Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Transverse spin gradient functional for non-collinear Spin Density Functional Theory[1] F.G. EICH[2], G. VIGNALE, Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211, USA, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany — The ab-initio description of non-collinear magnetism is essential for the search of new materials suitable for the construction of spintronic devices. We present a novel functional explicitly constructed for the description of non-collinear magnetism. It is formulated in terms of a Spin Gradient Extension (SGE) to the Local Spin Density Approximation, which introduces a dependence on the transverse gradients of the spin magnetization. While collinear Generalized Gradient Approximations provide a dependence on longitudinal spin gradients the SGE takes into account that longitudinal and transverse variations of the spin magnetization affect the energy differently. The explicit dependence on the transverse gradients is obtained from a reference systems which exhibits non-collinearity, i.e., the spin-spiral-wave state of the uniform electron gas. The inclusion of transverse spin gradients yields exchange-correlation magnetic fields that are non-collinear w.r.t. the spin magnetization. This implies that the spin-current density of the Kohn-Sham system does not vanish even if no external magnetic field is applied. As an example we present the application of the SGE to the non-collinear 120°-Néel state of a Chromium mono-layer.

[1]F.G.E. is supported by DOE grant No. DE-FG02-05ER46203
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Date submitted: 12 Nov 2012 Electronic form version 1.4