Modelling Atomic Arrangements in Multicomponent Alloys: A First-Principles-Based Approach

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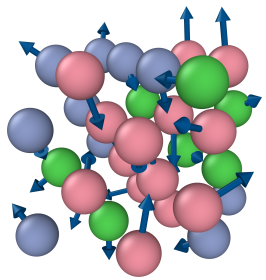
University of Warwick, Coventry, UK

Bristol Quantum Matter Seminar, 20th October 2023



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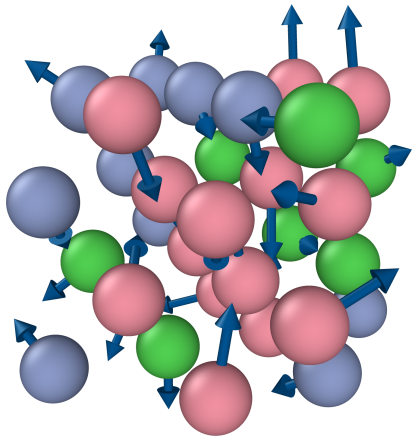

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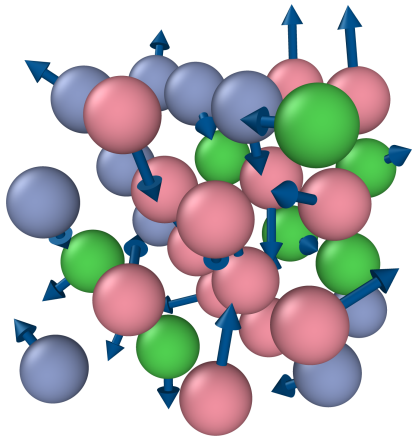

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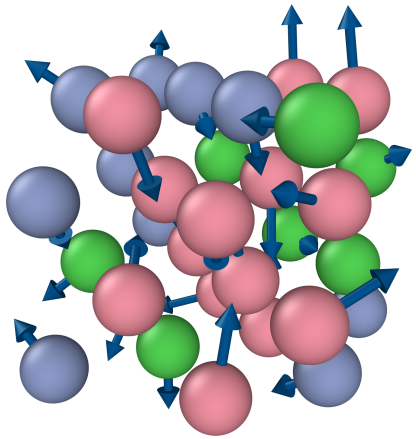

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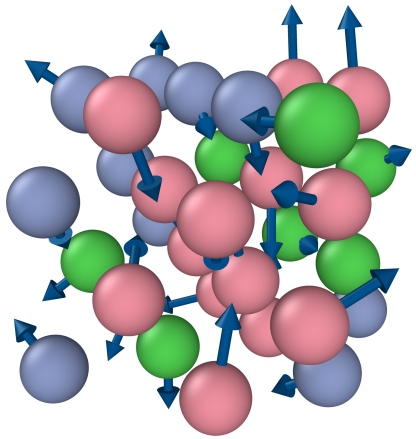

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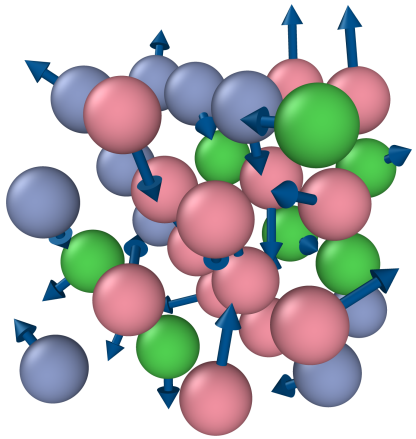

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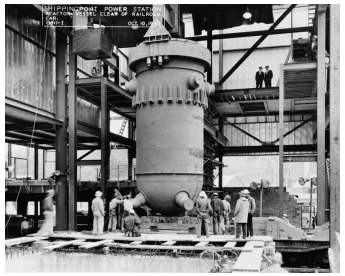

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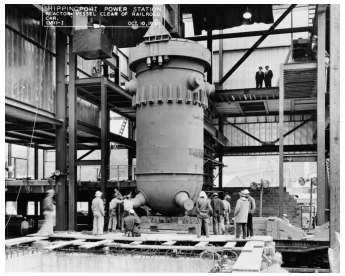

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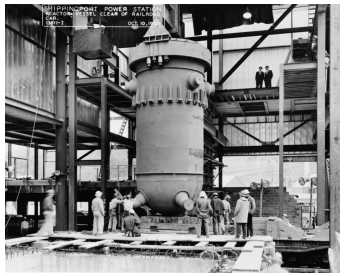

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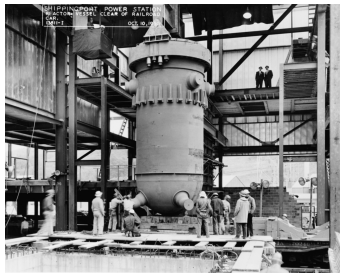

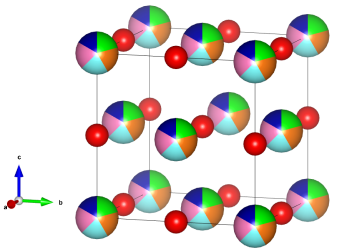

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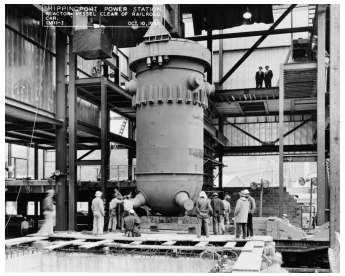

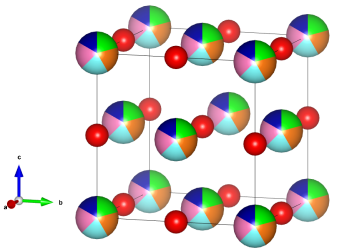

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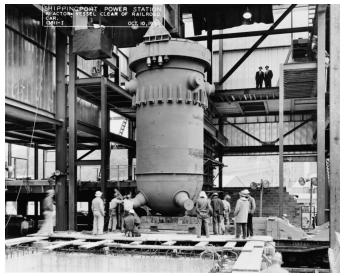
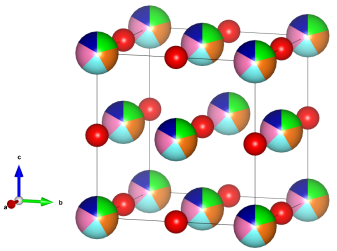
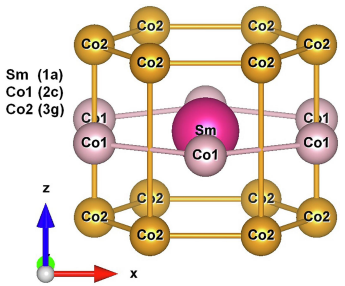
  - 'High Entropy Magnets', *e.g.* $SmCo_5 \rightarrow Sm(FeCoNi)_5$.







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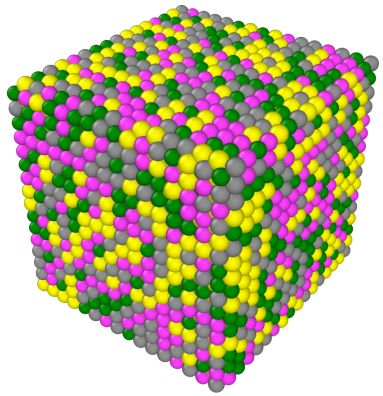

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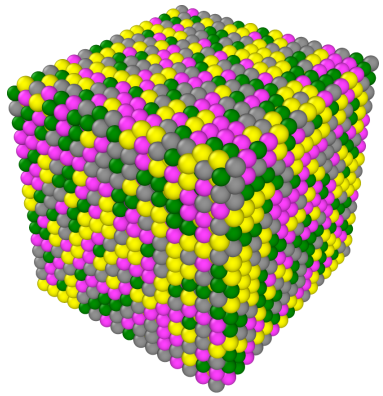

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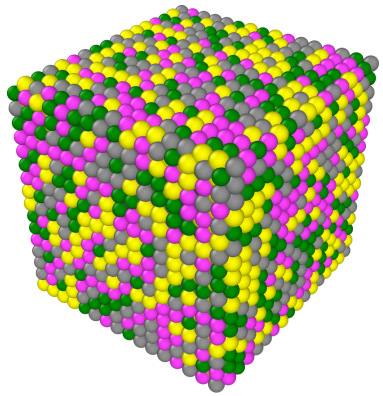

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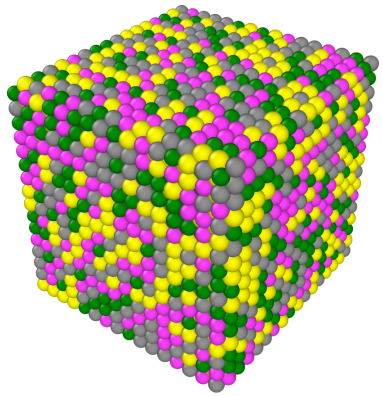

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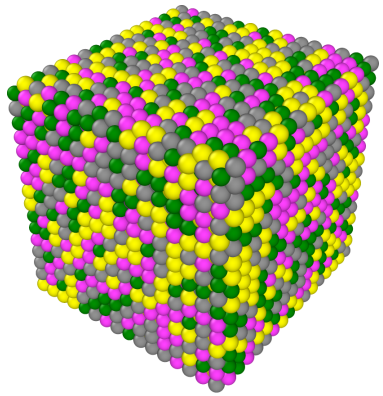

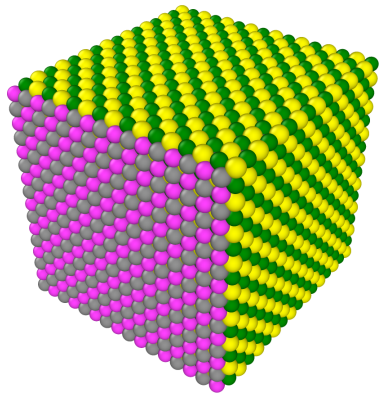

- At what temperature will order emerge? What is the nature of order? Short-range? Long-range? Effect on materials properties?

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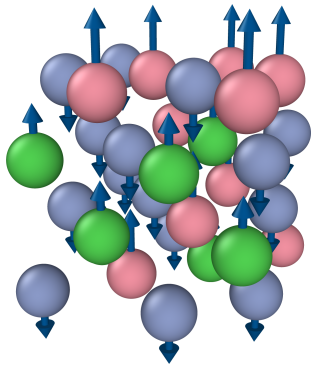

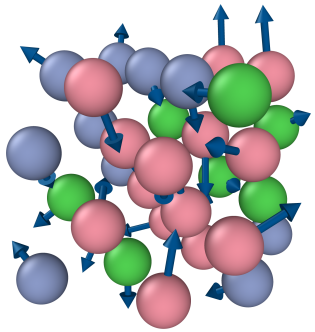

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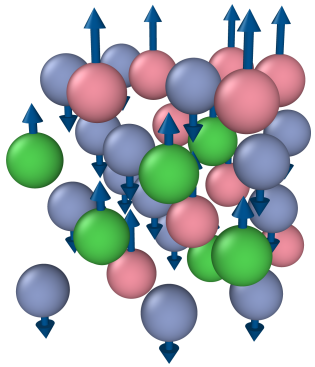
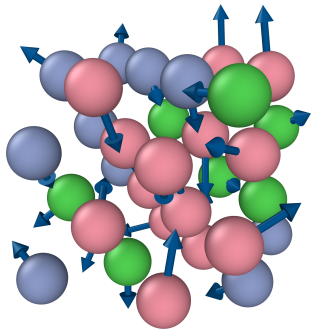
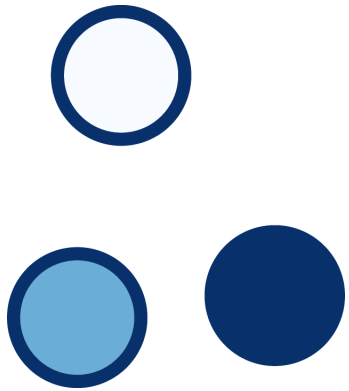




- Would like a *computationally efficient* modelling approach to assess phase stability. Can we do forward modelling?

