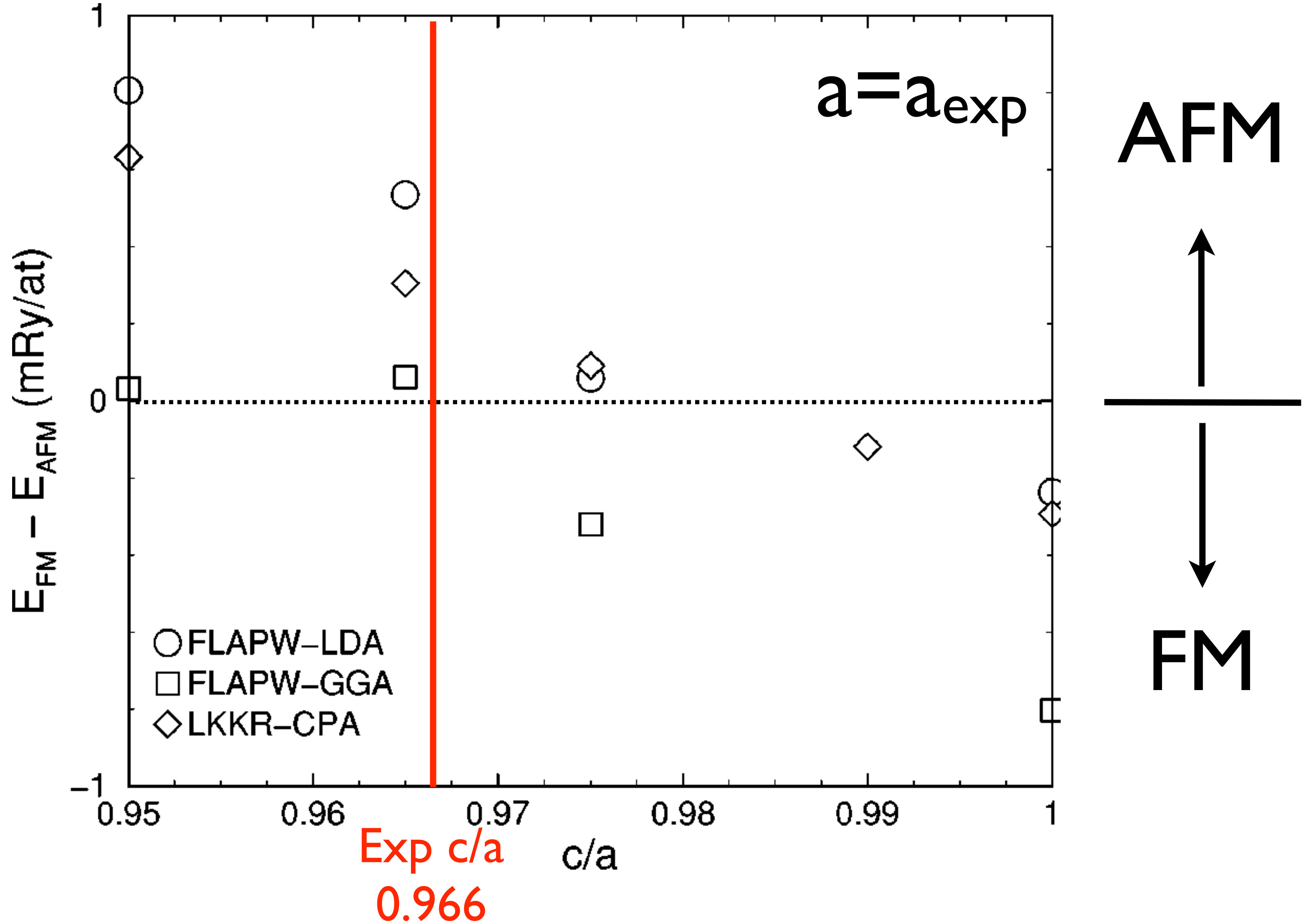
2. FM nanoparticles have been synthesized.

