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Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

Tuesday, 10 May 2022, 9:00 s.t., TU Darmstadt, Zoom

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Computational modelling of the physics of rare earth - transition metal permanent magnets

Abstract:

With the drive towards more energy efficient technologies, renewable energy supplies and further miniaturisation of devices, there is an urgent demand for stronger and cheaper magnetic materials. Most strong magnets contain both rare earth (RE) and transition metal (TM) elements and in this talk I will describe recently developed *ab initio* modelling to understand intrinsic magnetic properties. Each RE atom in the magnet has a magnetic moment which is set up by its nearly localised f-electrons. These moments are immersed in a glue of septillions of valence electrons coming from all the RE and TM atoms. Local magnetic moments associated with the TM atoms can also emerge from this complex electron fluid. The magnetic properties stem from how the RE and TM local moments affect and are affected by each other and the electron glue, on how the atoms are arranged and on the overall response to applied fields. I will discuss how the *ab initio* Density Functional Theory-based Disordered Local Moment theory [1] provides a parameter-free accurate account of the valence electrons and incorporates the effects of the fluctuating local moments by averaging over them so that temperature dependent effects can be described [2, 3]. Case studies will be outlined:- the RE-Co5 permanent magnet class [3], magneto-strictive FeGa (Galfenol) [4] and Tb/DyFe2 (Terfenol) [5] and the ubiquitous Nd2Fe14B magnet. The same interacting electrons which underpin the magnetism of a material are also responsible for determining the arrangements of its atoms. In the latter part of the talk, I will discuss how we are integrating our modelling of field- and temperature-dependent magnetic properties *ab initio* with compositional determination in multicomponent materials. I will illustrate the approach with our recent work on the prototypical high entropy alloy, NiCoFeMnCr, and its derivatives [6].

[1] B. L. Gyorffy et al., (1985), https://0-doi-org.pugwash.lib.warwick.ac.uk/10.1088/0305-4608/15/6/018
[2] E. Mendive-Tapia and J. B. Staunton, (2019), https://doi.org/10.1103/PhysRevB.99.144424
[3] C. E. Patrick and J. B. Staunton, (2019) https://doi.org/10.1103/PhysRevMaterials.3.101401
[4] G. A. Marchant et al., (2021), https://doi.org/10.1103/PhysRevB.103.094414
[5] C. E. Patrick et al. (2020), https://doi.org/10.1103/PhysRevApplied.14.01409
[6] C. D. Woodgate and J. B. Staunton, Phys. Rev. B, (2022), in press "*Compositional order in the mediumentropy and high-entropy Cantor-Wu alloys via ab initio theory and atomistic modelling*".

About the speaker:

Julie Staunton is a full professor at the Department of Physics, University of Warwick in the U.K. and heads its Theoretical Physics Group which has a strong tradition in materials modelling and collaborates extensively with experimental groups working on both hard condensed matter and bio-/soft matter. Her own research interests are in magnetic materials modelling and alloy physics, using a combination of theoretical techniques including *ab initio* simulations that require high performance computing. She leads the integrated theory-experiment PRETAMAG (Physics of Rare Earth -Transition metAl MAGnets) project where the predictive, *ab initio* computational model for rare earth - transition metal magnets, discussed in this talk, are tested by magnetic measurements on single crystal and powdered samples. She is also the inaugural Director of the Centre for Doctoral Training in Modelling of Heterogeneous Systems (HetSys) at Warwick which recruits students from across the physical sciences, mathematics and engineering to develop computational materials modelling skills and tackle a wide range of projects in quantum, atomistic and continuum research themes.