Magnetic ordering and magnetic interactions in rare earth materials described by an ab-initio electronic structure theory

J.B. Staunton¹, L. Petit², R. Banerjee¹, M. Lueders², Z. Szotek², D. Paudyal³, Y. Mudryk³, V.K. Pecharsky⁴, K.A. Gschneidner Jr.⁴

1) University of Warwick, Coventry CV4 7AL, U.K.
2) Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K.
4) The Ames Laboratory, U.S. Department of Energy and Department of Materials Science and Engineering, Iowa State University, Ames, Iowa 50011-3020, U.S.A.

Corresponding author: Julie Staunton (J.B.Staunton@warwick.ac.uk)

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. 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 [1]. We demonstrate the approach with an ab-initio theory of magnetocaloric effect (MCE) and results for gadolinium [2]. Finally 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 [3]. 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 [3].