Q. How do <u>size</u>, <u>disorder</u>, shape, concentration influence nanoscale magnetic properties of FePt?

Methods

1. Plane wave LDA DFT (VASP)
   - PAW method. Bulk and fully relaxed geometries
   - Periodic supercells. >10A vacuum between particles
   - Up to 807 atoms
2. Multiple scattering LDA DFT (LSMS)
   - Real space method
   - Not full potential. Use bulk or PAW geometries.
   - Future: Non-collinear magnetism. Model building

Bulk FePt is AFM in LDA

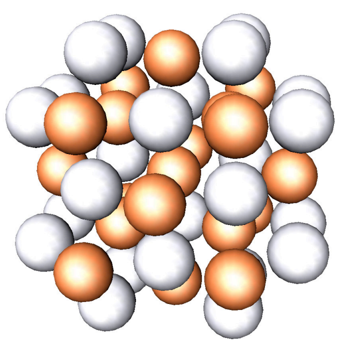


Strong sensitivity to c/a. Can force FM.

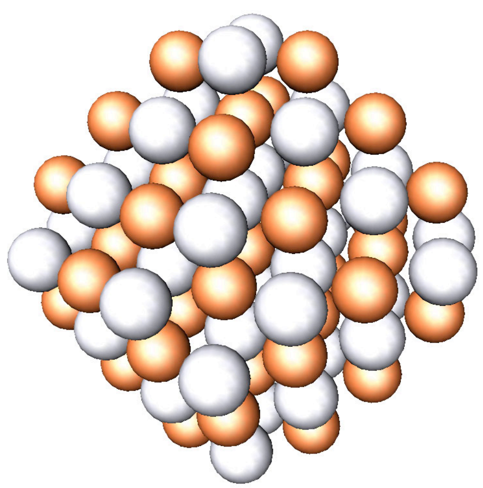
Brown et al. PRB 68 052405 (2003)

