Analysis of over-magnetization of elemental transition metal solids from the SCAN and related density functionals

Daniel Mejía-Rodríguez & Sam Trickey
University of Florida
Quantum Theory Project

APS March Meeting 2020
Denver, CO
DFT for matter under extreme conditions

Sam Trickey, Jim Dufty
Daniel Mejía-Rodríguez, Jeff Wrighton

Funding Acknowledgments:
US DOE Grant DE-SC0002139
US DOE Grant DE-SC0019330

Software & Publications:
http://qtp.ufl.edu/ofdft
SCAN over-magnetization

- Isaacs & Wolverton [PRM 2, 063801 (2018)]
- Jana et al. [JCP 149, 044120 (2018)]
- Romero & Verstraete [EPJB 91, 193 (2018)]
- Ekholm et al. [PRB 98, 094413 (2018)]
- Fu & Singh [PRL 121, 207201 (2018)]

BCC Fe fixed-spin moment curves
Mejia-Rodriguez & Trickey [PRB 100, 41113(R) (2019)]
SCAN over-magnetization

Ekholm et al. [PRB 98 094413 (2019)]

Fu & Singh [PRB 100, 045126 (2019)]
SCAN over-magnetization

Fu & Singh [PRB 100, 045126 (2019)]
SCAN over-magnetization

Zhang et al. [arXiv:1906.06467v2 (2019)]
SCAN XC energy functional

SCAN
Sun, Ruzsinszky, & Perdew

\textbf{PRL 115, 036402 (2015)}

\begin{equation}
F_x(p, \alpha) = \left( h_x^1(p, \alpha) + f_x(\alpha) \left[ 1.174 - h_x^1(p, \alpha) \right] \right) g_x(p)
\end{equation}

\begin{align*}
g_x(p) &= 1 - e^{-\alpha_1 p^{-1/4}} \\
h_x^1(p, \alpha) &= 1 + k_1 - \frac{k_1}{1 + x(p, \alpha)/k_1} \\
f_x(\alpha) &= \theta(1 - \alpha) e^{-\alpha_1 \alpha/(1 - \alpha)} - d_x \theta(\alpha - 1) e^{-\alpha_2 \alpha/(\alpha - 1)}
\end{align*}

\begin{align*}
p(n, \nabla n) &= \frac{|\nabla n|^2}{4(3\pi^2)^{2/3} n^{8/3}} \\
\alpha(n, \nabla n, \tau) &= \frac{\tau - \tau^{vW}}{\tau^{TF}} \\
\tau &= \frac{1}{2} \sum_i f_i |\nabla \phi_i|^2
\end{align*}
SCAN & SCAN-L XC energy functionals

SCAN
Sun, Ruzsinszky, & Perdew


\[ \alpha(n, \nabla n, \tau) \equiv \frac{\tau - \tau^{vW}}{\tau_{TF}} \]

SCAN-L
Mejía-Rodríguez & Trickey

*PRA* **96**, 052512 (2017)

\[ \alpha_L(n, \nabla n, \nabla^2 n) \equiv \frac{\tau^{PC_{opt}}(n, \nabla n, \nabla^2 n) - \tau^{vW}}{\tau_{TF}} \]
SCAN & SCAN-L XC energy functionals

**Stretched H$_2^+$**

![Graph showing binding energy vs. internuclear distance for H$_2^+$ with different functionals (HF, PBE, SCAN, SCAN-L).](image)

**Fractional Charge Error Mn (3+, 2+, 1+)**

![Graph showing deviation from linear segment for Mn states (3d$^1$, 3d$^5$, 3d$^5$4s$^1$) with different functionals (PBE, SCAN, SCAN-L).](image)
SCAN & SCAN-L XC energy functionals

MnO AFM density difference (VASP)
SCAN over-magnetization

- Isaacs & Wolverton [PRM 2, 063801 (2018)]
- Jana et al. [JCP 149, 044120 (2018)]
- Romero & Verstraete [EPJB 91, 193 (2018)]
- Ekholm et al. [PRB 98, 094413 (2018)]
- Fu & Singh [PRL 121, 207201 (2018)]

BCC Fe fixed-spin moment curves
Mejia-Rodriguez & Trickey [PRB 100, 41113(R) (2019)]
SCAN in BCC Fe

\[ f_x(\alpha) = \theta(1 - \alpha)e^{-c_1x\alpha/(1-\alpha)} - d_x \theta(\alpha - 1)e^{-c_2x/\alpha-1} \]

Angularly averaged switching function

Angularly averaged enhancement factor
SCAN in BCC Fe

\[ f_x(\alpha) = \theta(1-\alpha) e^{-c_1 x/\alpha(1-\alpha)} - d_x \theta(\alpha - 1) e^{-c_2 x/(\alpha-1)} \]
SCAN, SCAN-L & PBE DOS in BCC Fe
Summary

The SCAN-L enhancement factor is close enough to the original one, the only difference being the representation of the iso-orbital indicator.

The differences between the original and deorbitalized iso-orbital indicators correct, serendipitously, the erroneous over-magnetization predicted by SCAN.

The origin of the over-magnetization was traced back to the so-called switching function.