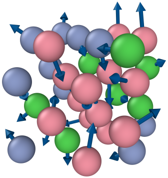
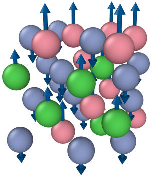
Connections Between Magnetism and Preferred Atomic Arrangements in Multicomponent Alloys

Christopher D. Woodgate

University of Warwick, Coventry, UK

CCP9 Conference 2024





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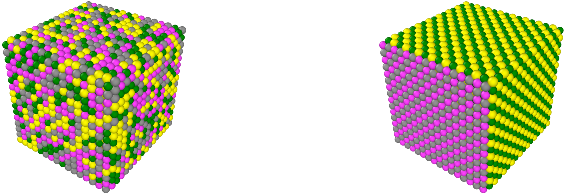

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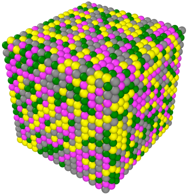
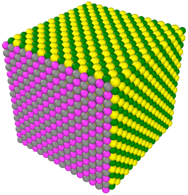
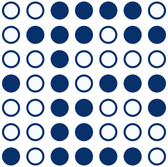




- At what temperature will order emerge? What is the nature of order? Short-range? Long-range? Materials properties?
- Challenging for modellers. Huge number of potential compositions and atomic configurations. Magnetic state for alloys containing Fe, Mn, Co?

Our Description

- Have lots of lattice-based configurations.



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

[2] Woodgate, Staunton, Phys. Rev. Mater. **7** 013801 (2023)

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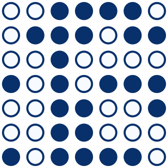

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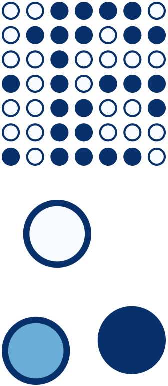

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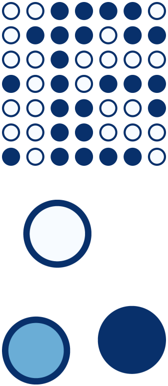

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- Construct an effective medium representing the average electronic structure of the disordered alloy; use the KKR-CPA to do this[1][2].

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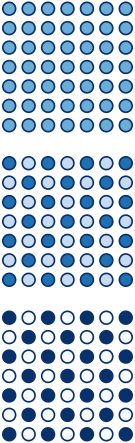
Key Idea

- Perturb high-T, homogeneous state $c_{i\alpha} = c_\alpha + \Delta c_{i\alpha}$ and see what favourable correlations are[1][2].



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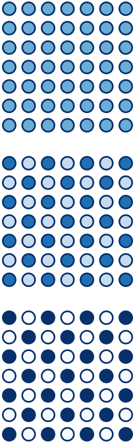

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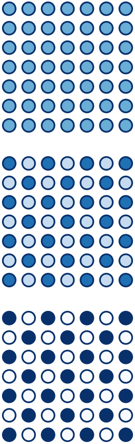

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- Get energetic costs via a perturbative analysis of CPA reference medium[3]; think DFPT.

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Understanding Ordering Tendencies

Two options:

- Apply Landau theory to free energy constructed via perturbative analysis[1][2].

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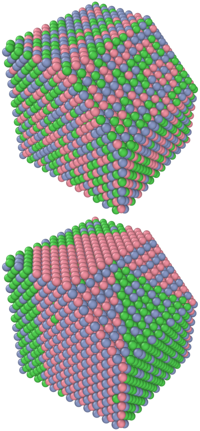

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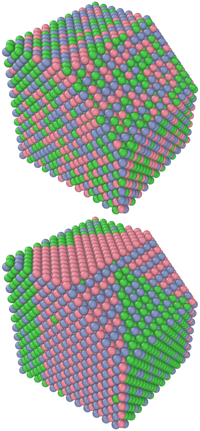
- **Generate physically-motivated configurations for subsequent study.**



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Successful Applications

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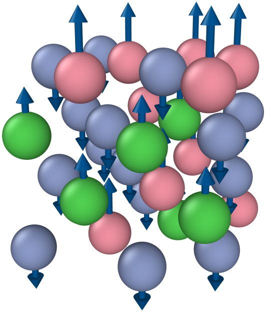
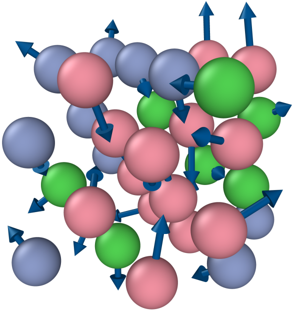
Case Study: CrCoNi