Describing Atomic Configurations



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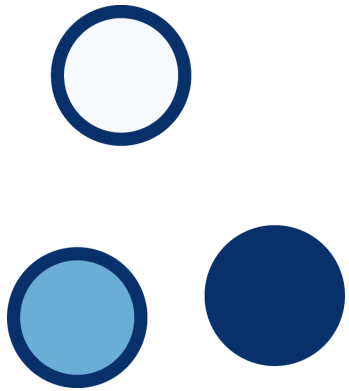

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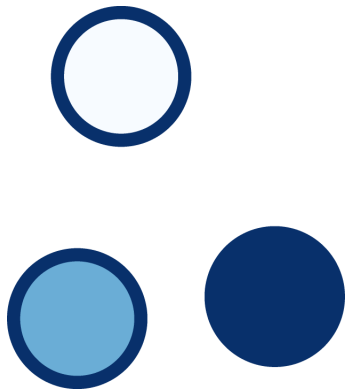

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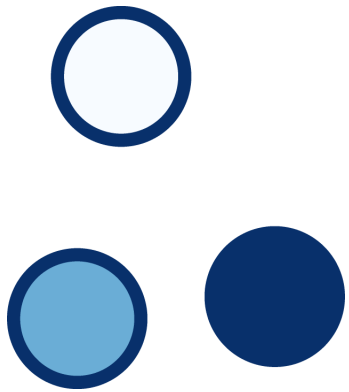

- Above order-disorder transition temperature, these are *homogeneous*:

$$\lim_{T \to \infty} c_{i\alpha} = c_\alpha.$$

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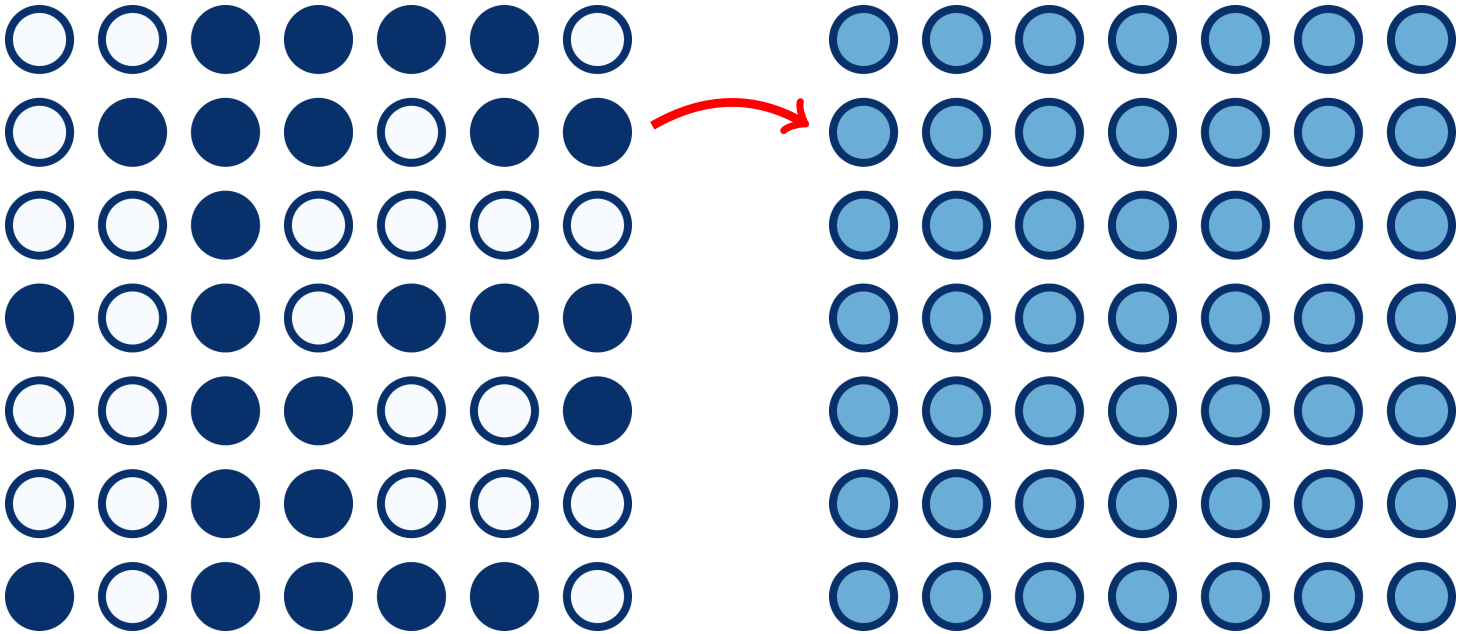

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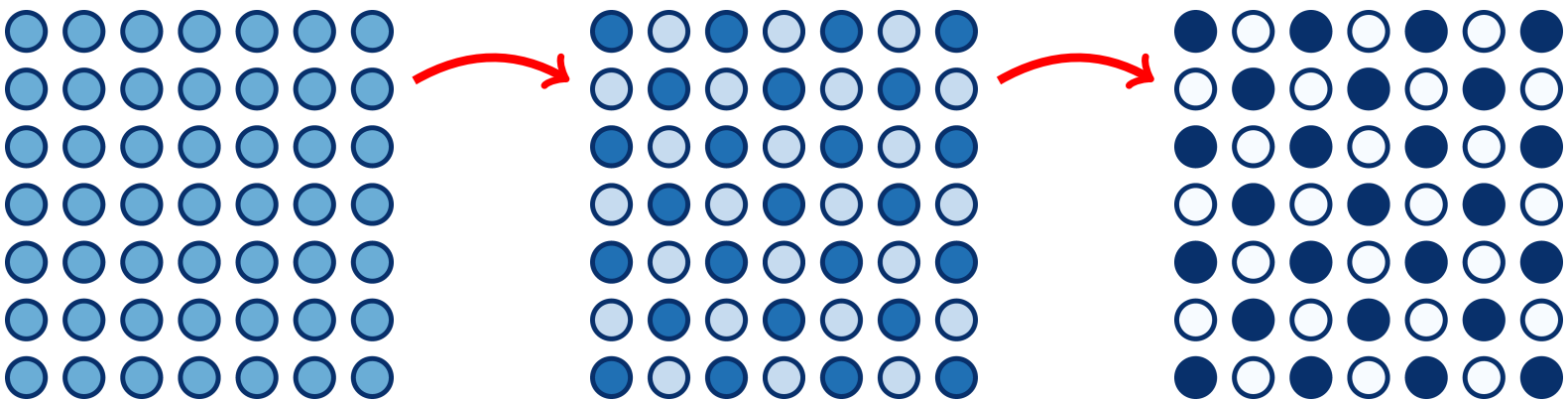

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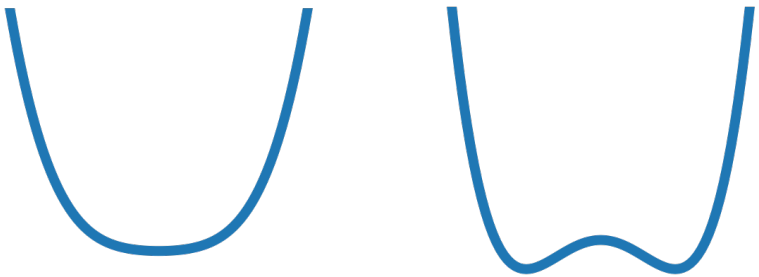
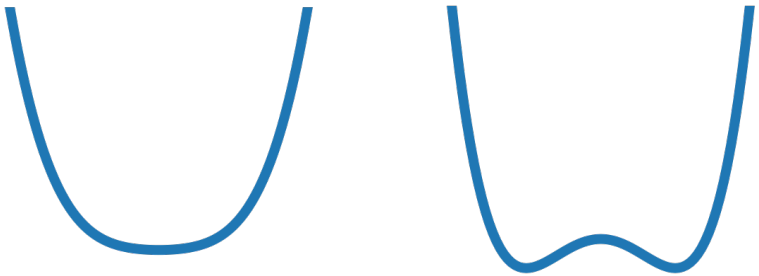
- Assess energetic cost of perturbations to homogeneous reference state.
  - Infer both short-range order and phase stability.



Landau Series Expansion



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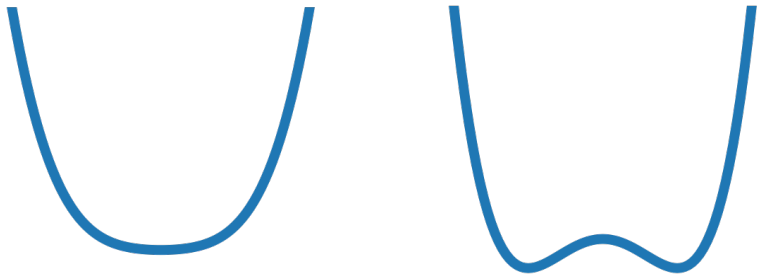

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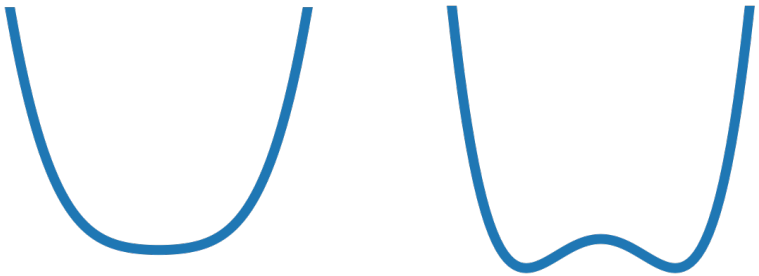
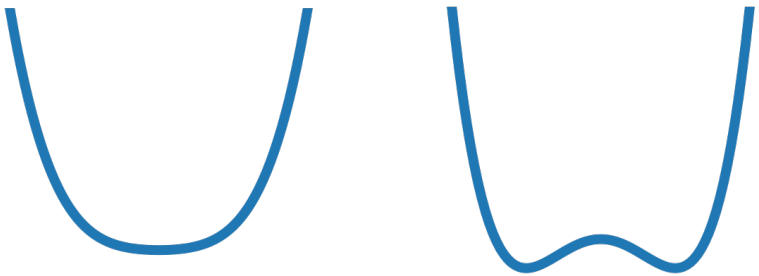
- Series expansion:

$$F\left[\{c_{i\alpha}\}\right] = F\left[\{c_\alpha\}\right] + \sum_{i\alpha} \left.\frac{\partial F}{\partial c_{i\alpha}}\right|_{\{c_\alpha\}} \Delta c_{i\alpha} + \frac{1}{2} \sum_{\substack{i\alpha \\ j\alpha'}} \left.\frac{\partial^2 F}{\partial c_{i\alpha} \partial c_{j\alpha'}}\right|_{\{c_\alpha\}} \Delta c_{i\alpha} \Delta c_{j\alpha'} + \ldots$$



