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

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DFT for matter under extreme conditions

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

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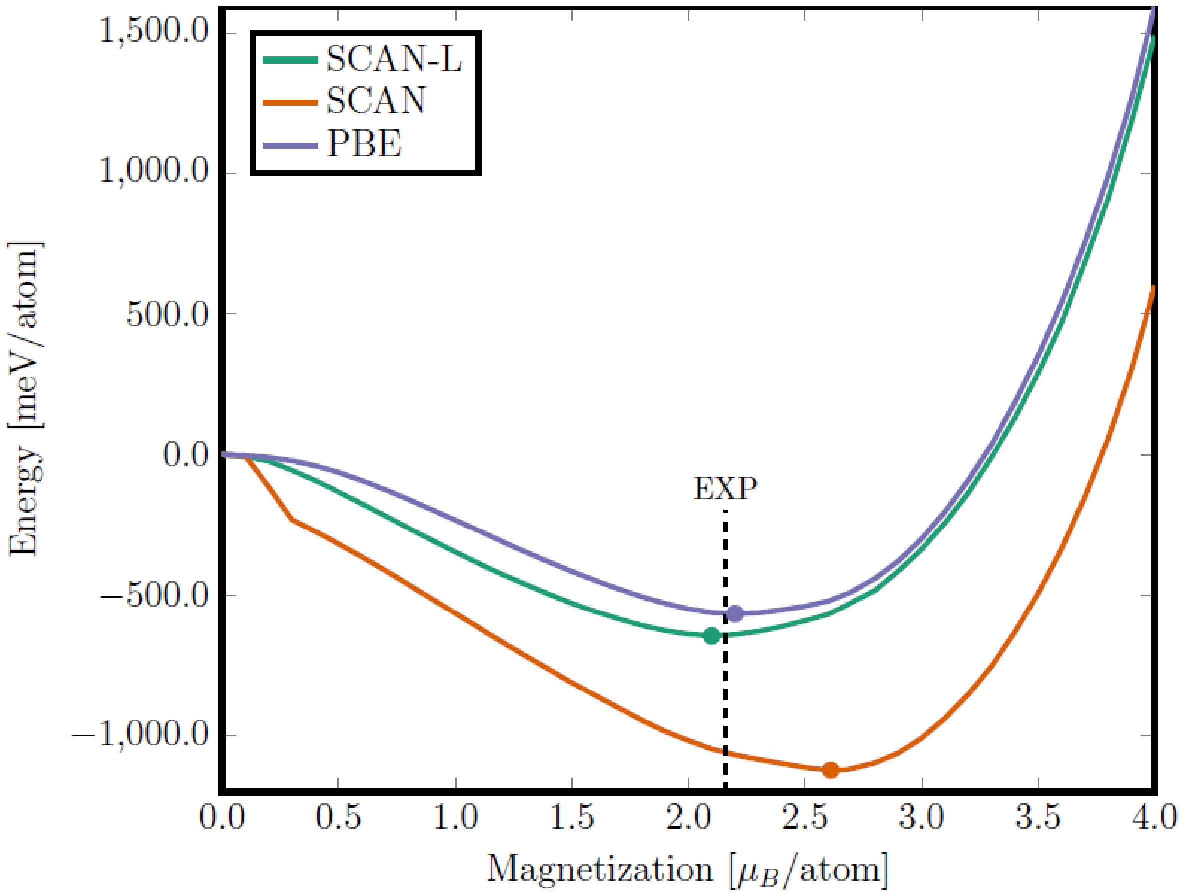
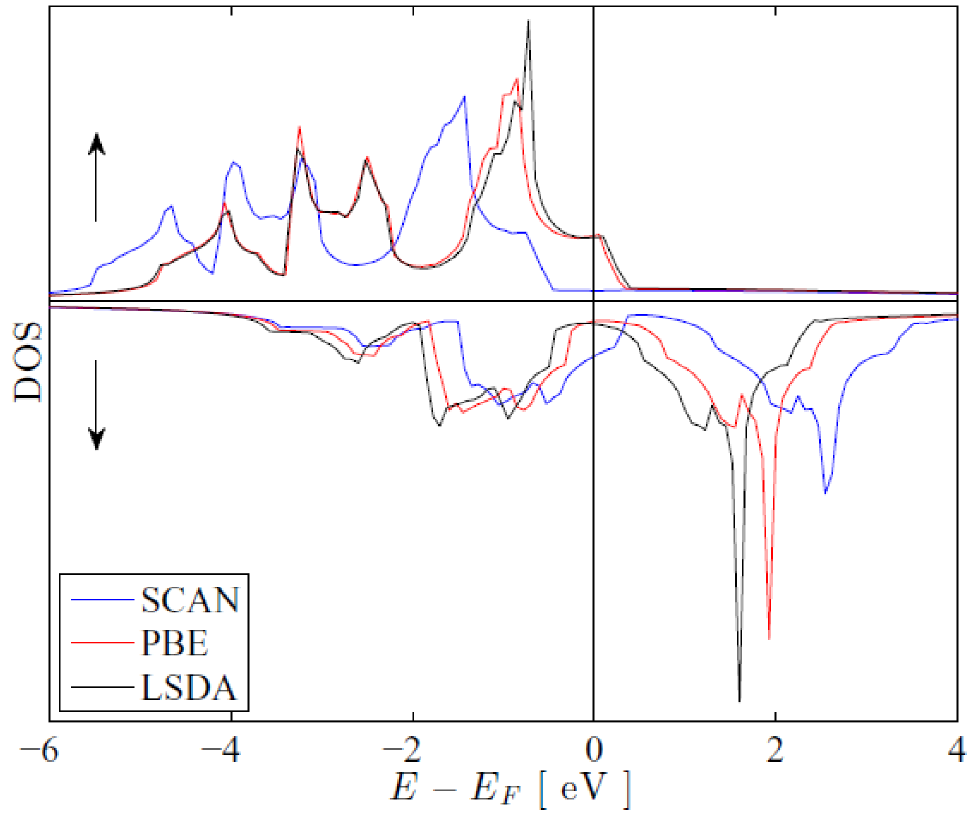
SCAN over-magnetization



