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LDA+DMFT Approach to Magnetocrystalline Anisotropy of Strong Magnets[1] JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, MARC JANOSCHEK, Los Alamos National Laboratory Los Alamos, New Mexico 87545, USA, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, FILIP RONNING, J.D. THOMPSON, MICHAEL A. TORREZ, ERIC D. BAUER, CRISTIAN D. BATISTA, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — The new challenges posed by the need of finding strong rare-earth-free magnets demand methods that can predict magnetization and magnetocrystalline anisotropy energy (MAE). We argue that correlated electron effects, which are normally underestimated in band structure calculations, play a crucial role in the development of the orbital component of the magnetic moments. Because magnetic anisotropy arises from this orbital component, the ability to include correlation effects has profound consequences on our predictive power of the MAE of strong magnets. Here we show [1] that incorporating the local effects of electronic correlations with dynamical mean-field theory provides reliable estimates of the orbital moment, the mass enhancement and the MAE of YCo_5.

[1] J.-X. Zhu *et al., Phys. Rev. X* **4**, *021027 (2014).*

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