Chemical Stability Matrix



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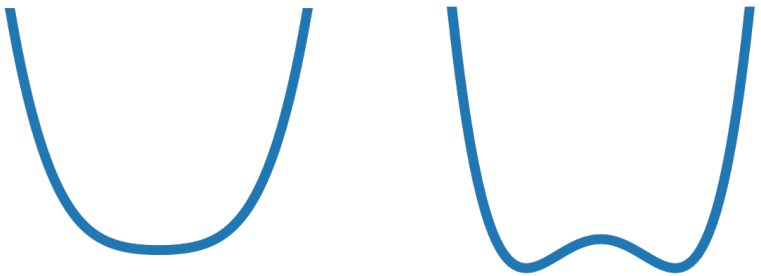

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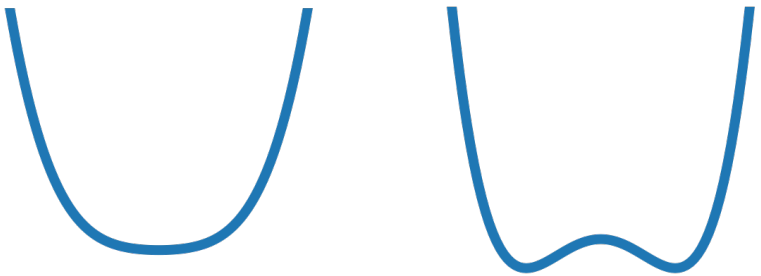
- *Or*, in reciprocal space:

$$\Delta F = \frac{1}{2} \sum_{\mathbf{k}} \sum_{\alpha\alpha'} \Delta c_\alpha(\mathbf{k}) \left[\beta \Psi^{-1}_{\alpha\alpha'}(\mathbf{k}) \right] \Delta c'_\alpha(\mathbf{k}) \qquad (4)$$



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- Recall that free energy has three terms:

$$F = -\beta^{-1} \sum_{i\alpha} c_{i\alpha} \log c_{i\alpha} - \sum_{i\alpha}{}' \nu_{i\alpha} c_{i\alpha} + \langle \Omega_{\mathrm{el}} \rangle_0 [\{c_{i\alpha}\}]$$

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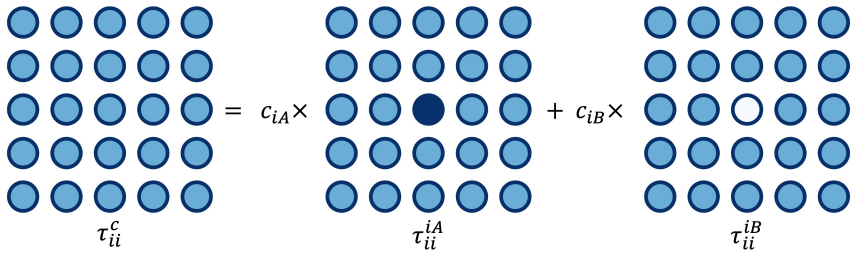
  - Third term more tricky.
- Can evaluate $\langle \Omega_{\mathrm{el}} \rangle_0 [\{c_\alpha\}]$ within KKR formulation of DFT, using CPA to average over disorder.



Evaluating Free Energy and its derivatives

[1] Khan, Staunton, Stocks, Phys. Rev. B **93** 054206 (2016)

Evaluating Free Energy and its derivatives

- Evaluating derivatives of DFT energy is non-trivial[1].

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VOLUME 50, NUMBER 5 PHYSICAL REVIEW LETTERS 31 JANUARY 1983

Concentration Waves and Fermi Surfaces in Random Metallic Alloys

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Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, and H. H. Wills Physics Laboratory, University of Bristol, United Kingdom

and

G. M. Stocks
Science and Engineering Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom, and Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

(Received 18 June 1982)

On the basis of a new first-principles, electronic model for the forces driving clustering and short-range order in metallic alloys, it is argued that observed concentration-dependent peaks in the x-ray and electron diffuse scattering intensities are due to parallel sheets of flat Fermi surface. The positions of the peaks are directly related to the spanning vector $\vec{k}_0$.

PACS numbers: 71.25.Mg, 71.10.+x, 71.25.Hc

[1] Khan, Staunton, Stocks, Phys. Rev. B **93** 054206 (2016)

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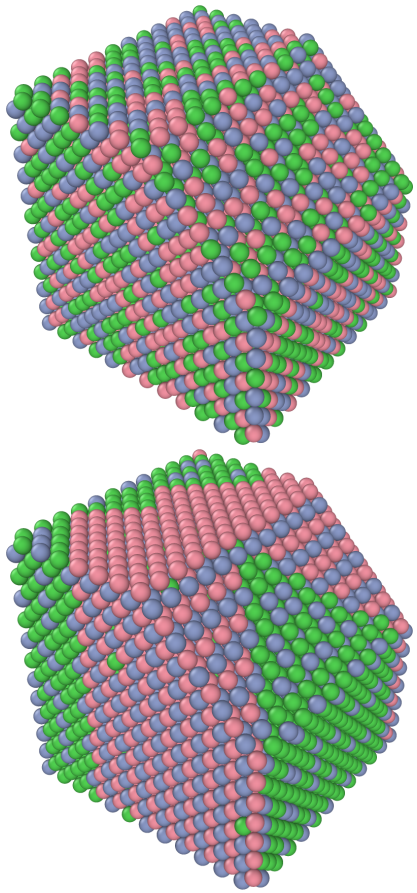
- End result is quantity:

$$S^{(2)}_{i\alpha;j\alpha'} \equiv \frac{\partial^2 \langle \Omega_{\mathrm{el}} \rangle_0}{\partial c_{i\alpha} \partial c_{j\alpha'}} \rightsquigarrow \Psi^{-1}_{\alpha\alpha'}(\mathbf{q})$$

[1] Khan, Staunton, Stocks, Phys. Rev. B **93** 054206 (2016)

Recover a simple, pairwise model ('interatomic potential')



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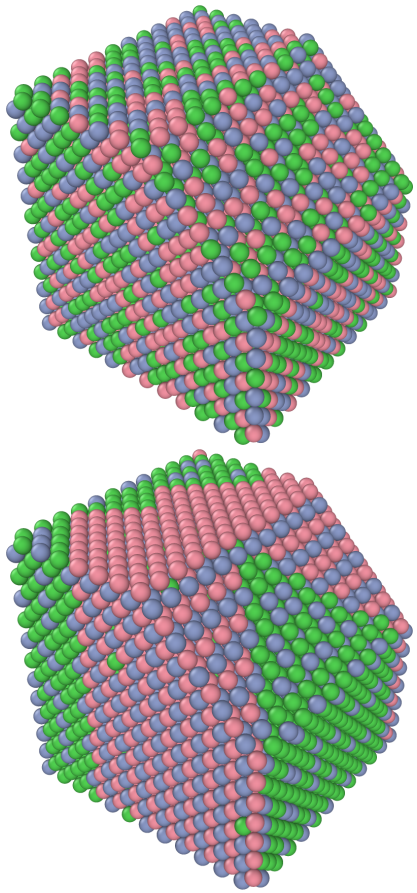
$$H(\{\xi_{i\alpha}\}) = \frac{1}{2} \sum_{\substack{i\alpha \\ j\alpha'}} V_{i\alpha;j\alpha'}\, \xi_{i\alpha}\xi_{j\beta}$$



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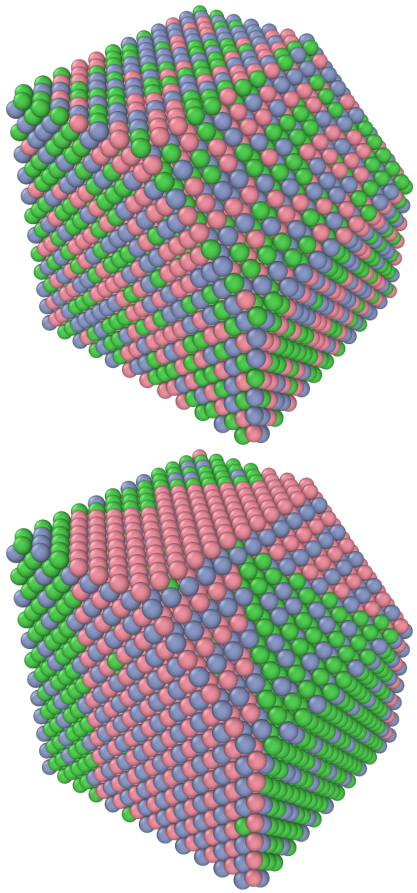
- If H as above, $V_{i\alpha;j\alpha'} = -S^{(2)}_{i\alpha;j\alpha'}$ *exactly*.



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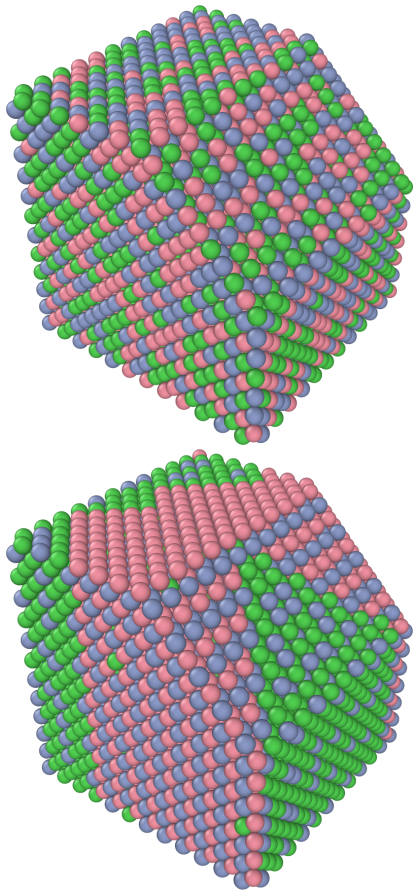
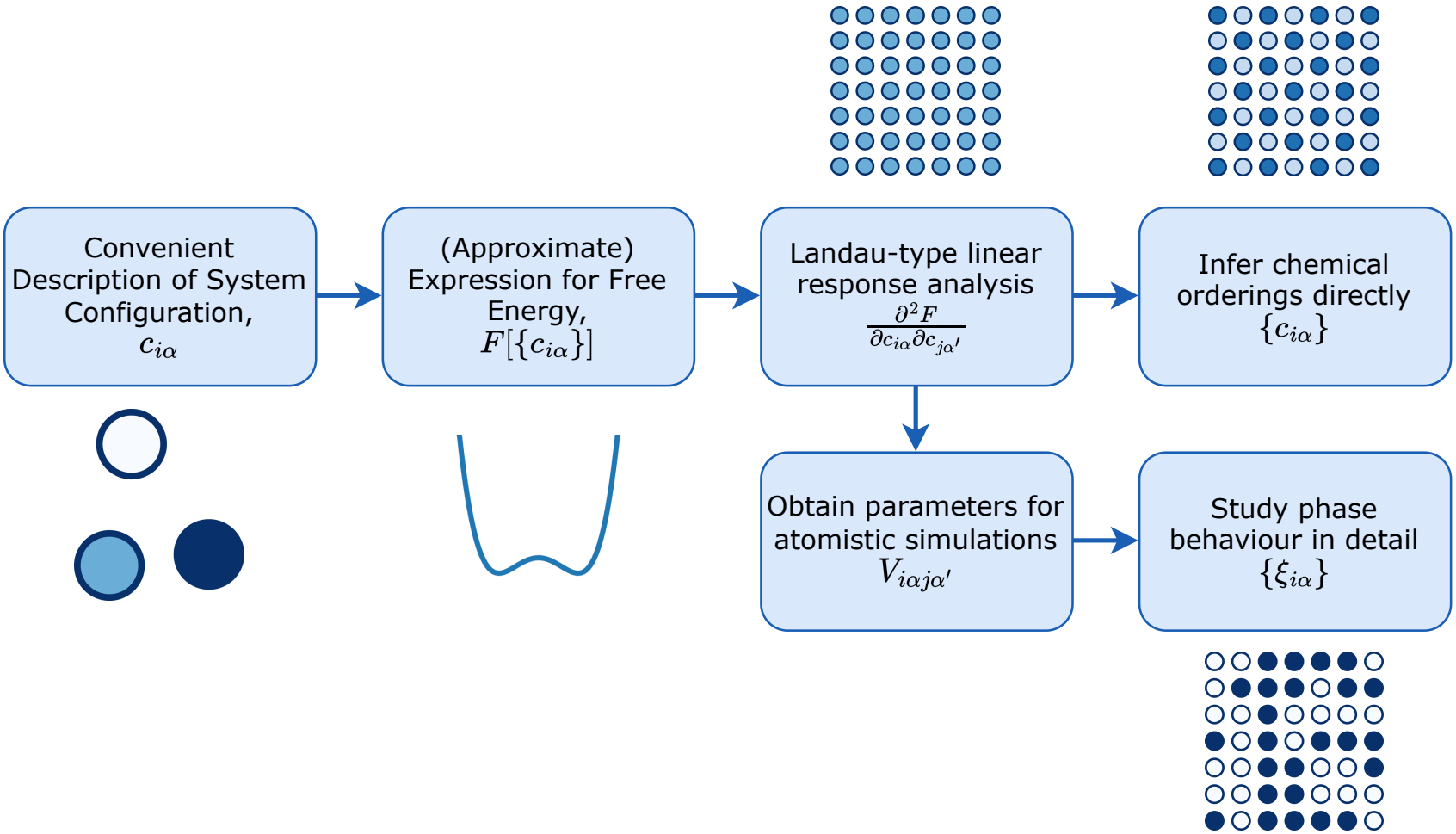
- If H as above, $V_{i\alpha;j\alpha'} = -S^{(2)}_{i\alpha;j\alpha'}$ *exactly*.
- Study phase behaviour using, *e.g.* Monte Carlo simulations.