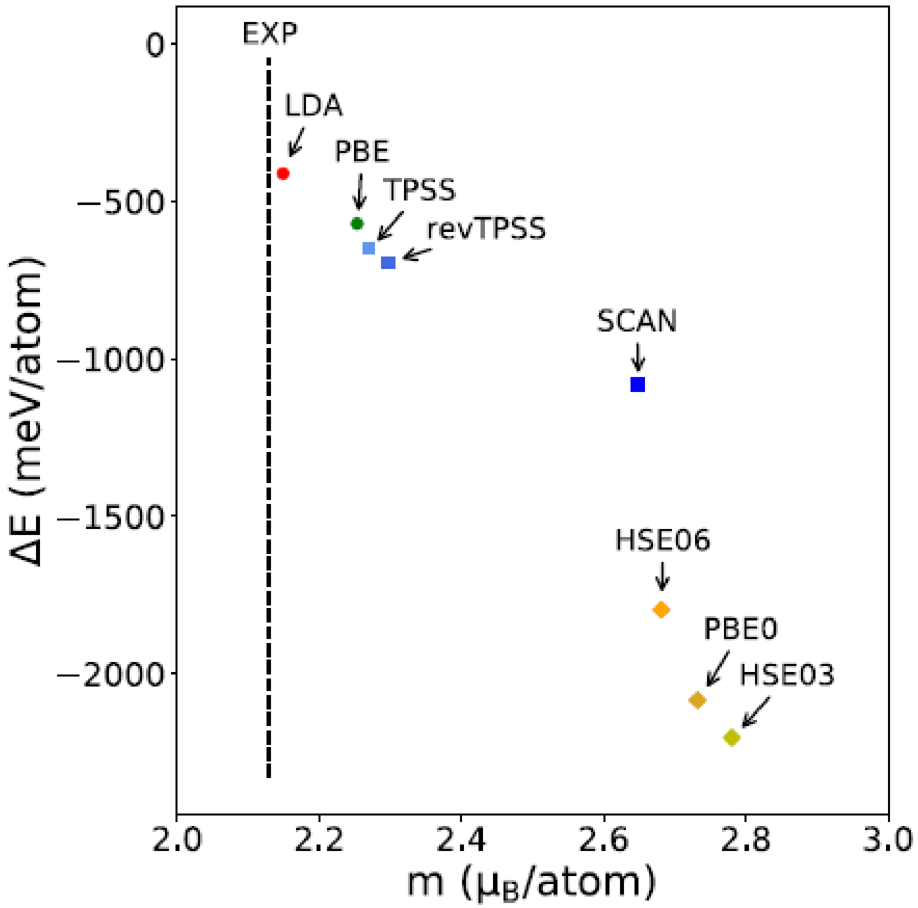
BCC Fe fixed-spin moment curves
Mejia-Rodriguez & Trickey [*PRB* ***100****, 41113(R) (2019)*]

- 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)*]