Fully relaxed gives AFM

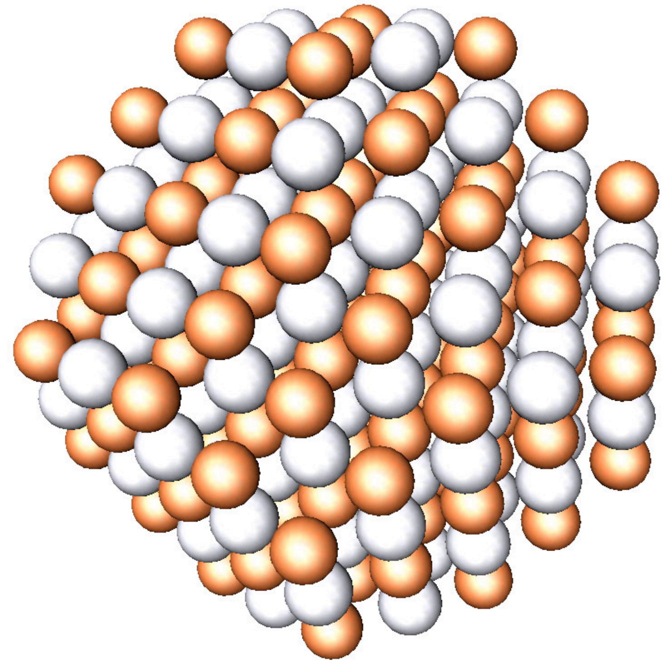
FePt structures



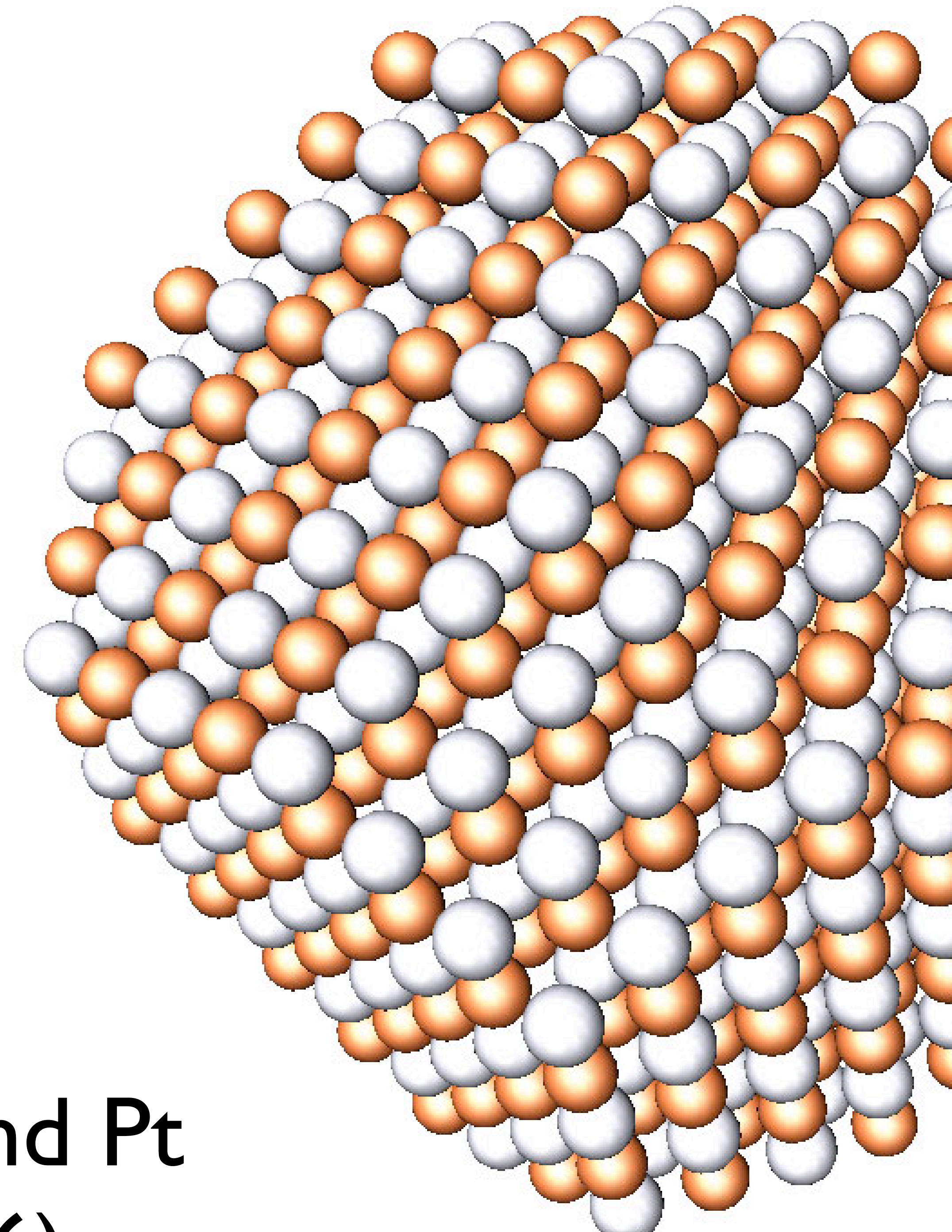
43 atoms



79 atoms