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

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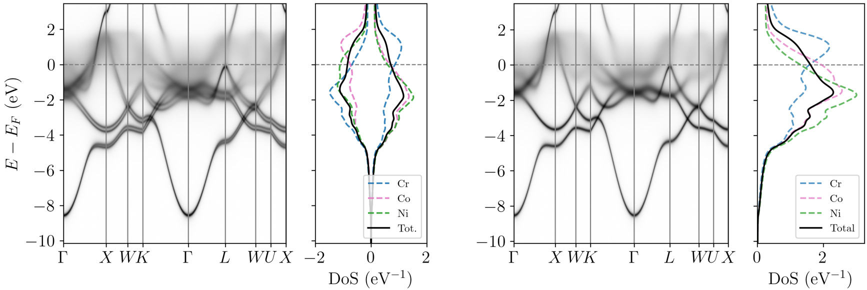
CrCoNi: Electronic Structure

Hutsepot



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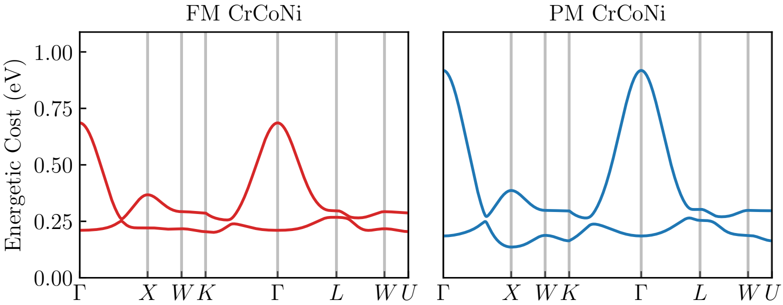
CrCoNi: Perturbative Analysis



- Shape of modes *and* location of minimum altered.

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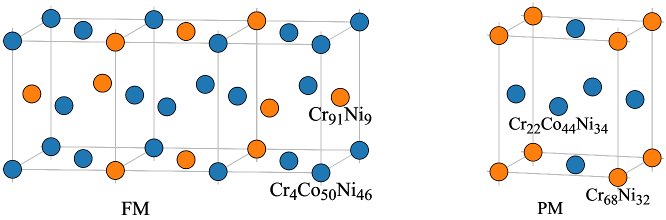
CrCoNi: Inferred Orderings



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

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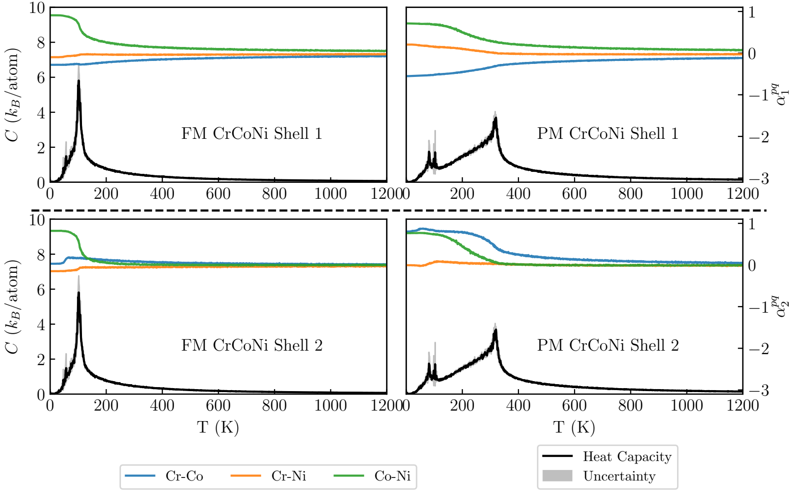
CrCoNi: Atomistic Modelling



Next Steps and Future Work

- Multicomponent alloys represent a *huge* playground.

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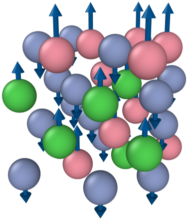
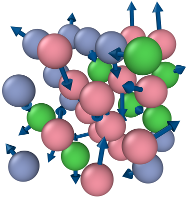
- Feed into more sophisticated techniques, *e.g.* use rapidly-generated configurations in training sets for machine-learned interatomic potentials[5].





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Take-Home Messages

When Modelling Alloys, Magnetism is *Important*

Nature of the magnetic state in an alloy can alter strength of interactions/correlations between elements.

Experimental Implications

Can some multicomponent alloys be processed in an applied magnetic field to tune atomic ordering?

Interface with other techniques

Can use computationally efficient approach to generate configurations for subsequent studies.

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- EPSRC (UK)
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Hutsepot

People

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- Christopher D. Woodgate
- Julie B. Staunton

Northeastern University, USA

- Laura H. Lewis

Our paper:
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