SCAN over-magnetization

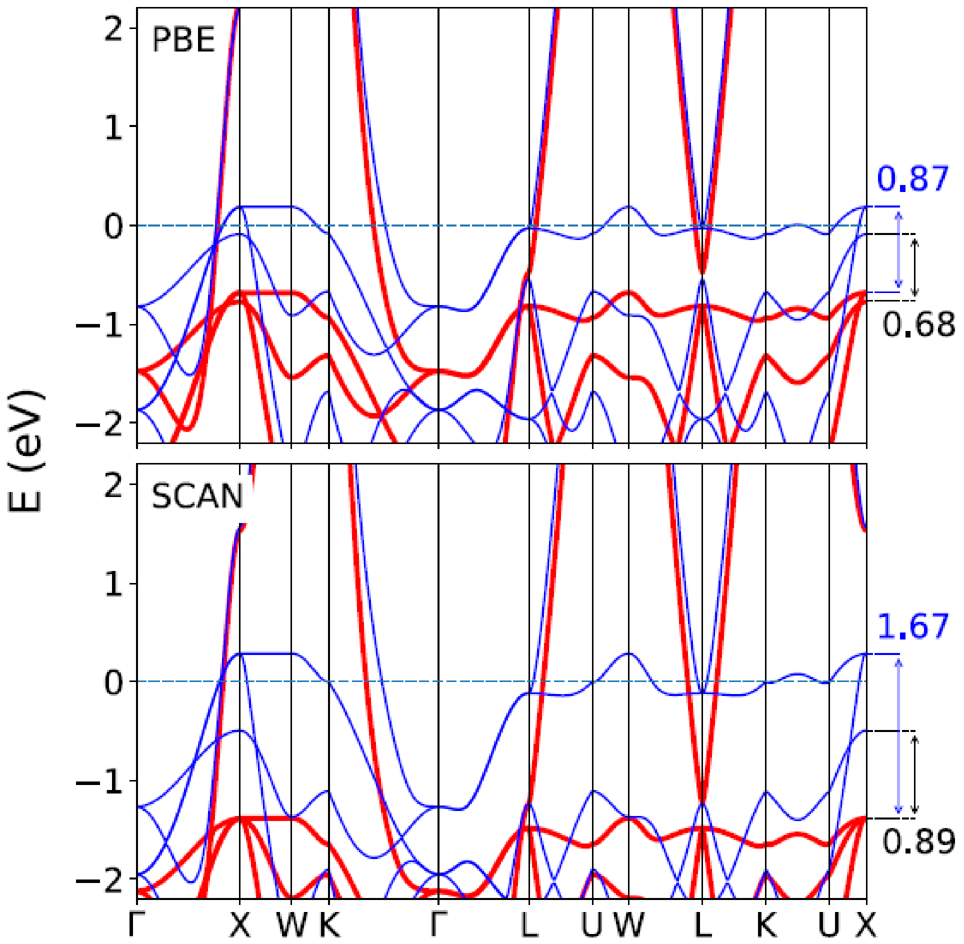


Ekholm *et al.* [*PRB **98** 094413 (2019)*]



Fu & Singh [*PRB **100**, 045126 (2019)*]

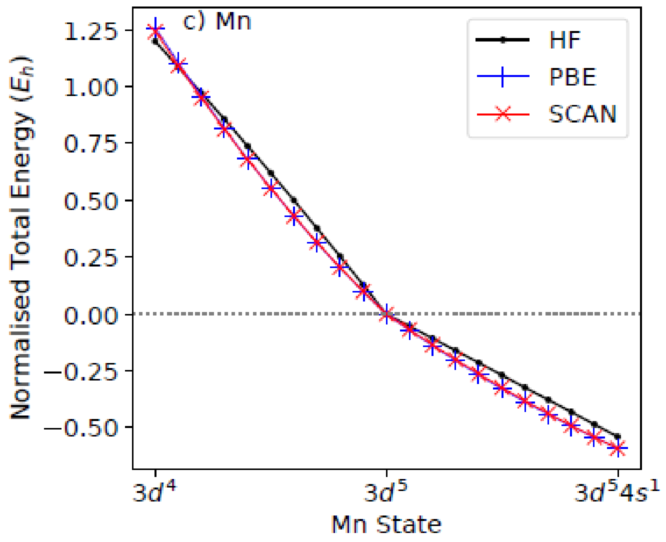
SCAN over-magnetization

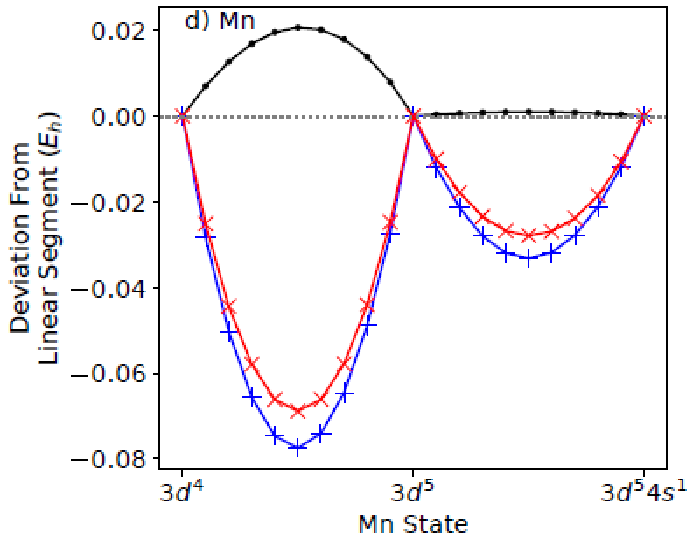


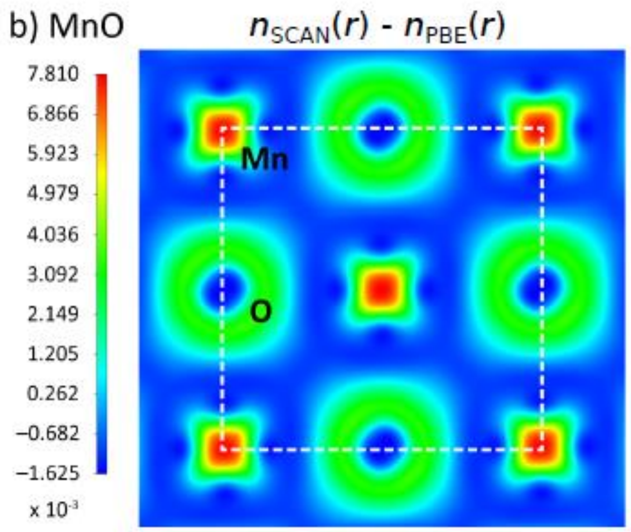
Fu & Singh [*PRB* ***100***, *045126 (2019)*]

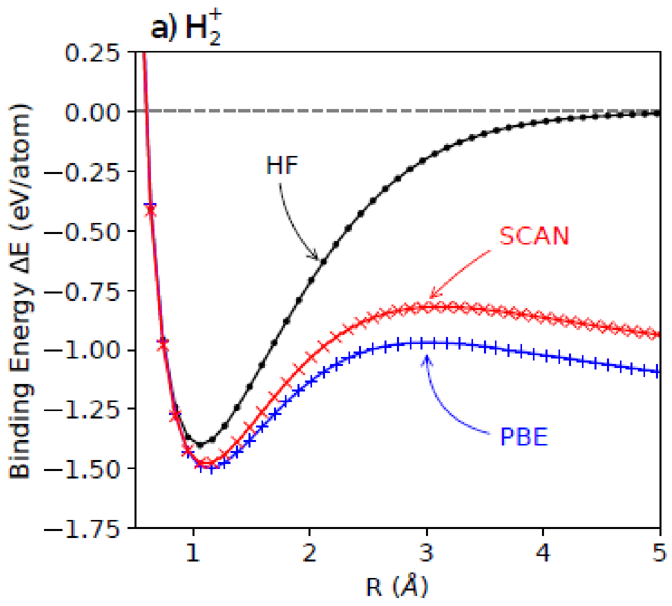
SCAN over-magnetization

Zhang *et al.* [*arXiv:1906.06467v2 (2019)*]









