Concentration waves in high-entropy alloys: Probing the (meta)stability of complex solid solutions within a DFT-based modelling framework

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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 not only because they are well-suited to a range of next-generation engineering applications, but also because they exhibit a range of interesting physical phenomena, including Fermi surface smearing, quantum critical behaviour, and superconductivity. From the perspective of theory and simulation, they represent a fascinating but challenging class of materials to study due to their chemical complexity and the huge space of potential compositions and atomic configurations.

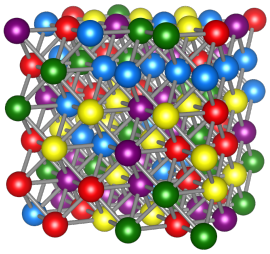

Figure 1:Figure 1: An indicative disordered configuration of a 5-component HEA.

In this talk, I will outline a new modelling approach [1-5] for studying the phase stability of these systems, which is based on representing atomic-scale chemical fluctuations as 'concentration waves' describing a range of potential ordered structures. By assessing the energetic costs of these fluctuations using density functional theory (DFT) calculations, it is possible to infer phase transitions directly, as well as to recover atomistic models suitable for further computational investigation. I will present results from case studies on a range of canonical high-entropy alloys, demonstrating that the approach 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. I will endeavour to keep the talk accessible to a broad audience and make links to experiment where appropriate.

References:

[1] C. D. Woodgate, J. B. Staunton, Phys. Rev. B **105**, 115124 (2022).
[2] C. D. Woodgate, J. B. Staunton, Phys. Rev. Mater. **7**, 013801 (2023).
[3] C. D. Woodgate, D. Hedlund, L. H. Lewis, J. B. Staunton, Phys. Rev. Materials **7**, 053801 (2023).
[4] C. D. Woodgate, J. B. Staunton, J. Appl. Phys. **135**, 135106 (2024).
[5] C. D. Woodgate, G. A. Marchant, L. B. Pártay, J. B. Staunton, npj Comput. Mater. **10**, 271 (2024).

Biography:
Chris received his PhD from the University of Warwick, where he also spent a short period as a postdoctoral researcher, before moving to the University of Bristol to take up an EPSRC Doctoral Prize Fellowship. 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.