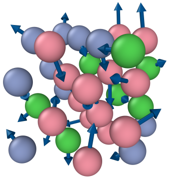
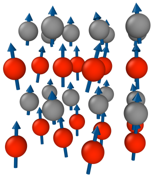
A (Spin) Polarised World: Multiscale Modelling of Magnetic Materials for Energy Applications

Christopher D. Woodgate, PhD

University of Warwick, Coventry, UK

18/04/2024





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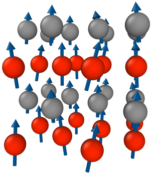

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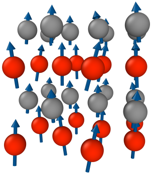

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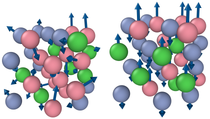

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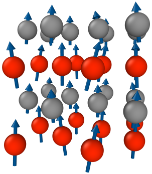

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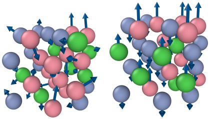

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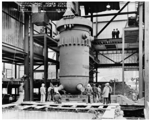

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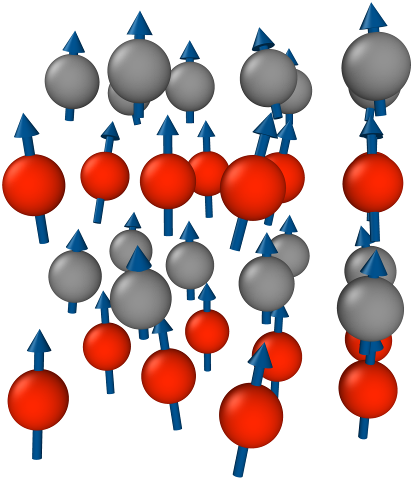

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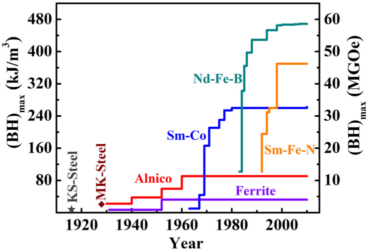

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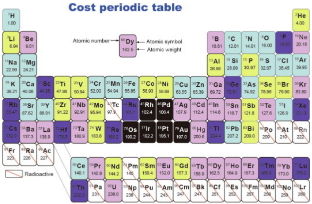

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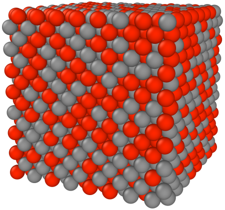

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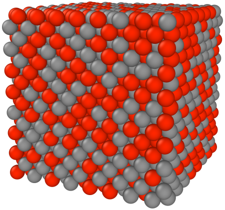

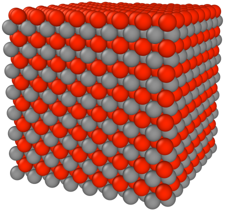

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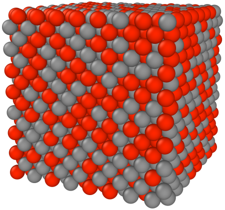

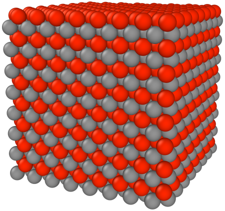

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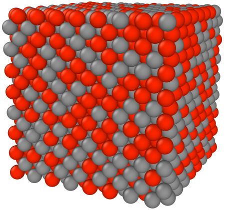
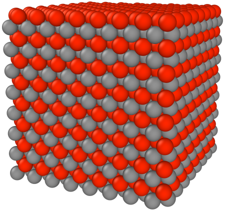
- If we don't wait anneal for long enough, get *partial* order.





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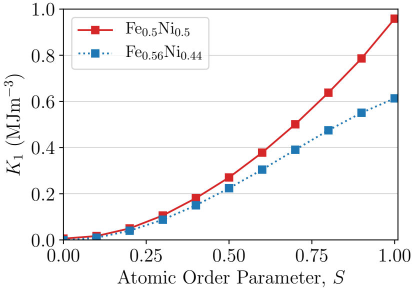

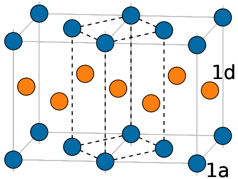

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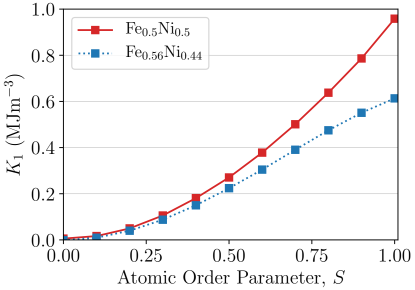

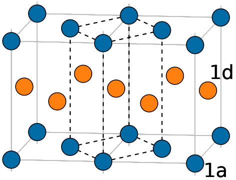

- Maximal order needed for good magnetic properties.