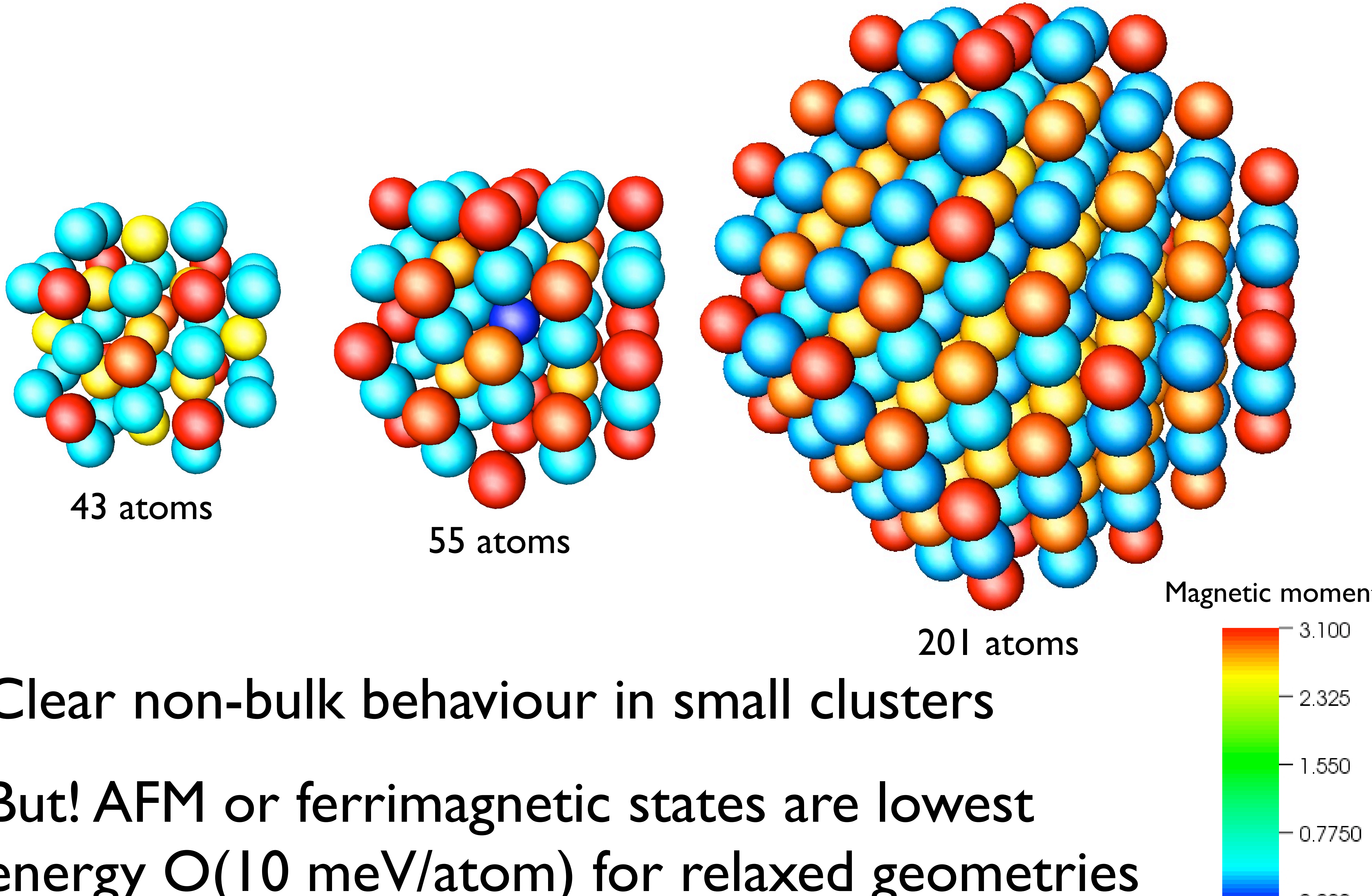
201 atoms



807 atoms

Perfect $L1_0$ ordered planes of Fe and Pt atoms cleaved from bulk (c/a=0.966). Nominally 1:1 ratio Fe:Pt.