SCAN XC energy functional

SCAN
Sun, Ruzsinszky, & Perdew
PRL ***115***, *036402 (2015)*

$$F_x(p,\alpha) = \left(h_x^1(p,\alpha) + f_x(\alpha)\left[1.174 - h_x^1(p,\alpha)\right]\right) g_x(p)$$

$$g_x(p) = 1 - e^{-a_1 p^{-1/4}}$$

$$h_x^1(p,\alpha) = 1 + k_1 - \frac{k_1}{1 + x(p,\alpha)/k_1}$$

$$f_x(\alpha) = \theta(1-\alpha)e^{-c_{1x}\alpha/(1-\alpha)} - d_x\theta(\alpha-1)e^{-c_{2x}/(\alpha-1)}$$

$$p(n,\nabla n) = \frac{|\nabla n|^2}{4(3\pi^2)^{2/3}n^{8/3}}$$

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

$$\tau = \frac{1}{2}\sum_i f_i|\nabla\phi_i|^2$$

SCAN & SCAN-L XC energy functionals

SCAN

Sun, Ruzsinszky, & Perdew

*PRL **115**, 036402 (2015)*

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

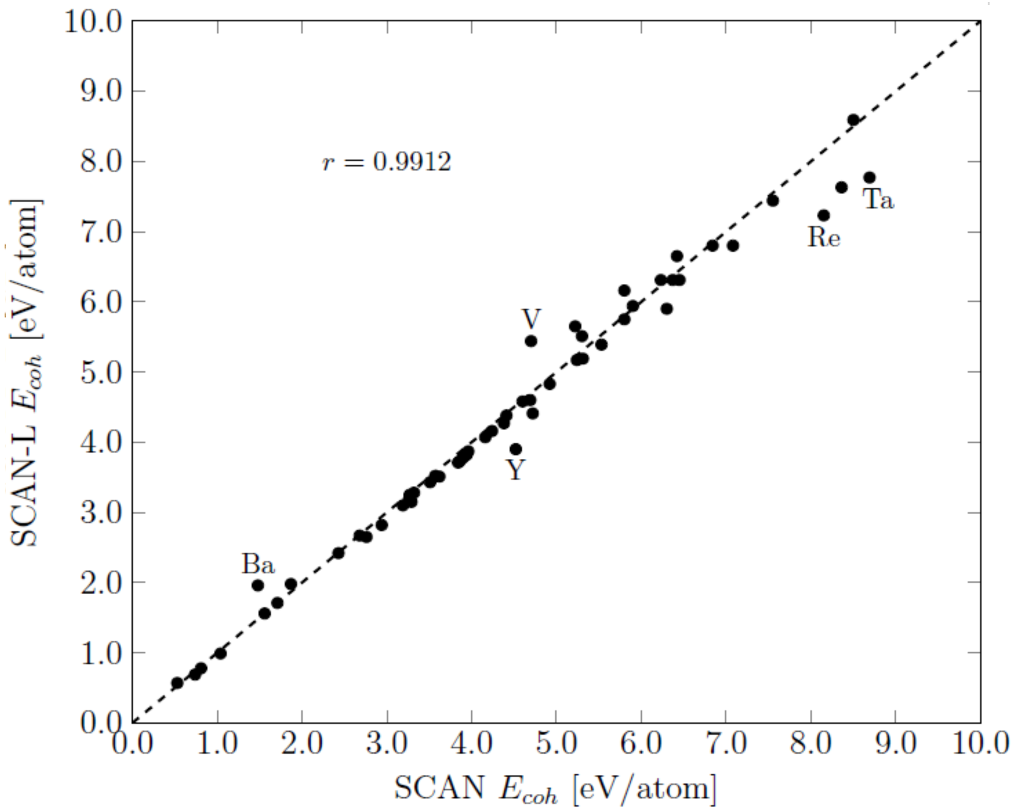
SCAN-L

Mejía-Rodríguez & Trickey

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

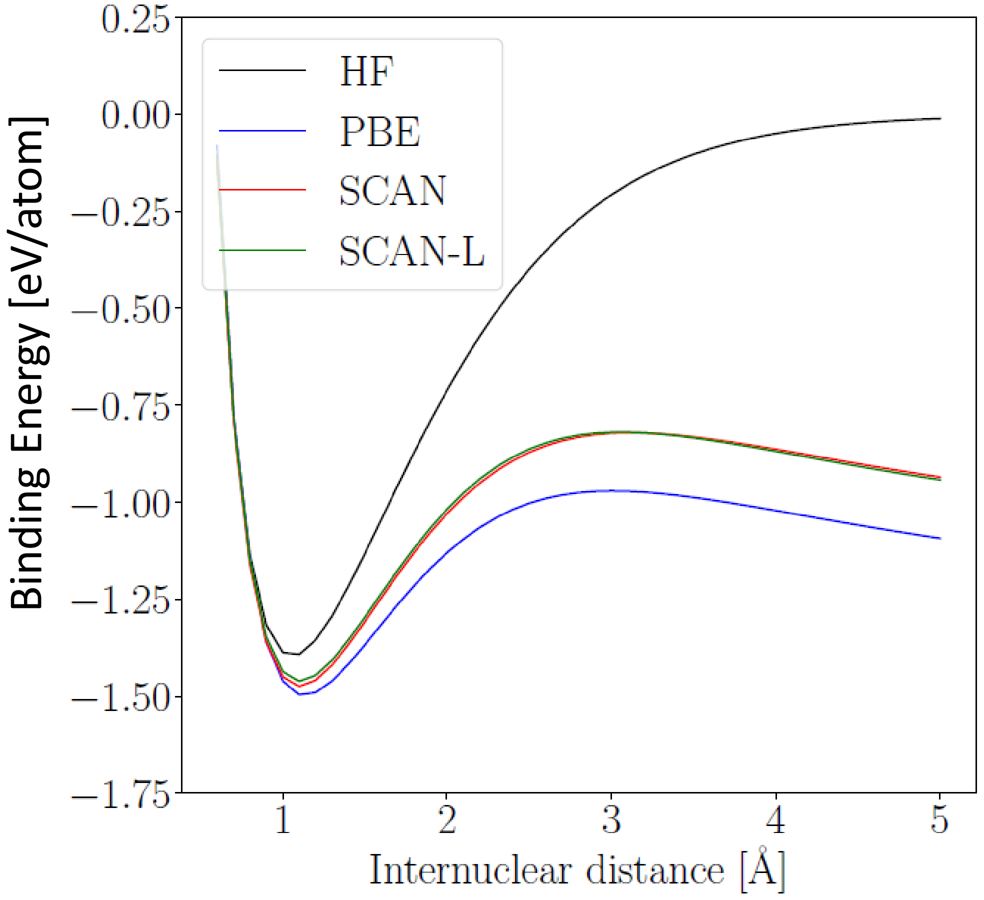
*PRB **98** ,115161 (2018)*

$$\alpha_L(n, \nabla n, \nabla^2 n) \equiv \frac{\tau^{PCopt}(n, \nabla n, \nabla^2 n) - \tau^{vW}}{\tau^{TF}}$$

