
Warwick Centre for Predictive Modelling Seminar Series

# Density functional theory and slowly varying fluctuations at finite temperature to describe alloy and magnetic phase diagrams

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**Abstract:** Density functional theory (DFT) is extensively used in ab-initio materials modelling. This can be extended by identifying different time scales amongst the collective electronic degrees of freedom. For example, it shows how relatively slowly fluctuating local moments can emerge from the interacting electrons of many materials. Such entities have rigid magnitudes and fluctuate their orientations from atomic site to atomic site on a timescale long compared to other electronic times.[1]. Averaging over these `local moment' degrees of freedom provides a quantitative description of the type and onset of magnetic order, high temperature paramagnetic phases and indeed magnetic phase diagrams[2,3]. We illustrate this disordered local moment (DLM) theory with recent work on transition metal and rare earth materials which have a broad range of applications as strong magnets, in high density magnetic recording and magnetic refrigeration. Fluctuating moments do not appear to establish naturally over such small regions for some other materials. We show how the DFT-DLM theory can be extended to these materials with the use of an effective cluster medium approach (the nonlocal Coherent Potential Approximation, NLCPA) to allow for more extensive, slow magnetic fluctuations[4]. The same technique can be adapted to order-disorder phenomena in alloys[5]. In the latter part of this talk I would like to begin the discussion with colleagues in the Predictive Modelling Centre on how to develop this further for ab-initio DFT-based descriptions of short- and long-range order in alloys and alloy phase diagrams.
[1] B.L.Gyorffy et al., J. Phys. F: Met. Phys. 15, 1337 (1985); [2] I.D. Hughes et al., Nature, 446, 650, (2007); [3] J.B. Staunton et al., Phys. Rev. B 89, 054427, (2014); [4]J.B. Staunton et al., J.Phys. Cond.Matt.:26, 274210, (2014):[5]D.A. Rowlands et al., Phys. Rev. B 73, 165122, (2006)

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