Strong size effects in magnetic moments

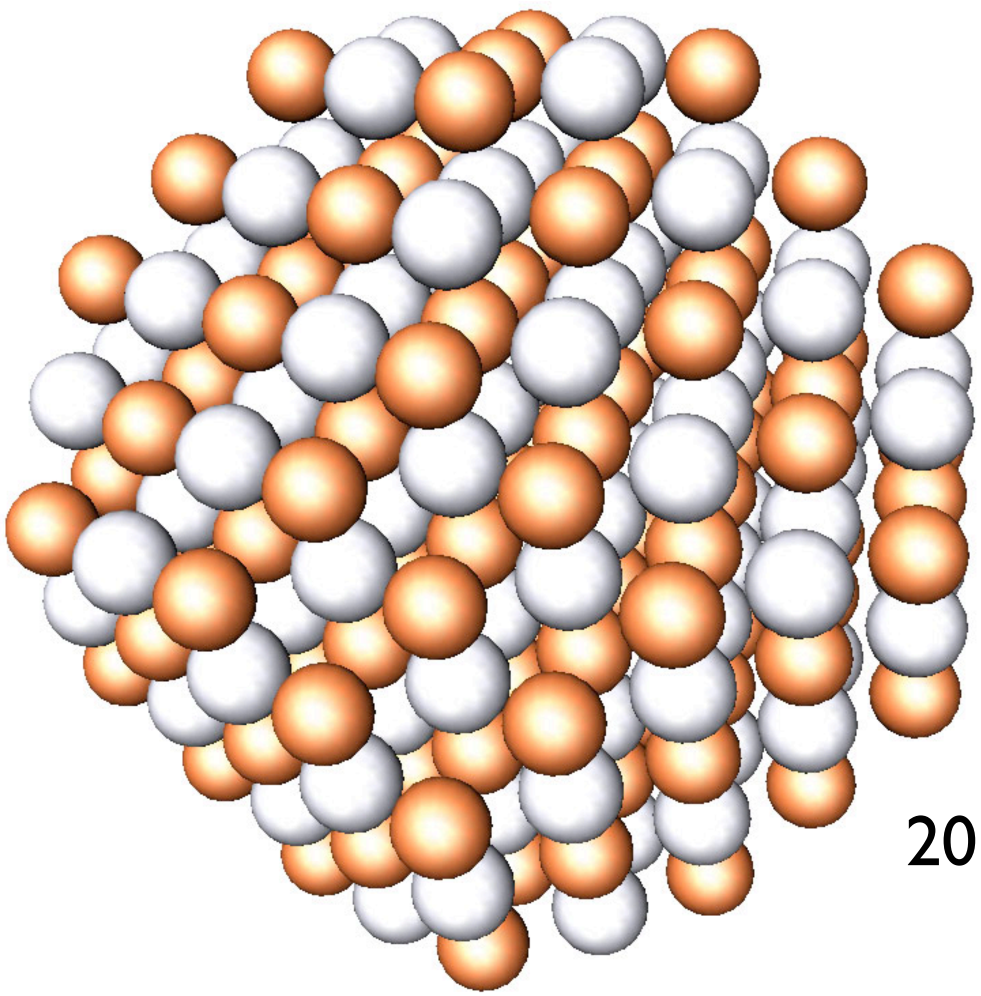


Clear non-bulk behaviour in small clusters

But! AFM or ferrimagnetic states are lowest energy O(10 meV/atom) for relaxed geometries