Workflow Summary



Refractory High-Entropy Alloys: Background

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

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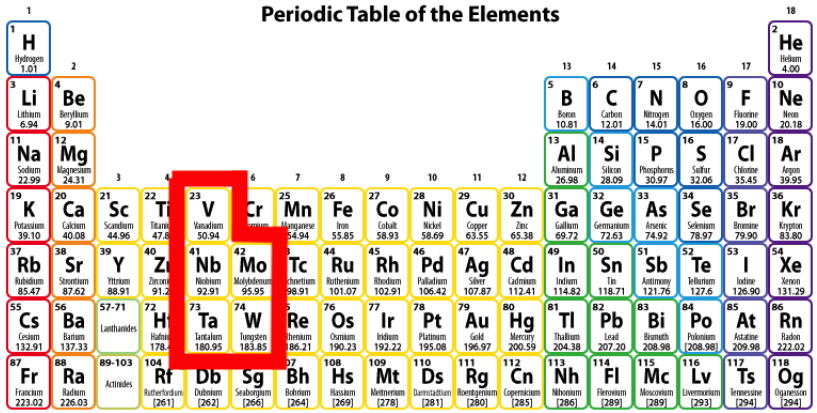
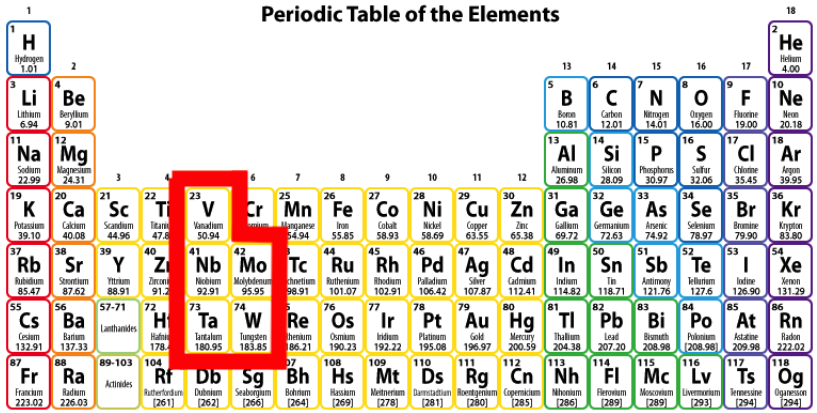


[2]Woodgate, Staunton, Phys. Rev. Mater. **7** 013801 (2023)

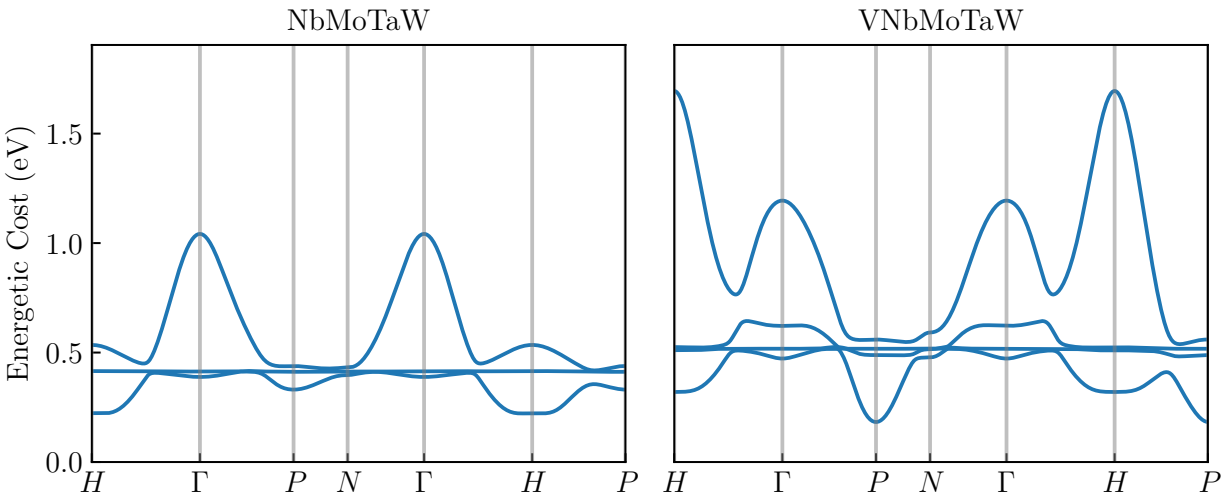
Refractory High-Entropy Alloys: Background

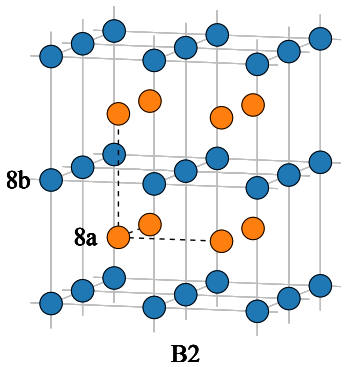
- First synthesised by Senkov around 2010.
- Excellent high-temperature performance, good radiation resistance.
- Previous studies of phase behaviour suggest interesting incipient ordering.

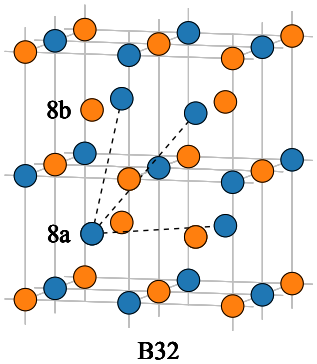


[2] Woodgate, Staunton, Phys. Rev. Mater. **7** 013801 (2023)

Refractory HEAs: Chemical Stability Matrices







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

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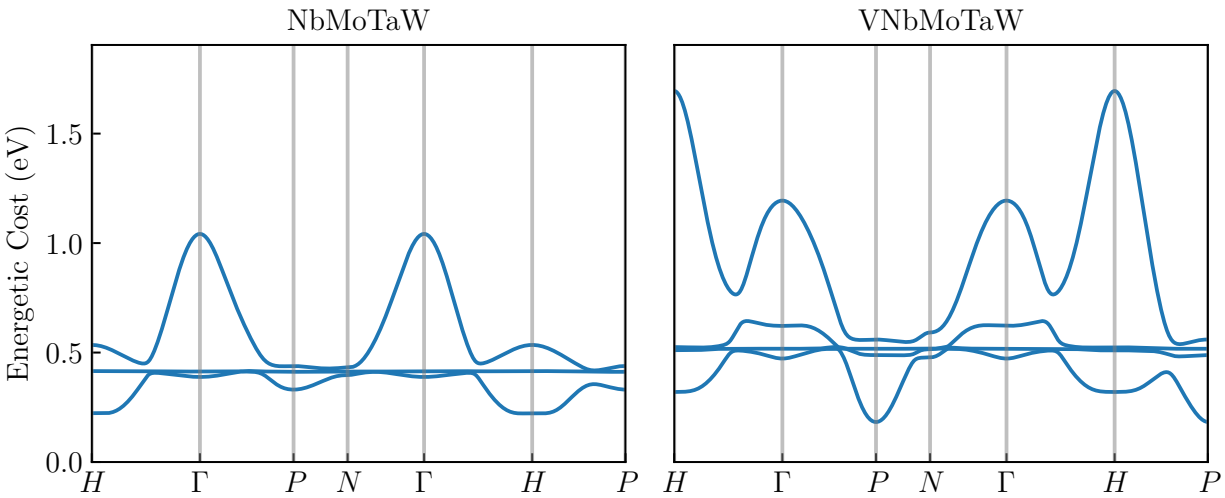
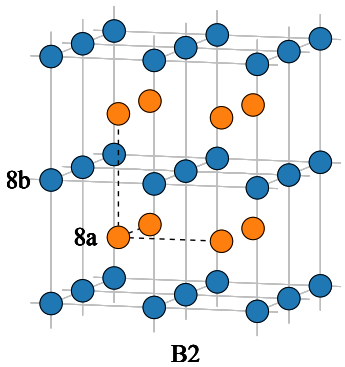
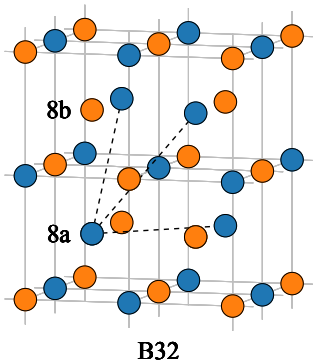


