The complex magnetism of lanthanide intermetallics: ab-initio disordered local moment theory

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The Density Functional Theory (DFT)-based 'disordered local moment' (DLM) picture for magnetism at finite temperatures shows how relatively slowly fluctuating local moments can emerge from the interacting electrons of many materials [1,2]. With a suitable description of the f-electron states, this is a good model for rare earth magnets providing a quantitative description of magnetic ordering and magnetic phase diagrams as demonstrated in an application to gadolinium and the other heavy rare earth elements [3]. We show an ab-initio theory of magnetocaloric effect (MCE) and results for gadolinium [4]. We explore an apparently simple prototypical class of lanthanide magnets (GdZn, GdCd and GdMg) with rich, complex and diverse magnetism. We explain why GdZn and GdCd are simple ferromagnets and predict a remarkably large increase of Curie temperature with pressure for GdCd which has been confirmed experimentally [5]. Moreover we find the origin of a ferromagnetic-antiferromagnetic competition in GdMg manifested by non-collinear, canted magnetic order at low temperatures. Replacing 35% of the Mg atoms with Zn removes this transition in excellent agreement with longstanding experimental data [5].

[1] B.L. Gyorffy et al.,J. Phys. F Met. Phys. **15**,1337, (1985).

[2] J.B. Staunton et al., Phys Rev B **89**,054427, (2014).

[3] I.D. Hughes et al., Nature, **446**, 650, (2007).

[4] J.B. Staunton et al., J. Phys. Condens. Matter **26**,274210, (2014).

[5] L. Petit et al., Phys. Rev. Lett. **115**, 207201, (2015).