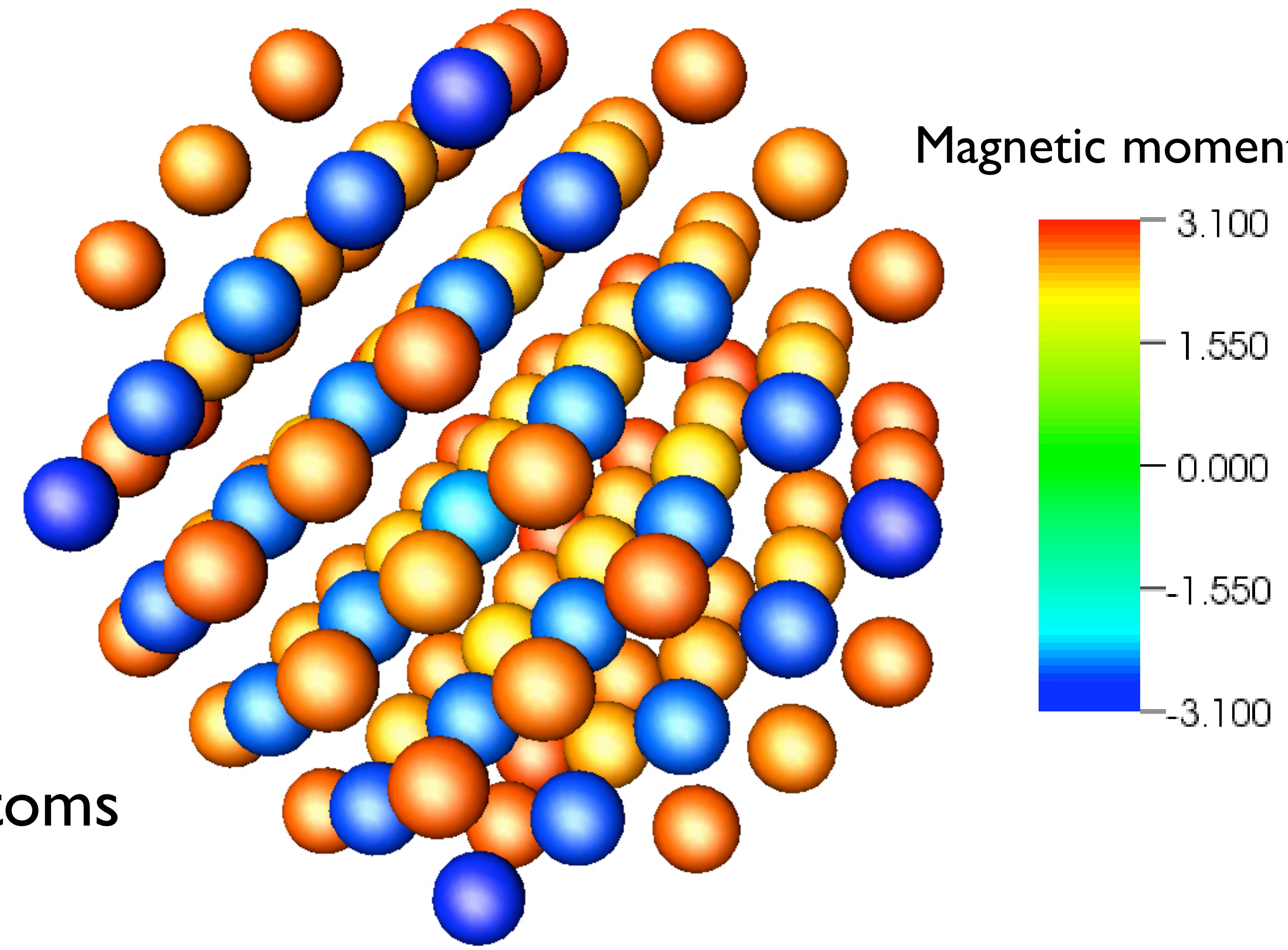
AFM results

Structure

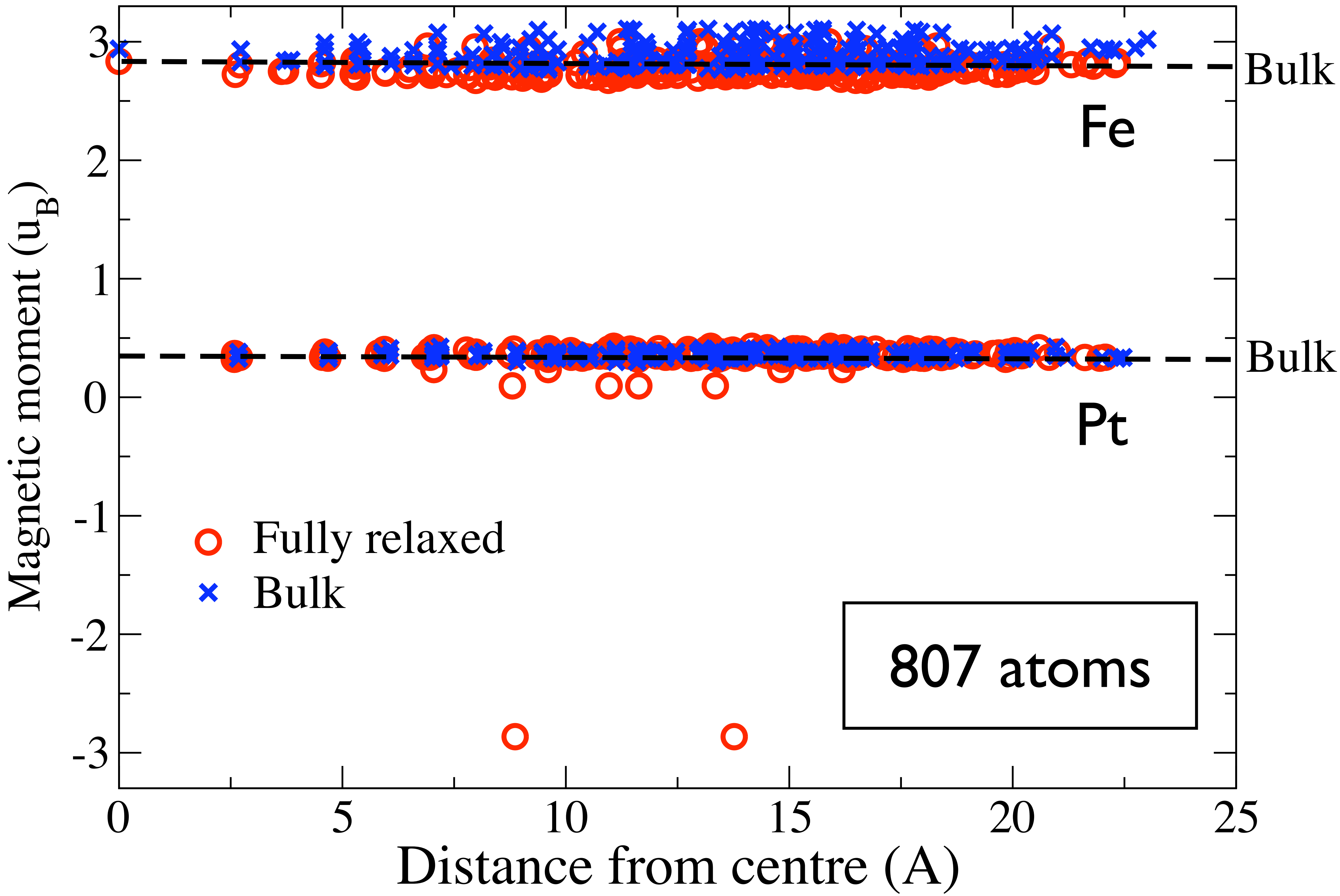


201 atoms

Moments (Fe only)