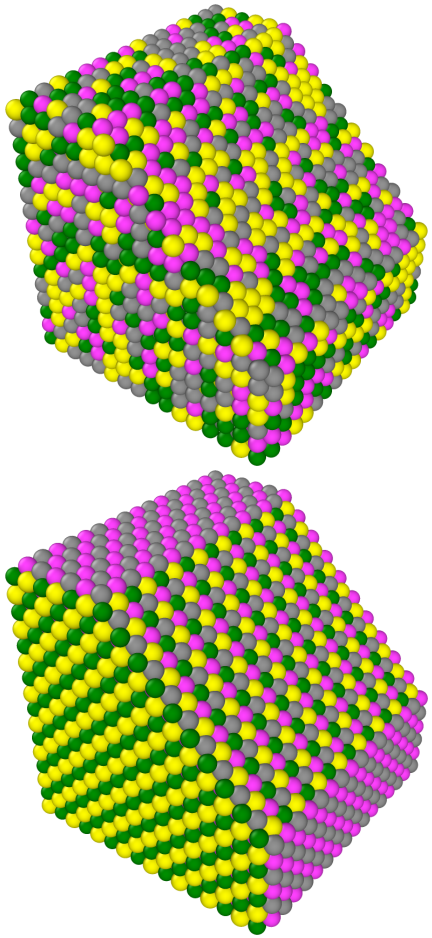


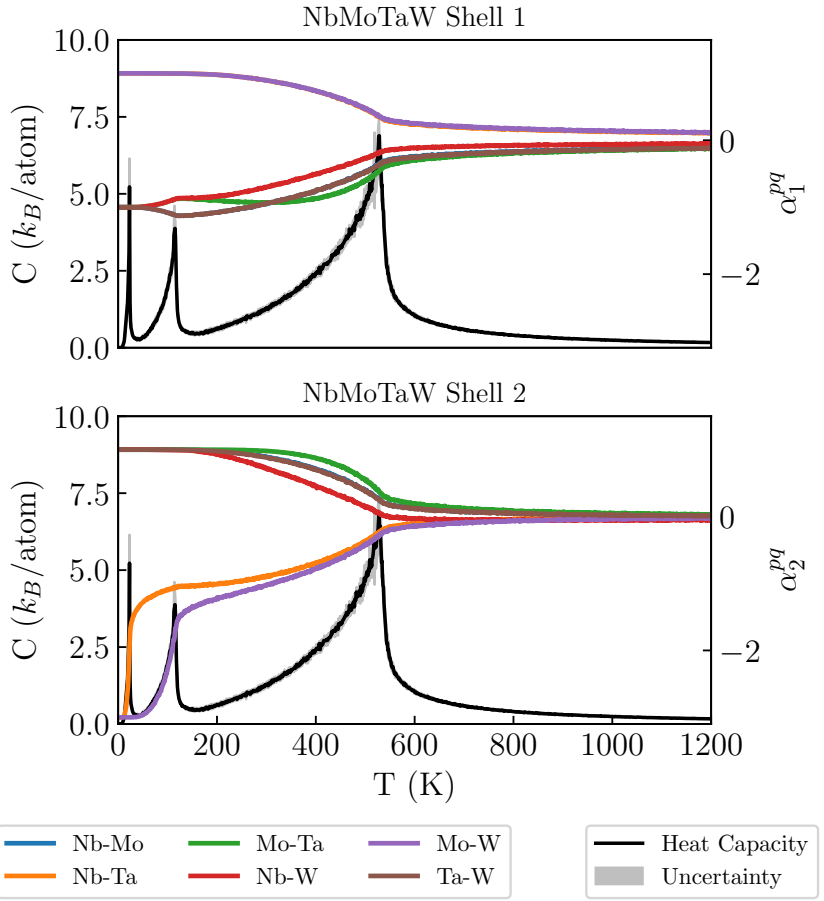


- NbMoTaW[2]: $T_{\text{ord}} = 559$ K.
- VNbMoTaW[2]: $T_{\text{ord}} = 742$ K.

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

Refractory HEAs: Atomistic Modelling





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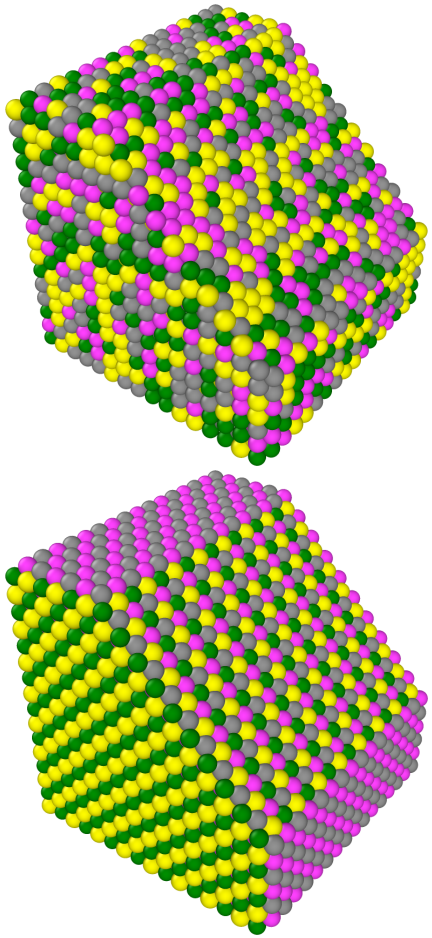
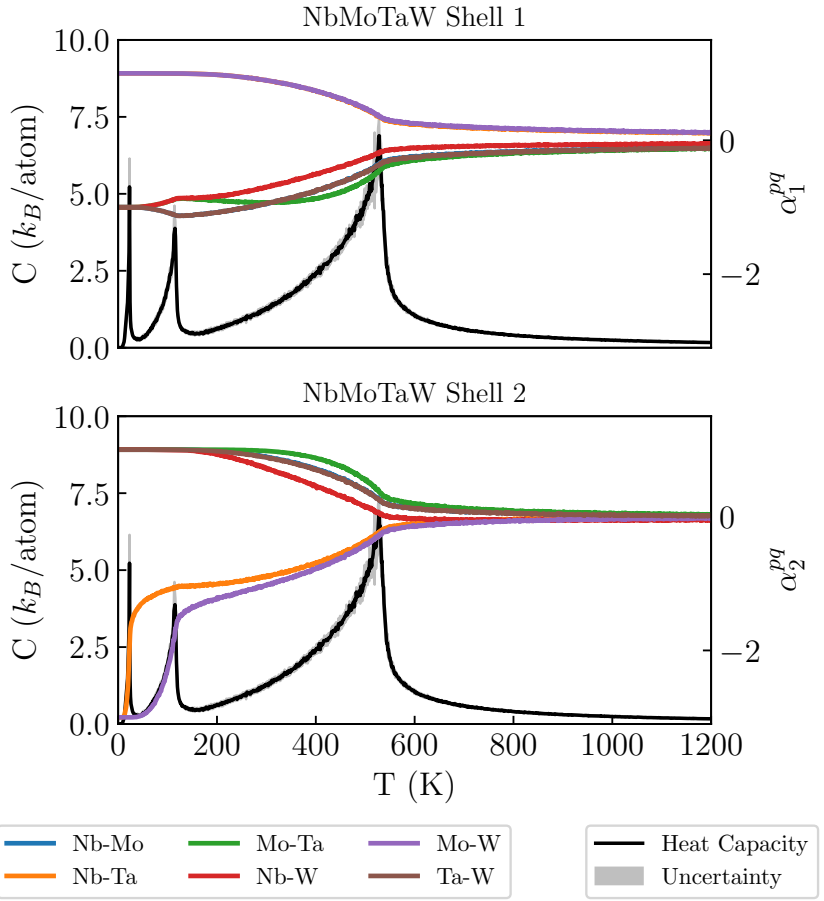




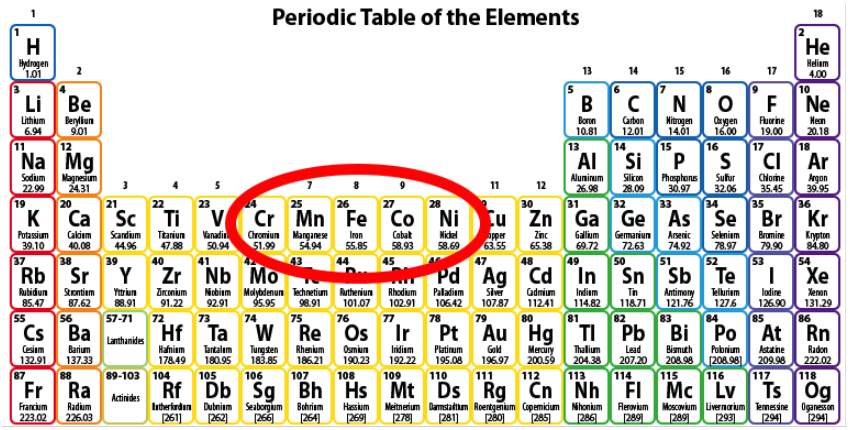
- NbMoTaW: predicted single-phase Heusler-like ground state[2].

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

Cantor Alloy & its Derivatives: Background

[3] Woodgate, Staunton, Phys. Rev. B **105** 115124 (2022). (Editors' Suggestion.)

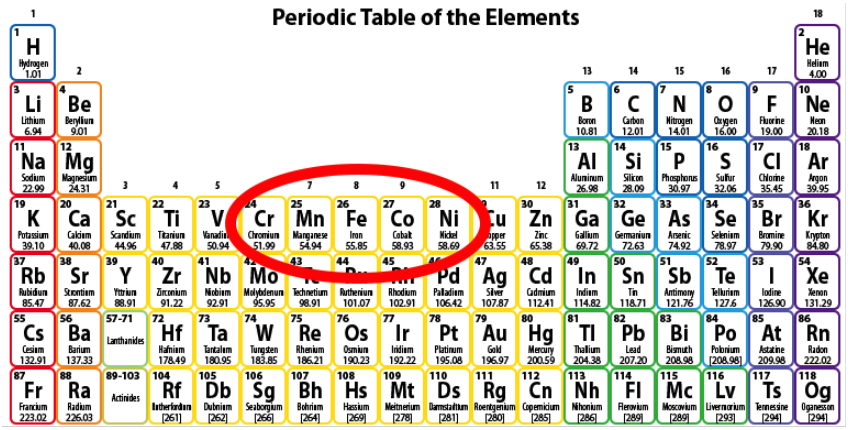
Cantor Alloy & its Derivatives: Background



[3] Woodgate, Staunton, Phys. Rev. B **105** 115124 (2022). (Editors' Suggestion.)

Cantor Alloy & its Derivatives: Background

- First synthesised by Cantor around 2004.
- Prototypical fcc high-entropy alloys.
- Experimentally observed atomic short-range order.



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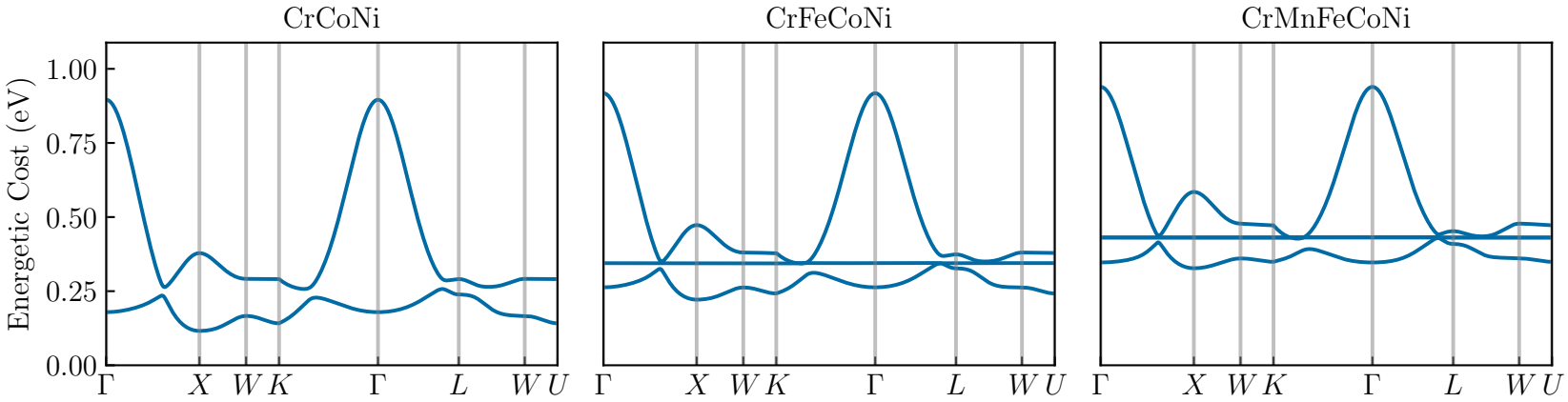
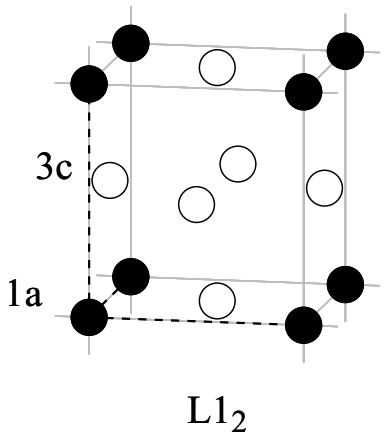
Cantor Alloy & its Derivatives: Chemical Stability Matrices