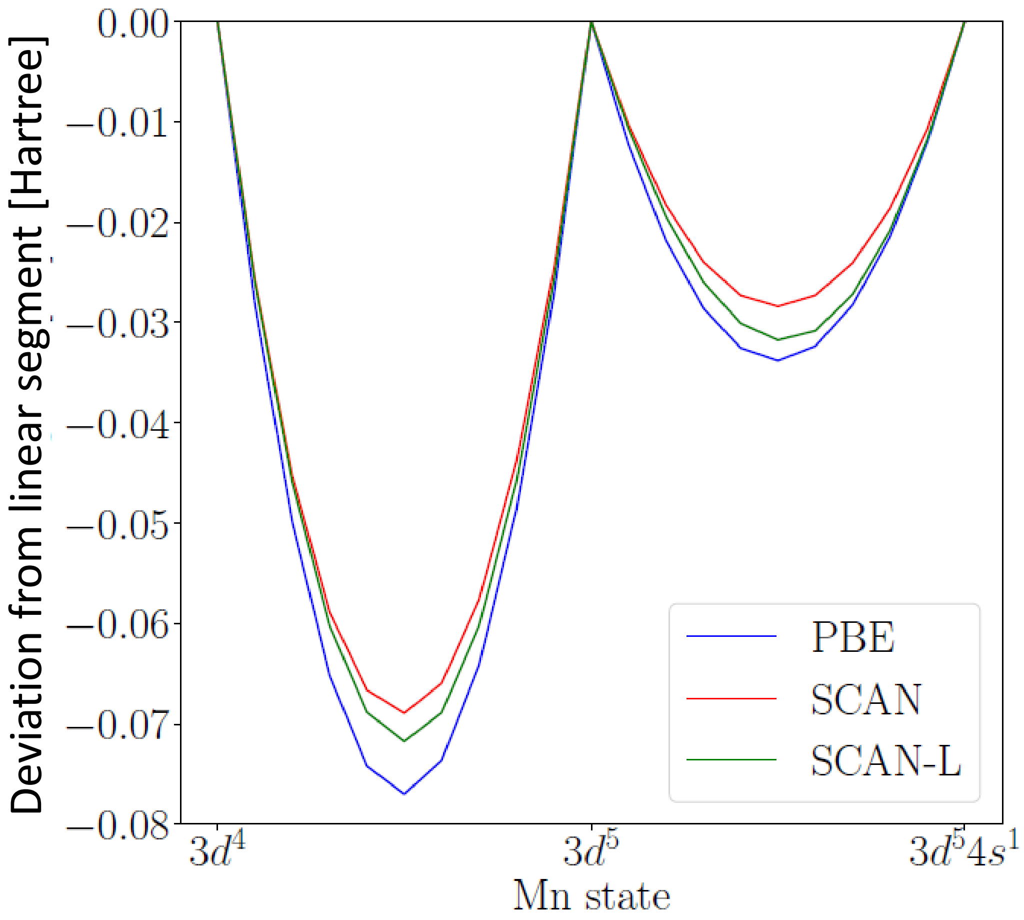


SCAN & SCAN-L XC energy functionals

Stretched H_2^+