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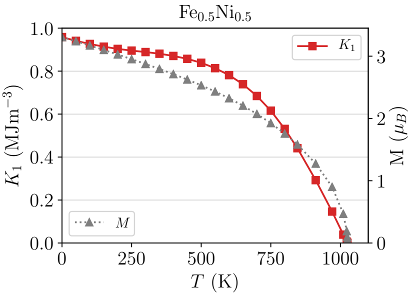

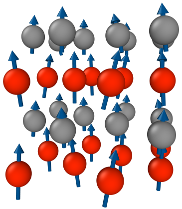

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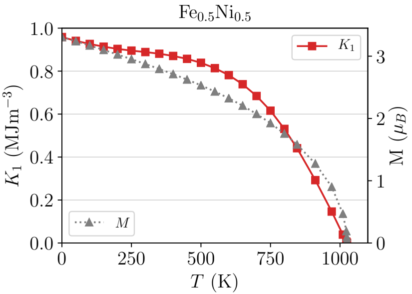

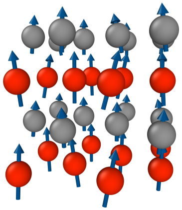

- Finite-temperature performance is excellent.

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Take-Home

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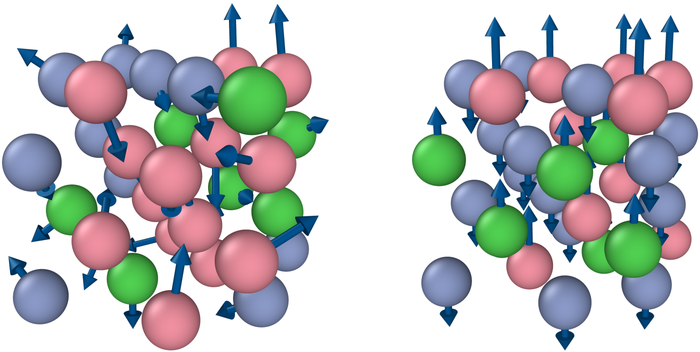
Story 1: L1$_0$ FeNi

Behaviour at the *atomic* scale affects *macroscopic* materials properties. Crucial for magnet design.

Story 2: Magnetism in High-Entropy Alloys



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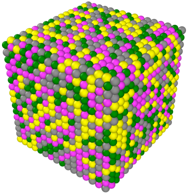

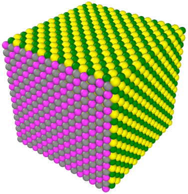

- At what temperature will order emerge? What is the nature of order? Short-range? Long-range? Materials properties?

Case study: Cantor Alloy (CrMnFeCoNi) and Derivatives

[4] Woodgate, Staunton, Phys. Rev. B **105** 115124 (2022).
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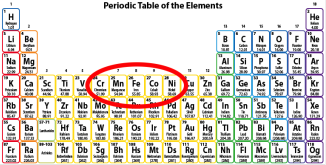

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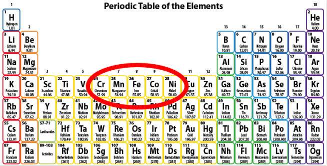

- Up to five mid- to late- 3*d* transition metals: magnetism *matters*.