$L1_2$

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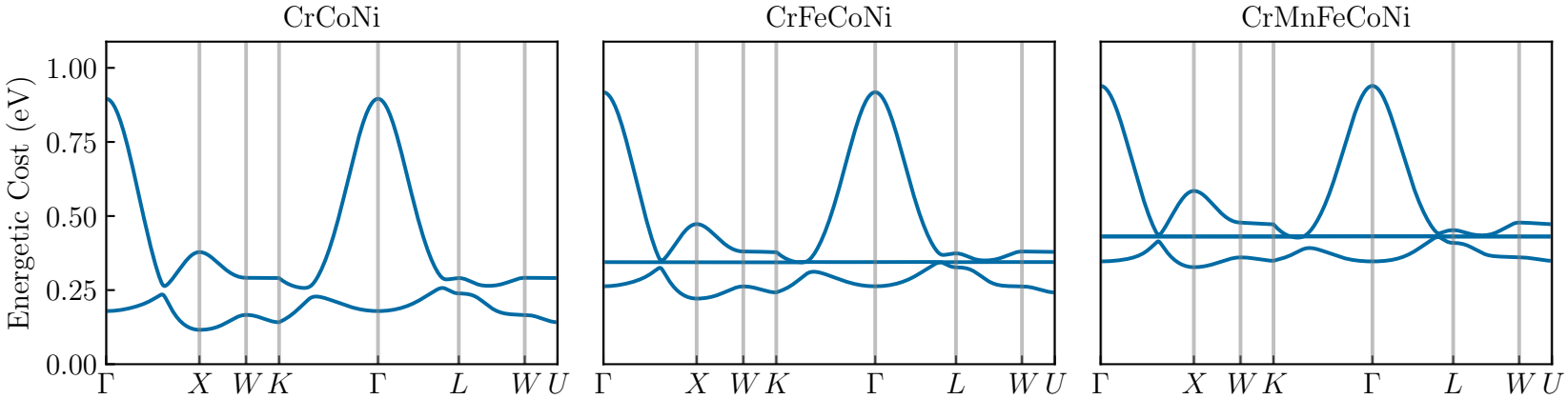
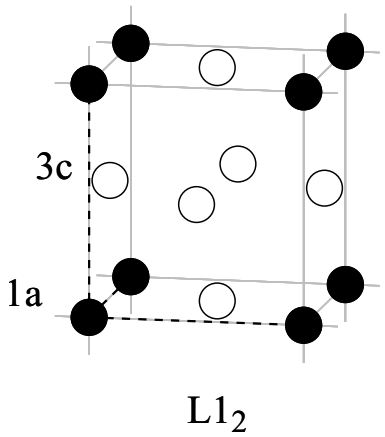


- $CrCoNi^3$: $T_{ord} = 606$ K.
- $CrFeCoNi^3$: $T_{ord} = 404$ K.
- $CrMnFeCoNi^3$: $T_{ord} = 281$ K.



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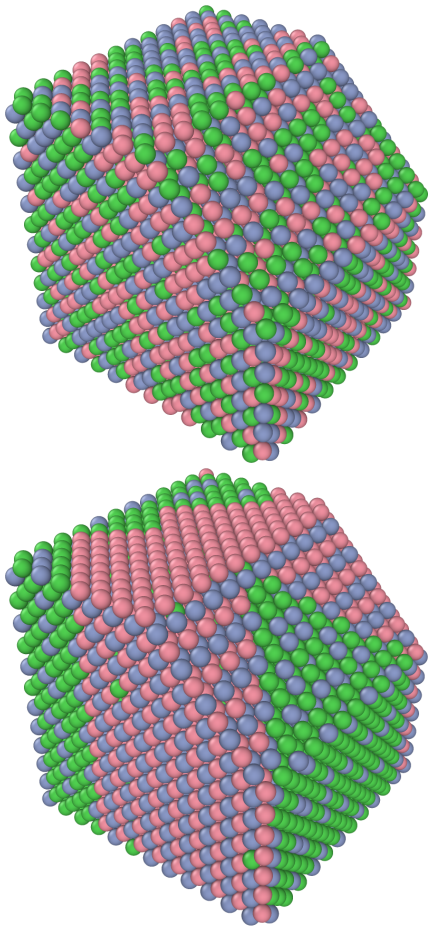
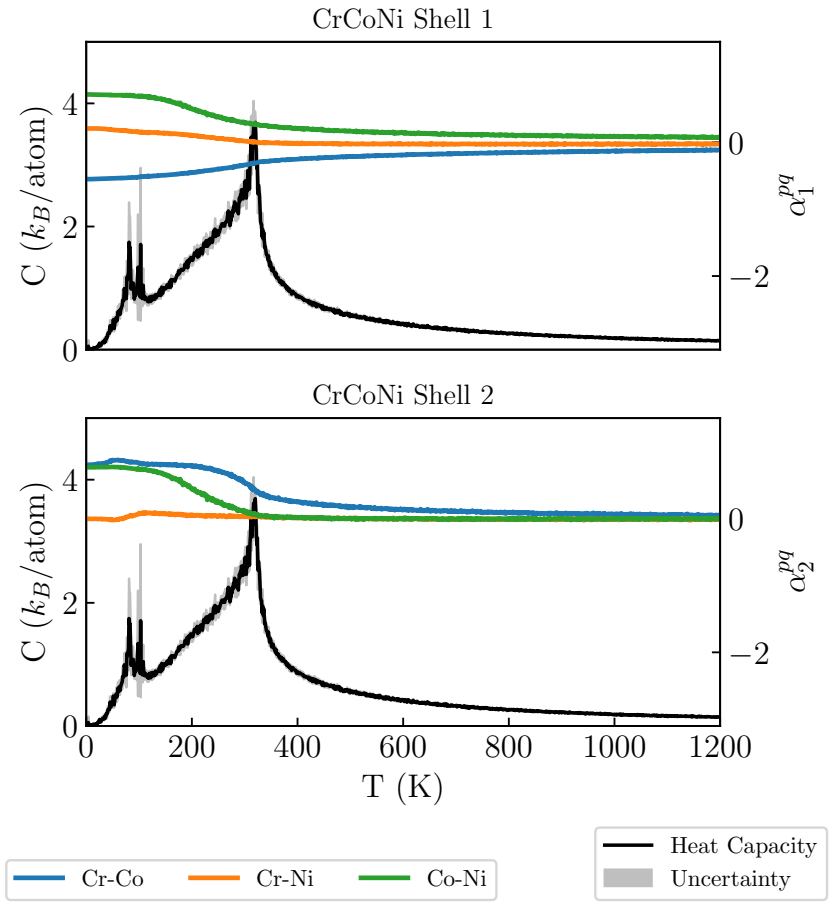
Cantor Alloy & its Derivatives: Atomistic Modelling





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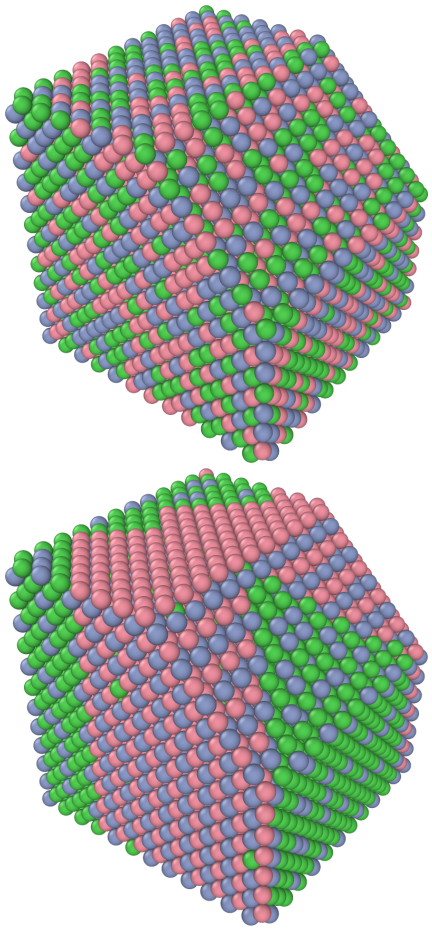
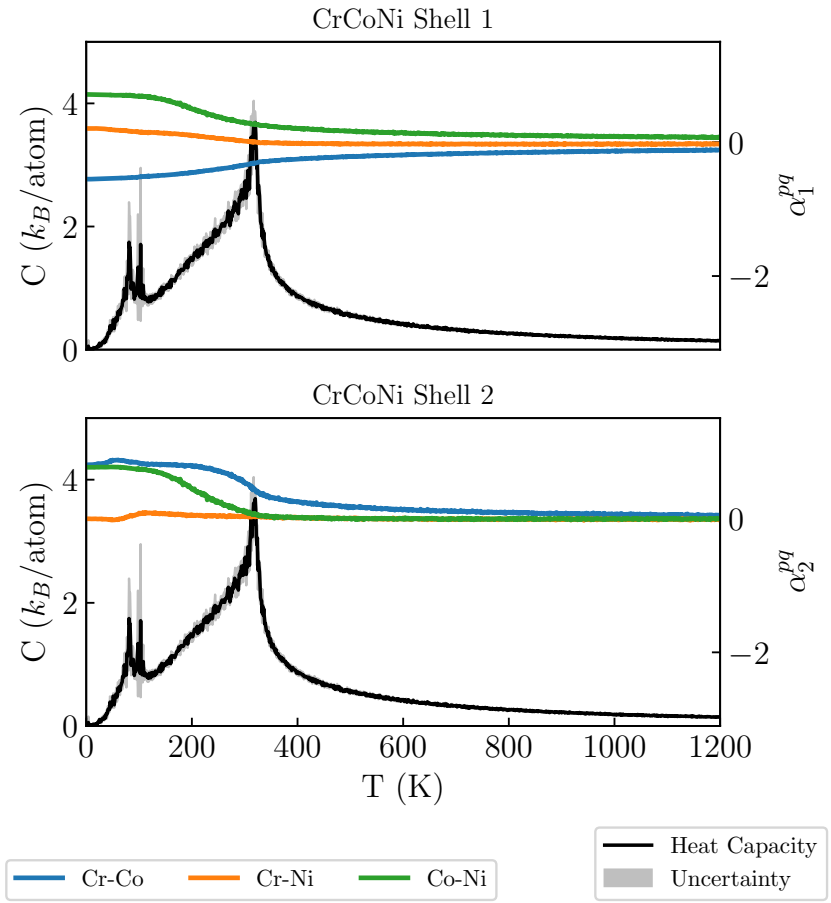
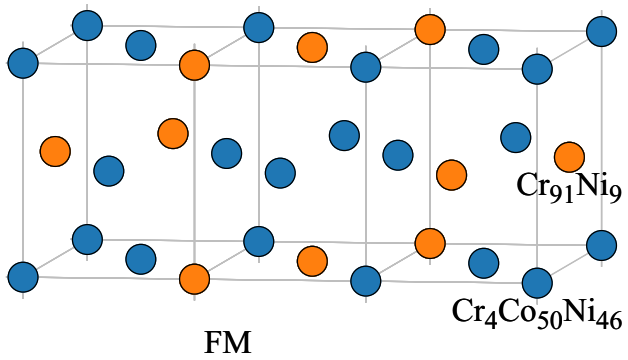


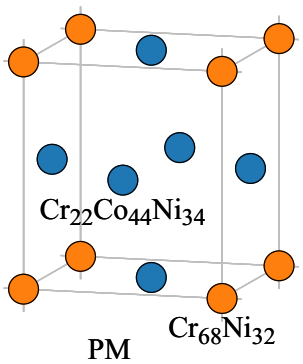


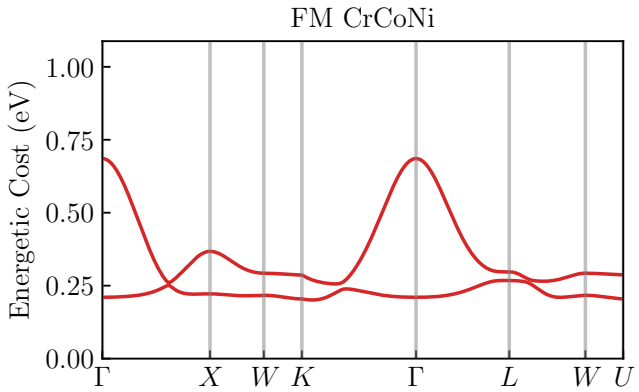
- No single-phase ground state[3].

