Maximal Disorder: Using the Coherent Potential Approximation to Study the Phase Behaviour of High-Entropy Alloys

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Abstract:
So-called 'high-entropy alloys' (HEAs)—those alloys containing four or more elements combined in near-equal ratios—are of interest for a range of next-generation engineering applications. Moreover, from a fundamental science perspective, they represent a fascinating but challenging class of materials to study. 'Fascinating' because the large entropy of mixing in such systems stabilises single-phase solid solutions containing combinations of elements which do not readily form binary alloys. 'Challenging' because the size of the phase space grows combinatorically with the number of chemical species considered, and because inclusion of elements at arbitrary concentrations frequently necessitates the use of comparatively large, computationally expensive, supercells in theoretical studies.

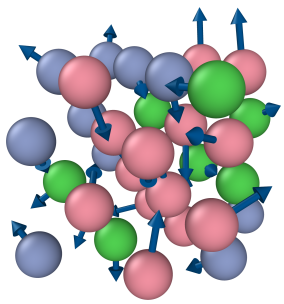

Figure 1: An illustration of the paramagnetic state of the 'medium-entropy' CrCoNi alloy.

In this talk, I will present results demonstrating that an old idea—the Coherent Potential Approximation (CPA)—combined with a new, perturbative approach developed for analysing the energetic cost of chemical fluctuations in multicomponent alloys [1-5], can provide a computationally inexpensive and physically insightful method for examining the phase stability of these complex systems. I will present results from case studies on a range of prototypical high-entropy alloys demonstrating that the approach successfully captures the phase behaviour of these systems, as well as providing fundamental physical insight into the electronic (and occasionally magnetic [3]) origins of atomic ordering tendencies.

References:
[1] Woodgate, Staunton, Phys. Rev. B **105**, 115124 (2022).
[2] Woodgate, Staunton, Phys. Rev. Mater. **7**, 013801 (2023).
[3] Woodgate, Hedlund, Lewis, Staunton, Phys. Rev. Materials **7**, 053801 (2023).
[4] Woodgate, Staunton, J. Appl. Phys. **135**, 135106 (2024).
[5] Woodgate, Marchant, Pártay, Staunton, arXiv: 2404.13173.

Biography:
Chris gained his PhD from the University of Warwick (UK), the same institution as that at which he is currently a Research Fellow in the Department of Physics. His research focusses on computational modelling of the physics of alloys and magnetic systems. Outside of research, Chris finds time to practice the sport of archery and the hobby of English-style change ringing.