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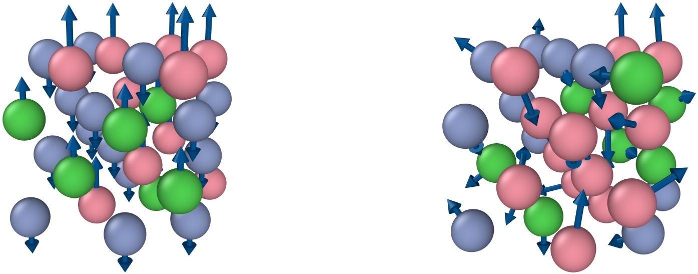

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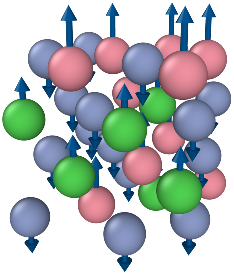

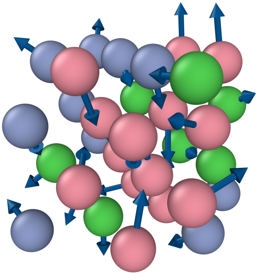

- Cr aligns antiparallel, Ni and Co parallel with total moment.

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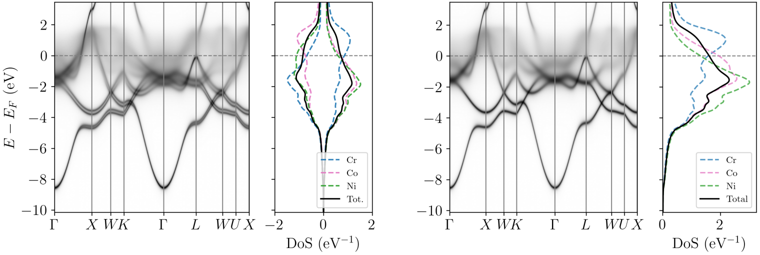

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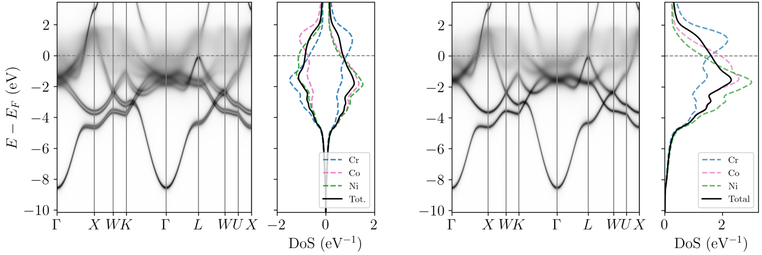

- Different magnetic state, different bandstructure.

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How does the magnetic state affect atomic ordering?

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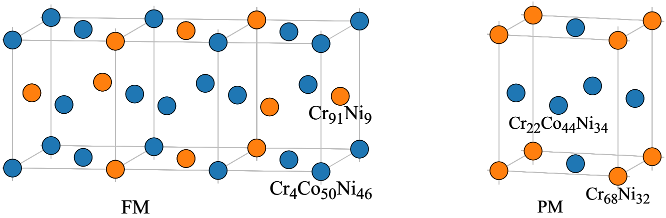

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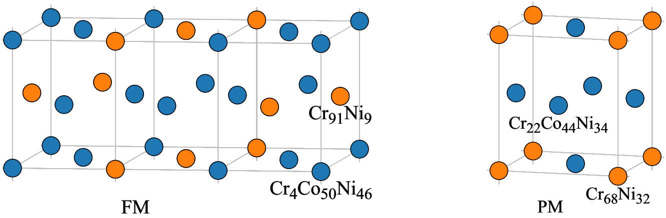

- Different predicted chemical orderings based on magnetic state! Can we observe this experimentally in some systems?

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Take-Home

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Story 2: Magnetism in High-Entropy Alloys

Magnetism (and magnetic state) affects how atoms preferentially arrange themselves. Can we tune materials properties?

Story 3: Machine-Learning for Materials Modelling

PHYSICAL REVIEW MATERIALS **8**, 033804 (2024)

Collinear-spin machine learned interatomic potential for Fe_7Cr_2Ni alloy

Lakshmi Shenoy,[1,*] Christopher D. Woodgate,[2] Julie B. Staunton,[2] Albert P. Bartók,[1,2] Charlotte S. Becquart,[3] Christophe Domain,[4] and James R. Kermode[1]

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(Received 4 October 2023; accepted 27 February 2024; published 22 March 2024)

Example Application: Reactor Pressure Vessels (RPVs)

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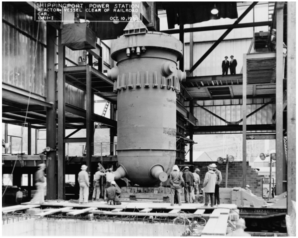
- Used *everywhere*, including in RPVs.



