Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Correlations, spin-charge separation, and magnetic anisotropy** RALPH SKOMSKI, PRIYANKA MANCHANDA, Department of Physics and Astronomy and NCMN, University of Nebraska, Lincoln, NE 68588 — Much of the physics of condensed matter reflects electron-electron correlations. On an independent-electron level, correlations are described by a single Slater determinant with broken spin symmetry. This approach includes Hund's rule correlations as well the LSDA and LSDA+U approximations to density-functional theory (DFT). However, from Kondo and heavy-fermion systems it is known that the independent-electron approach fails to describe spin-charge separation in strongly correlated systems, necessitating the use of two or more Slater determinants. Using first-principle and model calculations, we show that spin-charge separation strongly affects the leading rare-earth anisotropy contribution in top-end permanent magnet materials such as $Nd_2Fe_{14}B$ and $SmCo_5$. Explicit correlation results are obtained for two limiting cases. First, we derive the density functional for tripositive rare-earth ions in a Bethe-type crystal field. The potential looks very different from the LSDA(+U) potentials, including gradient corrections. Second, we use a simple model to show that Kondo-type spin-charge separation yield a rare-earth anisotropy contribution absent in the independent-electron approach. This research is supported by DOE (DE-FG02-04ER46152).

Ralph Skomski
Department of Physics and Astronomy and NCMN,
University of Nebraska, Lincoln, NE 68588

Date submitted: 14 Nov 2014 Electronic form version 1.4