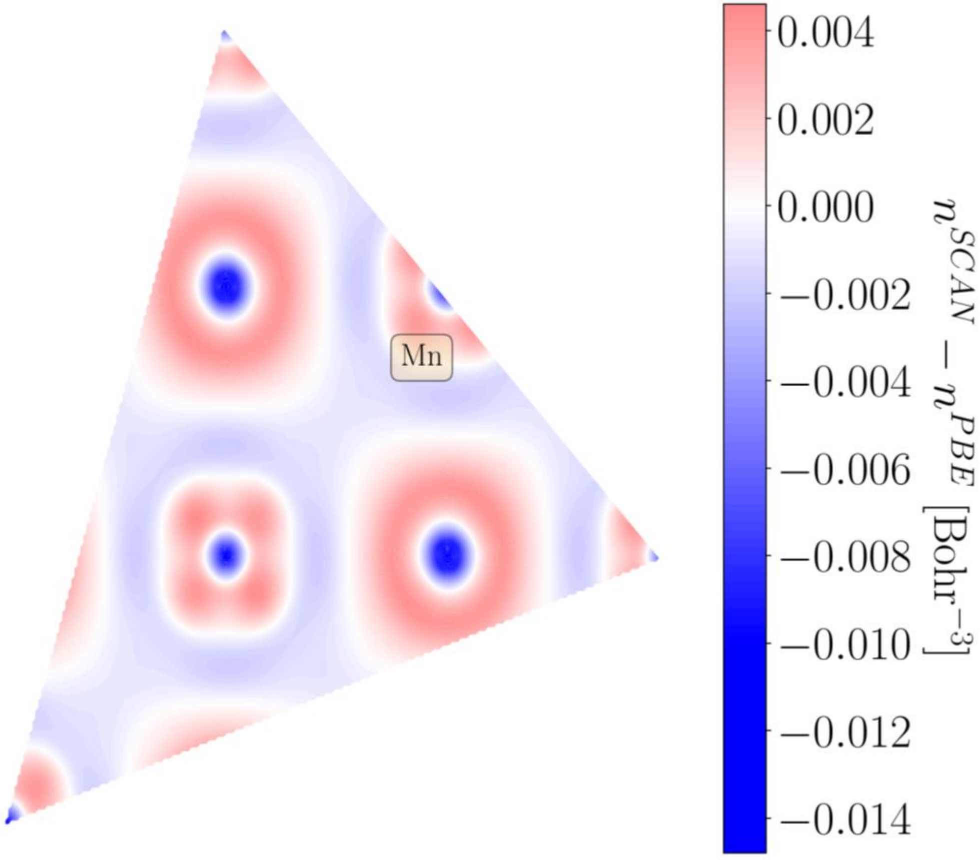


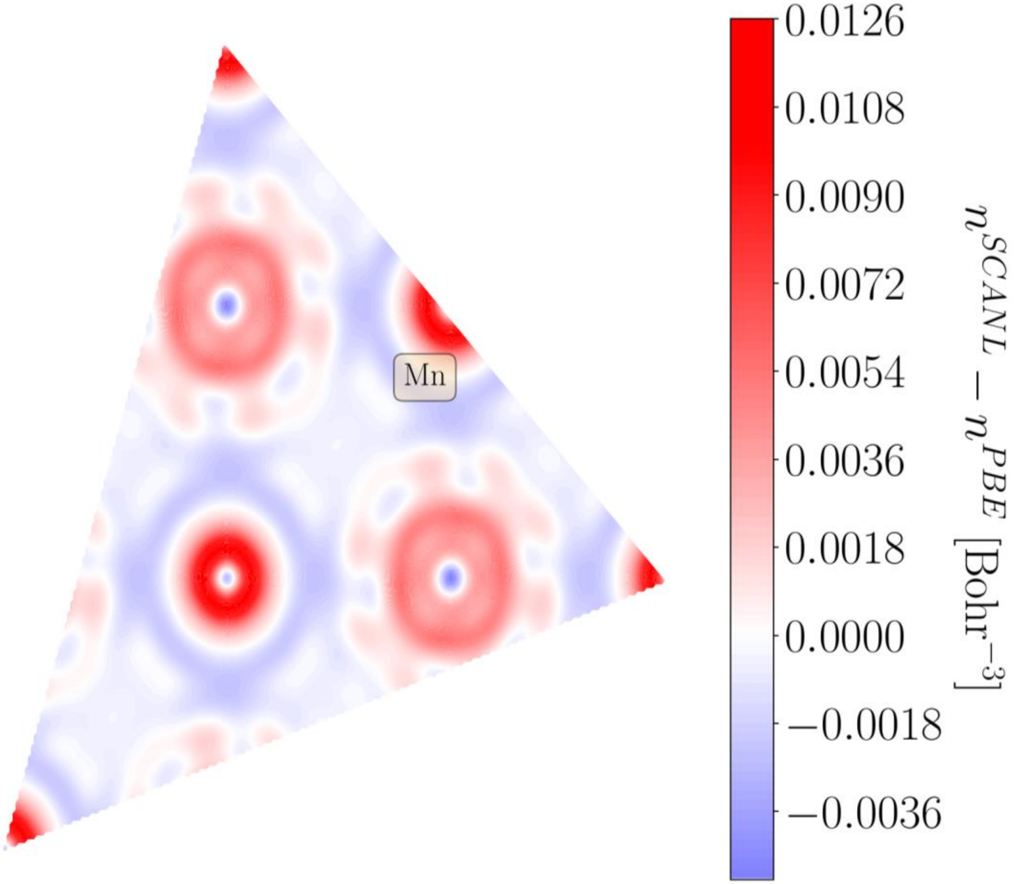
Fractional Charge Error Mn (3+, 2+, 1+)



