Understanding permanent magnets through first-principles calculations: progress and challenges

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First-principles calculations, particularly those based on density-functional theory, are extremely popular across a wide range of materials science research areas. Whilst improvements in computer power have allowed researchers to tackle increasingly complex systems with these techniques, it remains the case that the calculations are usually performed on highly idealized models. With this in mind, it is natural to ask to what extent such calculations can be used to interpret experimental measurements made on real samples. Here I will attempt to answer this question in the case of permanent magnets by describing some research performed as part of the joint computational/experimental "PRETAMAG" project [1]. In particular I will present examples comparing calculations and experiment for magnetization curves [2], torque magnetometry [3], spin reorientation transition temperatures [4] and phase diagrams. I will then discuss to what extent the available techniques might be hoped to understand the performance of commercial permanent magnets.

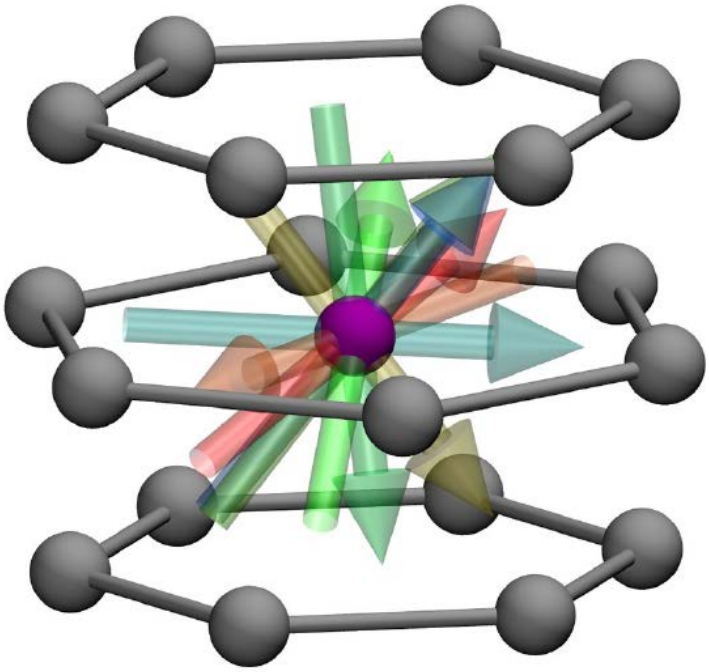

Fig. 1. Schematic representation of the finite temperature local moment disorder in RCo5

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[2] C E Patrick, S Kumar, G Balakrishnan, R S Edwards, M R Lees, L Petit, and J B Staunton, Phys. Rev. Lett. 120, 097202 (2018)

[3] S Kumar *et al.,* submitted (2019)

[4] C E Patrick and J B Staunton, Phys. Rev. Materials 3, 101401 (2019)