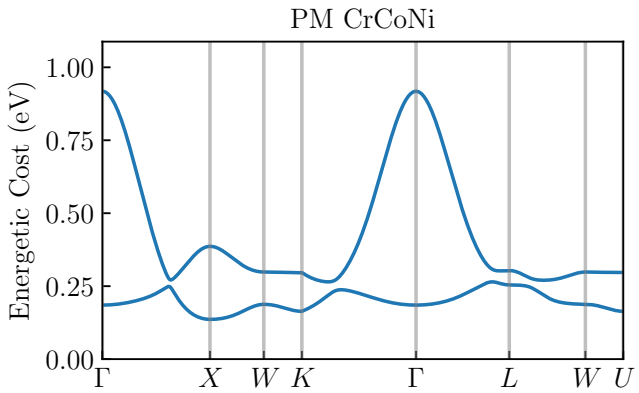
[3] Woodgate, Staunton, Phys. Rev. B **105** 115124 (2022). (Editors' Suggestion.)

Importance of the Magnetic State



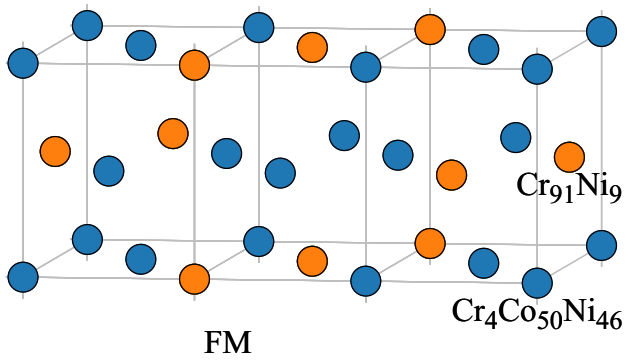


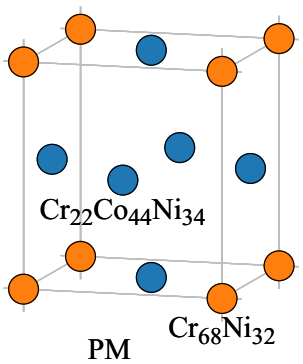


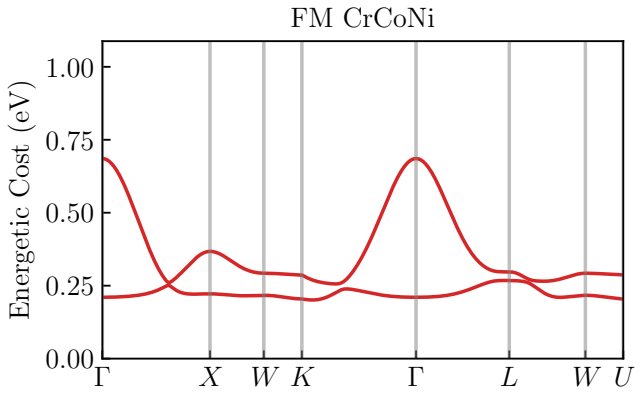


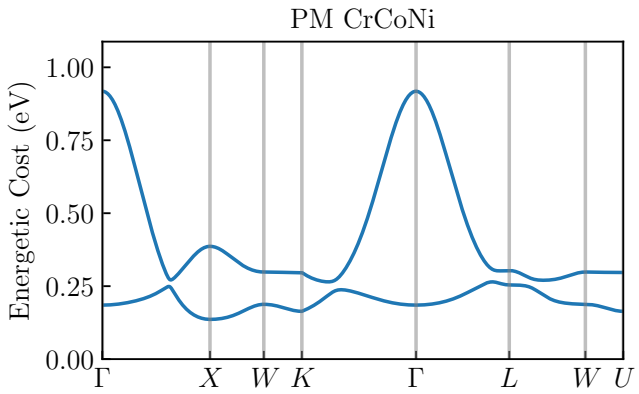
[4] Woodgate, Hedlund, Lewis, Staunton, Phys. Rev. Mater. **7** 053801 (2023)

Importance of the Magnetic State





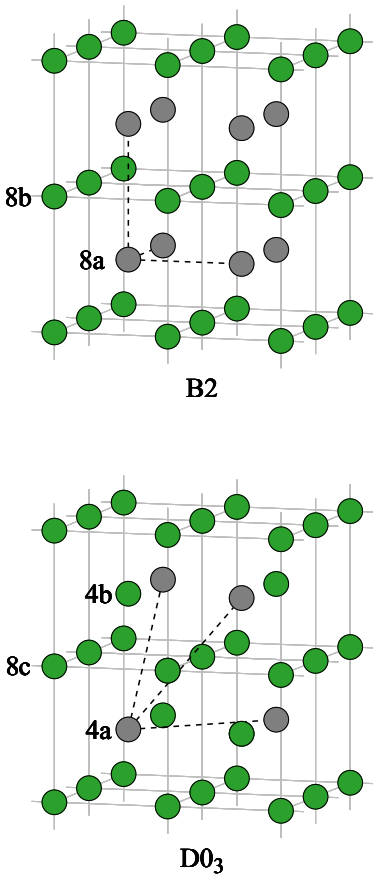


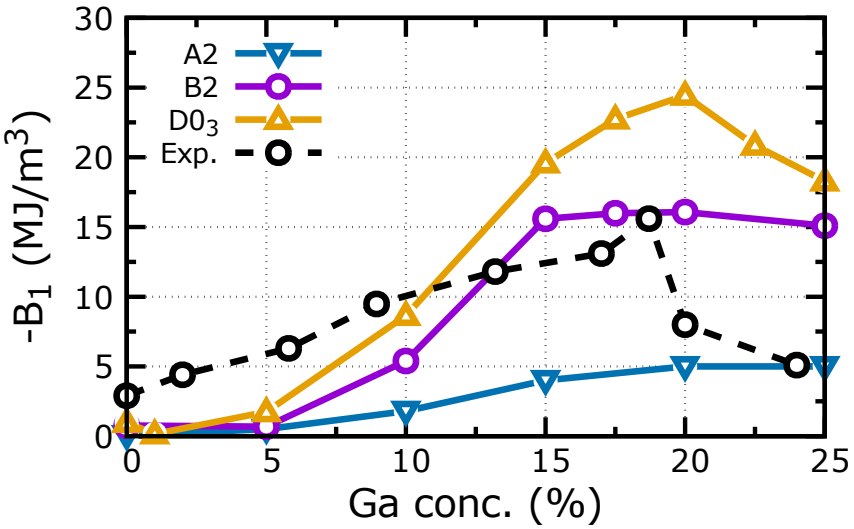


- Different magnetic state results in different orderings[4].

[4] Woodgate, Hedlund, Lewis, Staunton, Phys. Rev. Mater. **7** 053801 (2023)

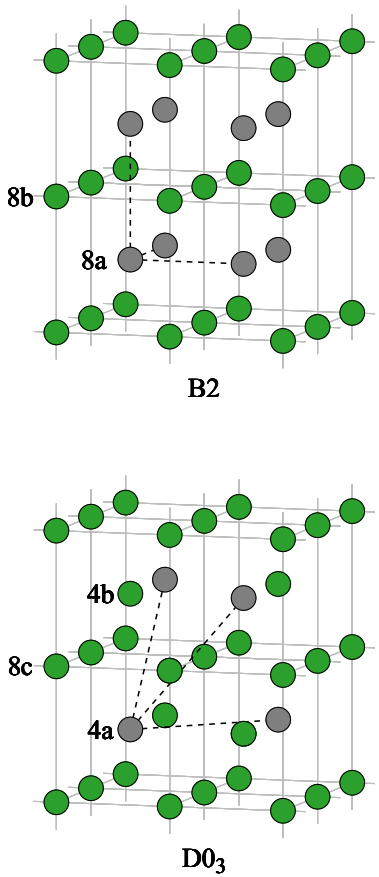
Impact of atomic arrangements on magnetic properties

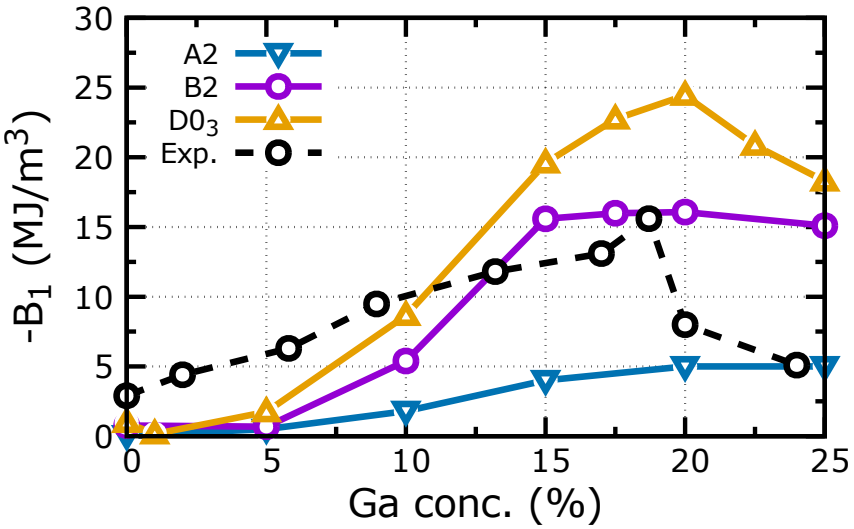




[5] Marchant, Woodgate, Patrick, Staunton, Phys. Rev. B **103**, 094414 (2021)