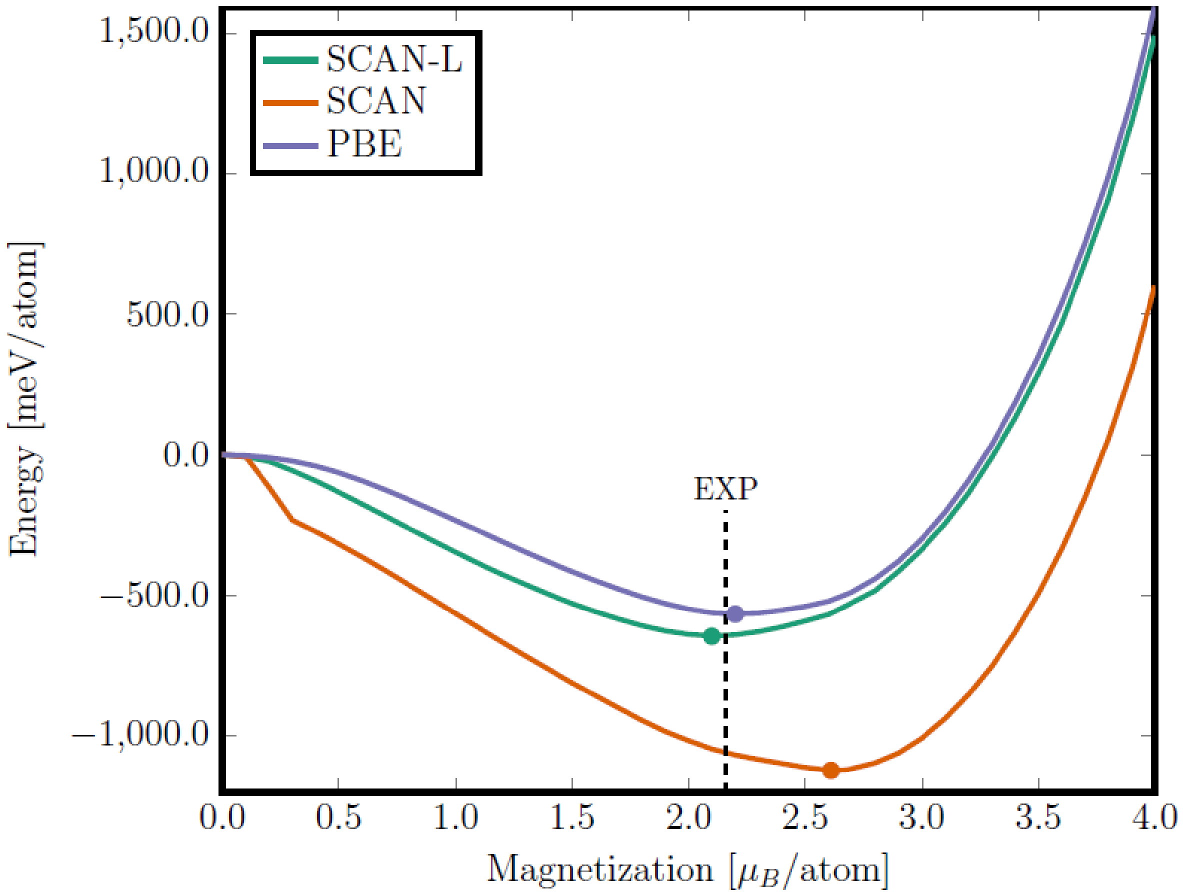
SCAN & SCAN-L XC energy functionals

MnO AFM density difference (VASP)





SCAN over-magnetization



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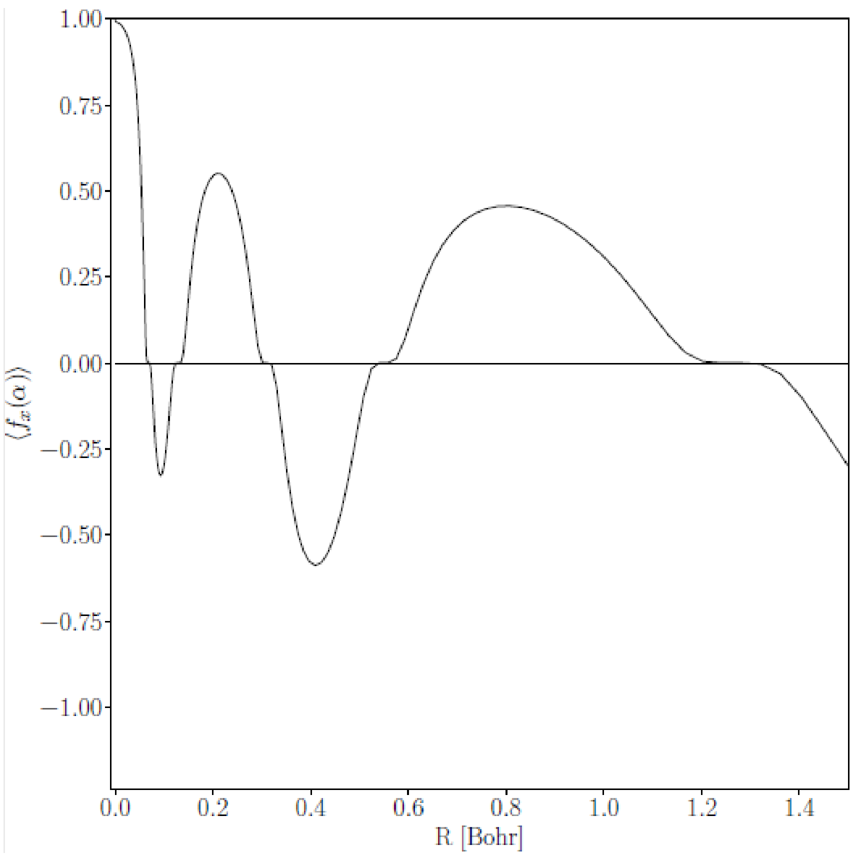
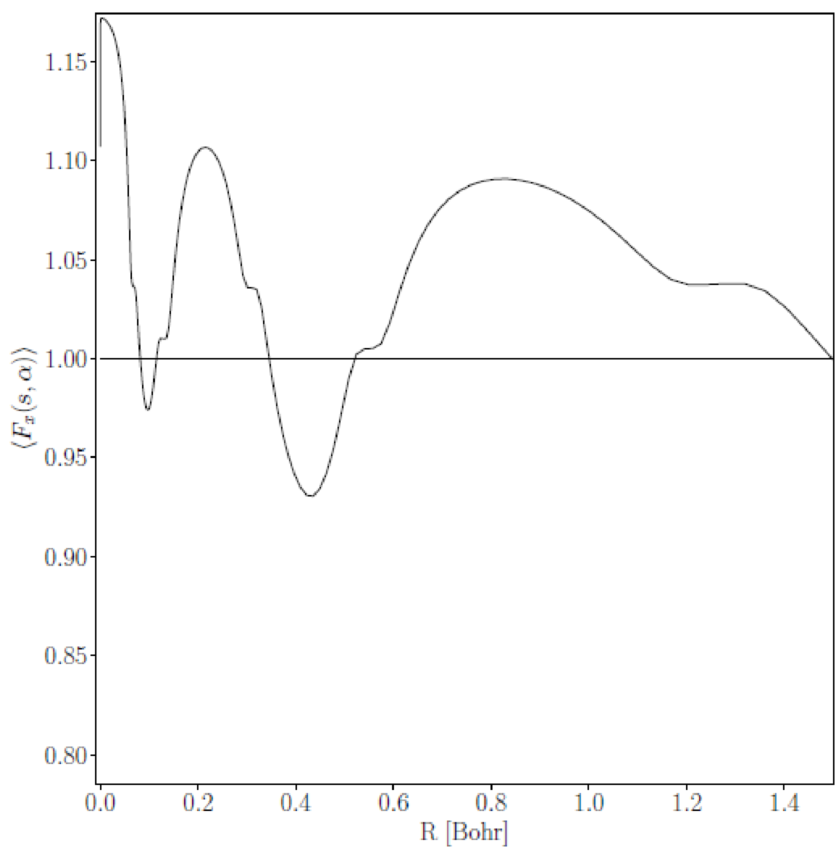
- Fu & Singh [*PRL* ***121****, 207201 (2018)*]