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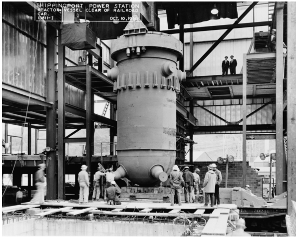
Example Application: Reactor Pressure Vessels (RPVs)

- Prototypical austenitic stainless steel: $Fe_{70}Cr_{20}Ni_{10}$.
- Used *everywhere*, including in RPVs.
- Need to understand how this material ages to be confident of reactor safety.



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Challenges and Opportunities

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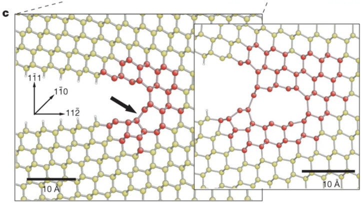

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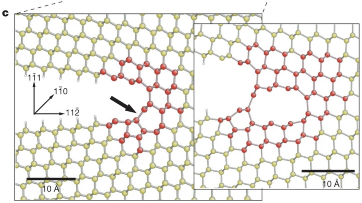

- Question: Can machine-learning help?

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Machine-Learned Interatomic Potentials (MLIPs)

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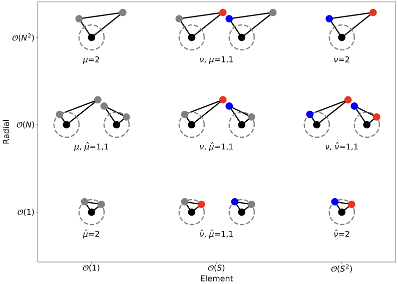

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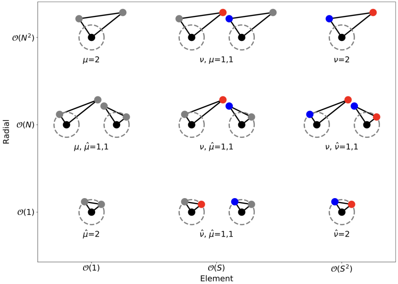

- We use the 'Gaussian Approximation Potential' (GAP).

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Handling Magnetic Elements: Fe, Cr, Ni?

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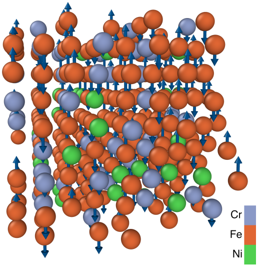

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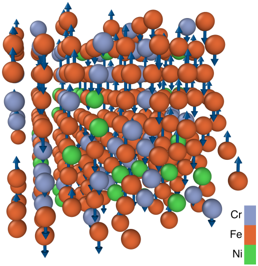

- Solution: treat different 'spins' as different 'chemical' species.

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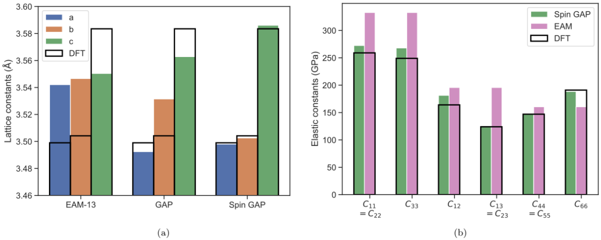

FIG. 4. (a) Lattice constants (a), (b), (c) averaged over 400 configurations predicted by EAM, GAP, and spin GAP for the AFM state,

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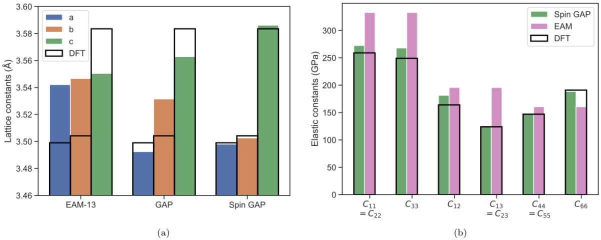

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- 'Spin GAP' does better than most.

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Acknowledgements

Funding

- C.D.W. supported by a studentship within EPSRC-funded CDT: warwick.ac.uk/hetsys
- EPSRC (UK)
- NSF (US)
- DOE (US)

People

University of Warwick, UK

- Lakshmi Shenoy
- James R. Kermode
- Albert P. Bartók
- George A. Marchant
- Julie B. Staunton

Northeastern University, USA

- Laura H. Lewis

University of Oxford, UK

- Christopher E. Patrick