Ab-Initio Calculation of Magnetic Anisotropy in Transition Metal Compounds: Correlation Effects

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1 Long-term Research Objective

Provide a working methods for predicting materials properties from first principles, with particular emphasis in materials where the correlations are strong. Explain this idea why it may be useful.

2 ST Objectives

3 Approach

Describe what I am doing. Including spin orbit coupling in DMFT equations. Formulating the magnetic anisotropy as a response quantity.

4 S&T Completed

5 Impact /Navy Relevance

why the navy might care.

6 planned reserach efforts

7 Other Sponsored Science and Technology

1) Petroleum Reserach Fund. 2) NSF 3) DOE

8 reference