Impact of atomic arrangements on magnetic properties

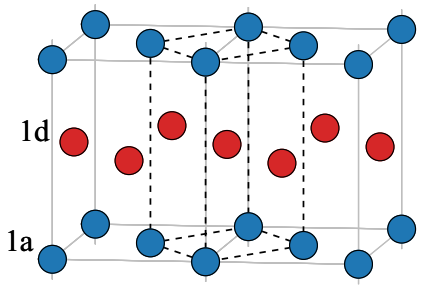


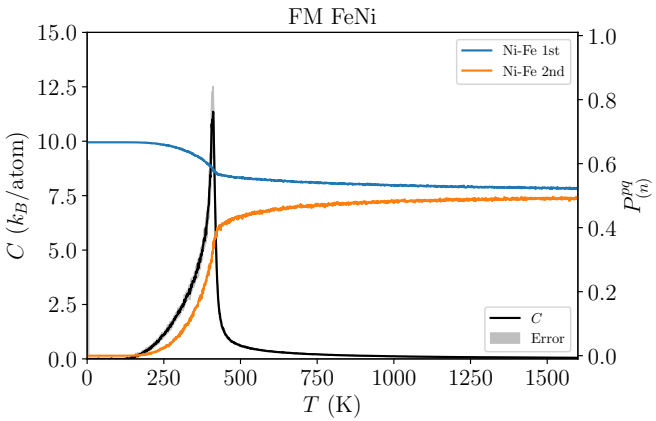


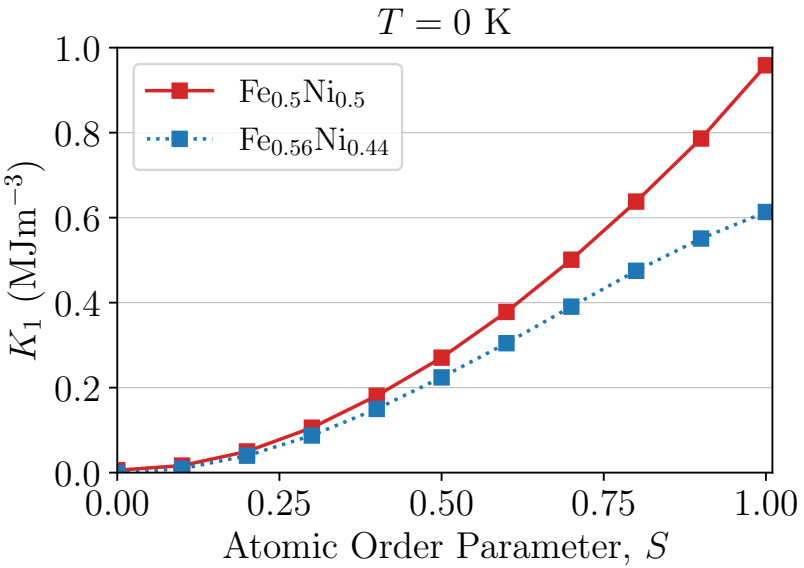
- Atomic ordering affects magnetostriction[5].

[5] Marchant, Woodgate, Patrick, Staunton, Phys. Rev. B **103**, 094414 (2021)

Impact of atomic arrangements on magnetic properties

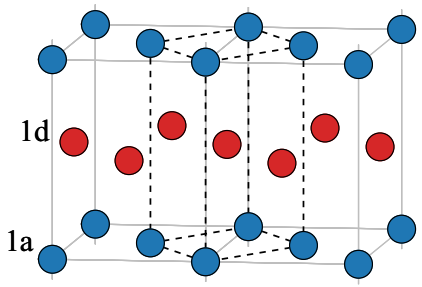


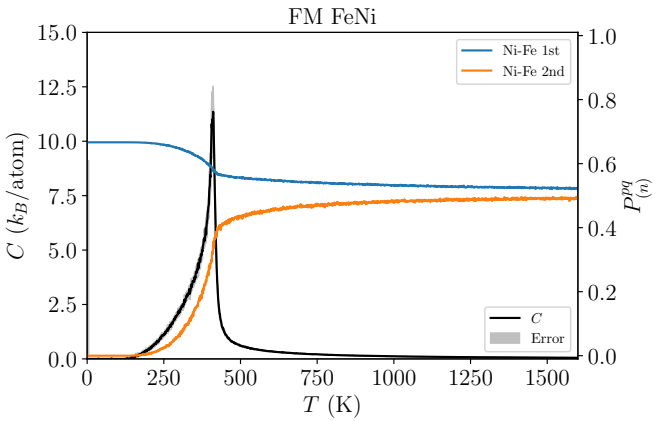


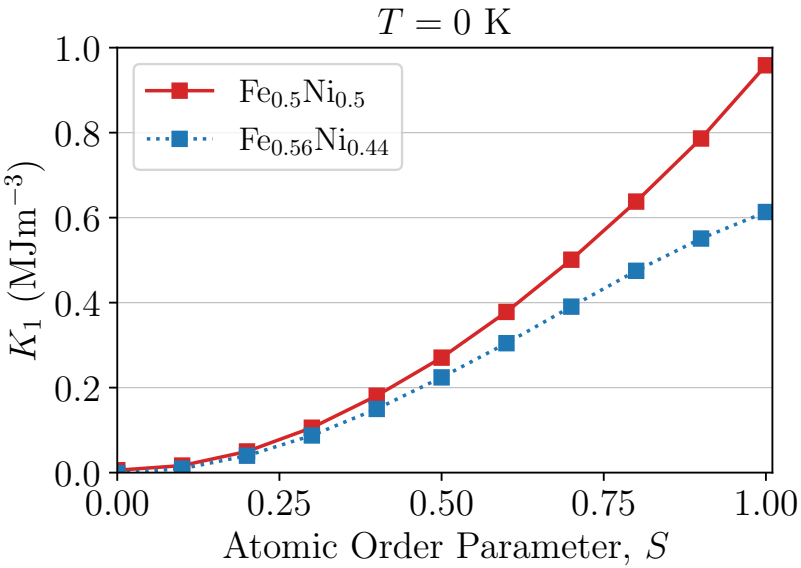


[6] Woodgate, Patrick, Lewis, Staunton, **arXiv:2307.15470**.
[7] Woodgate, Patrick, Lewis, Staunton, in preparation.

Impact of atomic arrangements on magnetic properties



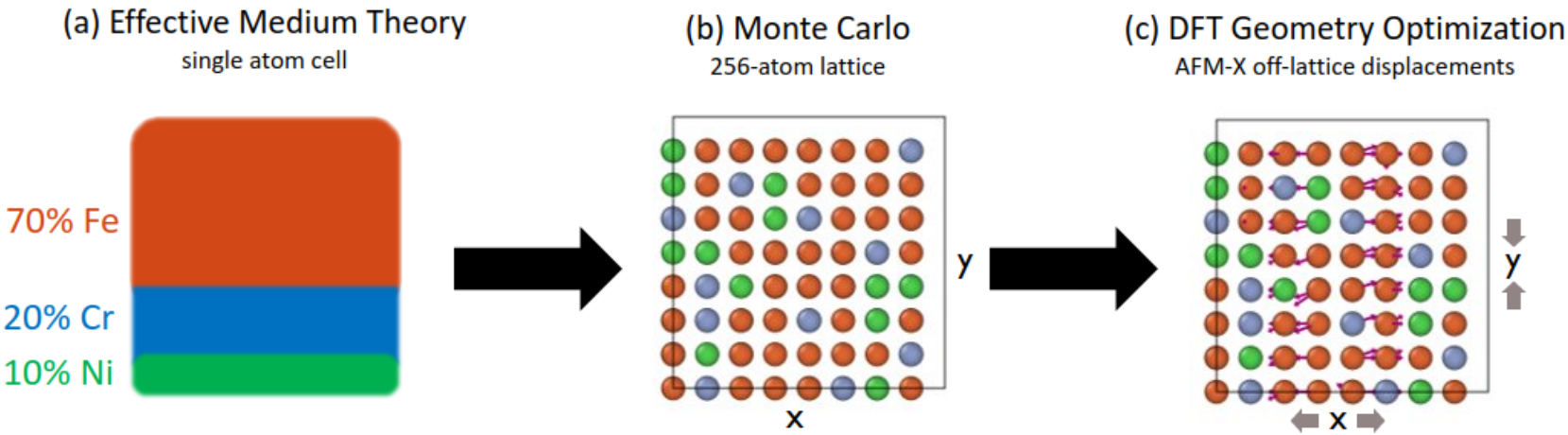




- Atomic ordering affects magnetic anisotropy[6,7].

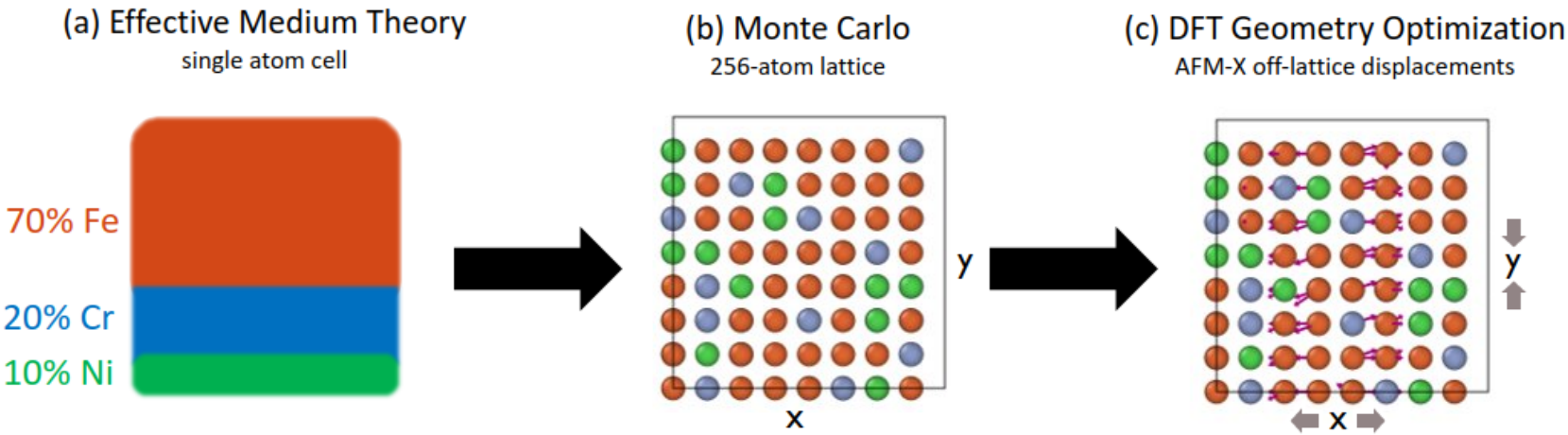
[6] Woodgate, Patrick, Lewis, Staunton, **arXiv:2307.15470**.
[7] Woodgate, Patrick, Lewis, Staunton, in preparation.

Feeding into Other Simulation Techniques



[5] Shenoy, Woodgate, *et al.*, **arXiv:2309.08689**.

Feeding into Other Simulation Techniques



- Can use physically motivated configurations in training data for machine-learned interatomic potentials[8].

[5] Shenoy, Woodgate, *et al.*, **arXiv:2309.08689**.

Next Steps and Future Work

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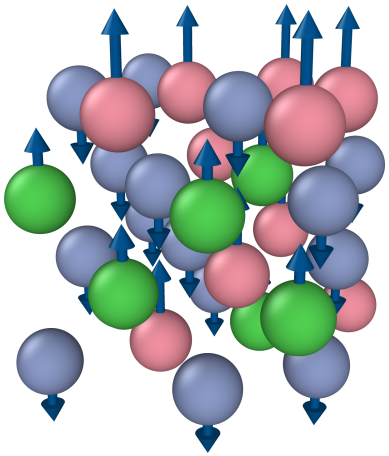
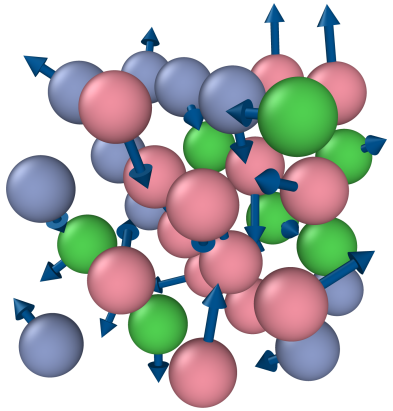
- Broaden approach to modelling general high-entropy oxides, carbides, etc.?.





Take-Home Messages

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Computationally efficient, DFT-based methodology predicts ordering and gives physical insight.

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Examples where atomic ordering impacts materials' magnetic properties.

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Interface with other techniques

Use physically motivated configurations in subsequent studies using other modelling techniques.

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