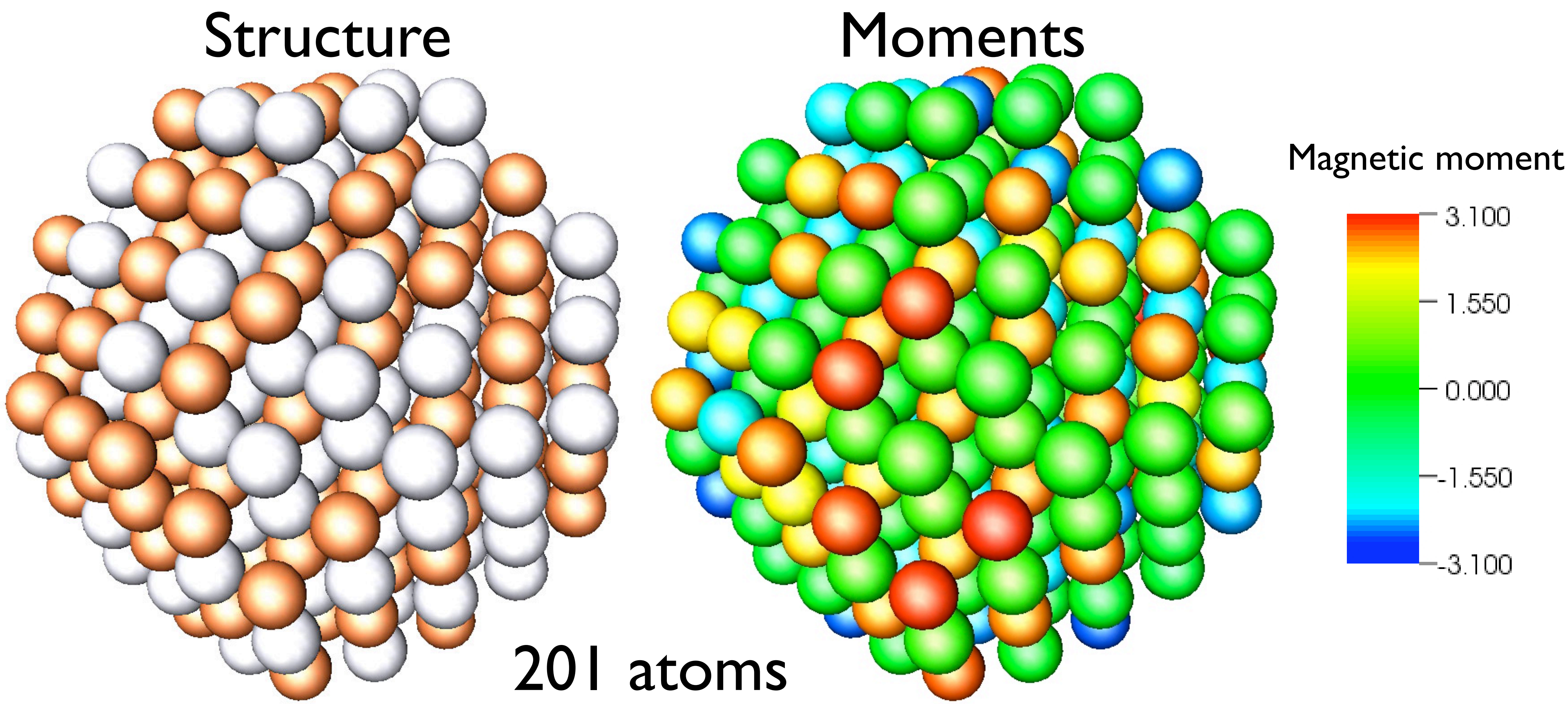


- Preferred ordering: AF planes
- AFM or ferri' depending on size, geometry, symmetry
- Small size alone is insufficient to stabilise strong FM



