Addressing Disorder: Modelling Alloys and Magnetic Materials Across Length Scales

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Abstract:
It is exceedingly rare for real-world materials to be as pristine as those considered in the examples to be found in the pages of our undergraduate textbooks. Indeed, a wide range of technologically relevant materials contain a degree of 'disorder' of some kind. Examples include *glasses*, where there is no well-defined underlying crystal lattice; *alloys*, where atoms of different chemical identities occupy lattice sites at random; and *magnetic materials*, where the effects of finite temperature cause magnetic moments first to 'wobble' and then to disorder entirely as a material enters its paramagnetic phase. It is crucial that modelling techniques are developed which can accurately simulate such disordered materials and provide insight into experimental studies.

In this talk, I will discuss means by which chemical and magnetic disorder can be studied computationally at the sub-atomic and atomic length scales via application of density functional theory (DFT) calculations, interatomic potentials, and machine learning techniques. Through application of methods from statistical physics, I will then demonstrate how it is then possible to extract quantities such as alloy disorder-order transitions and materials' magnetic critical temperatures—quantities which can be studied by experimental collaborators in a laboratory setting. Example applications will include structural materials [1], high-entropy alloys [2], and rare-earth-free permanent magnets [3, 4].

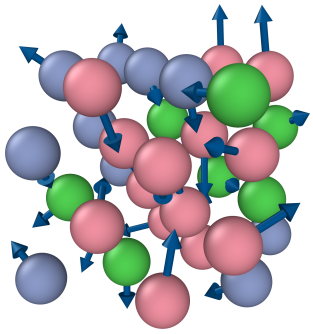

Figure 1: Visualisation of the paramagnetic state of an alloy, where both compositional and magnetic disorder are present.

References:
[1] Shenoy, Woodgate, Staunton, *et al.*, Phys. Rev. Materials **8**, 033804 (2024).
[2] Woodgate, Hedlund, Lewis, Staunton, Phys. Rev. Materials **7**, 053801 (2023).
[3] Woodgate, Patrick, Lewis, Staunton, J. Appl. Phys. **135**, 163905 (2023).
[4] Woodgate, Lewis, Staunton, npj Comput. Mater. **10**, 272 (2024).

Biography:
Chris gained his PhD from the University of Warwick (UK), where he worked on developing modelling techniques for studying alloy phase behaviour. He stayed on at Warwick for a short postdoctoral position, before moving to the University of Bristol to take up an EPSRC Doctoral Prize Fellowship. His research focusses on modelling the physics of alloys and magnetic systems, with extensive experimental collaboration. Outside of research, Chris finds time to practice the sport of archery and the hobby of English-style change ringing.