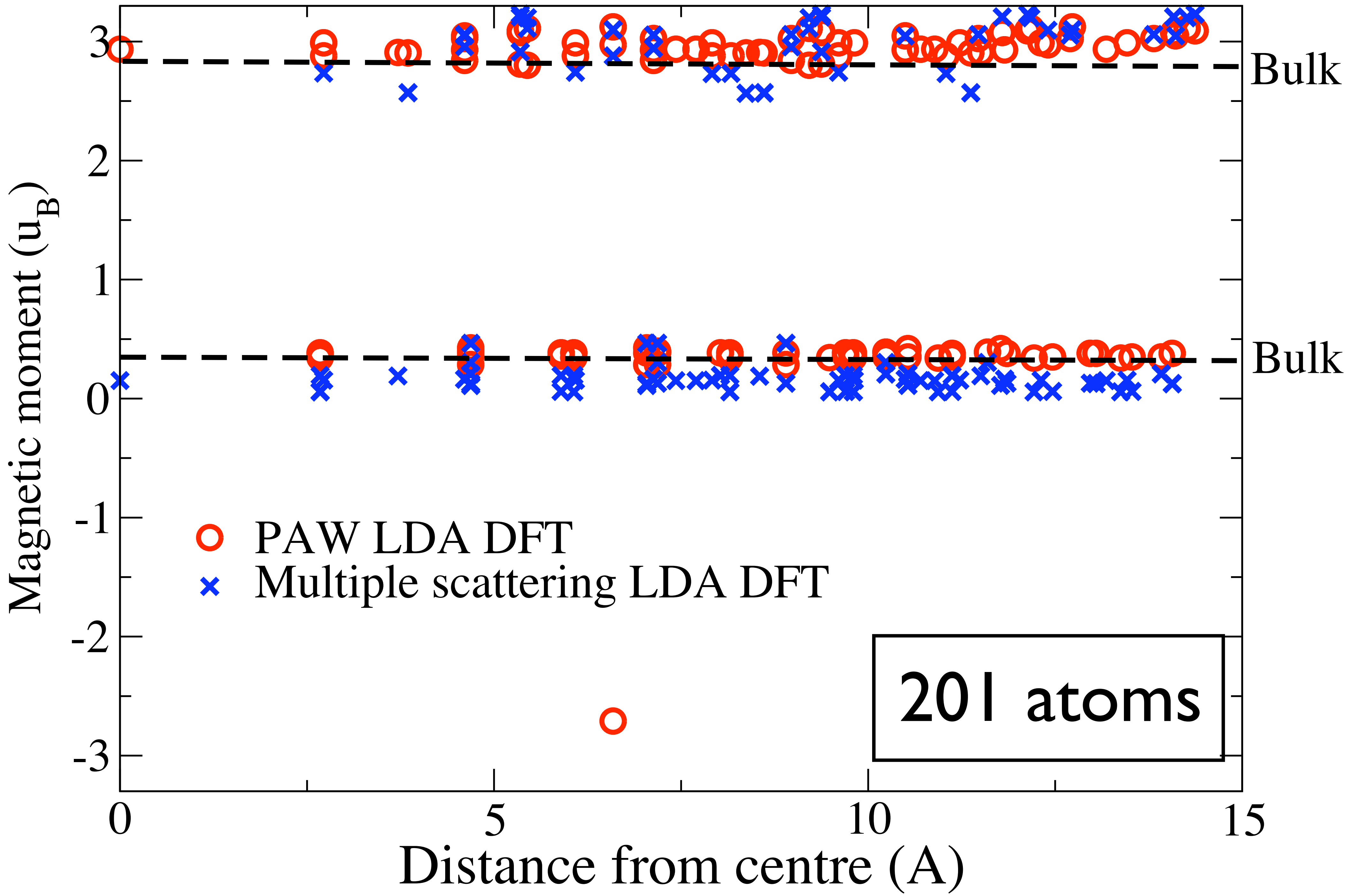
- Near-surface Fe atoms have enhanced moment
- Relaxations can be significant. AF spins!

Disorder



- Random occupations with LRO c[Fe]-c[Pt]=0.80
- Partial FM order stabilised via Fe on Pt planes
- Configuration dependent. Delicate competition between FM (via Fe on Pt sites) and AFM (FePt)

Multiple scattering



- Modest agreement with PAW. Smaller moments.
- Difficult convergence!

Conclusions

Disorder required to stabilize FM/non-AFM. ***Nanoscale alone is insufficient***

Magnetic moments FePt nanoparticles strongly dependent on size, disorder

Multiple scattering close to PAW results