SCAN in BCC Fe

$$f_x(\alpha) = \theta(1-\alpha)e^{-c_{1x}\alpha/(1-\alpha)} - d_x\theta(\alpha-1)e^{-c_{2x}/(\alpha-1)}$$



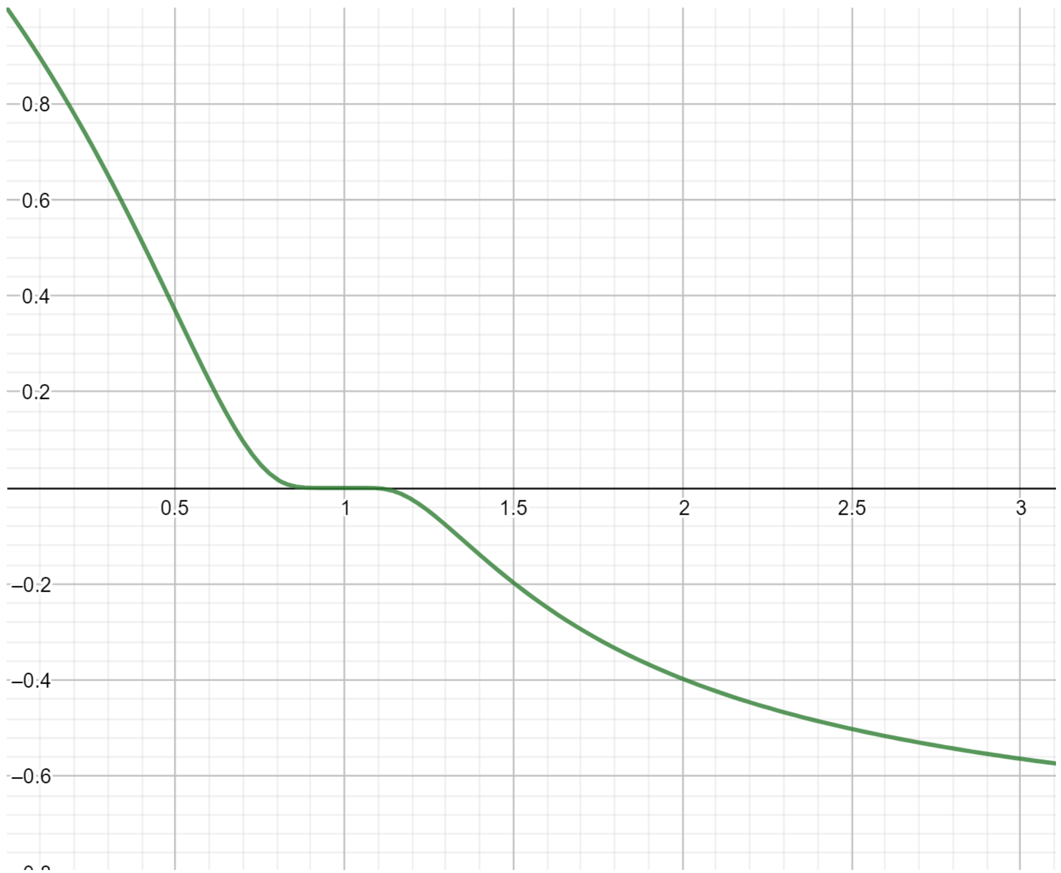
Angularly averaged switching function

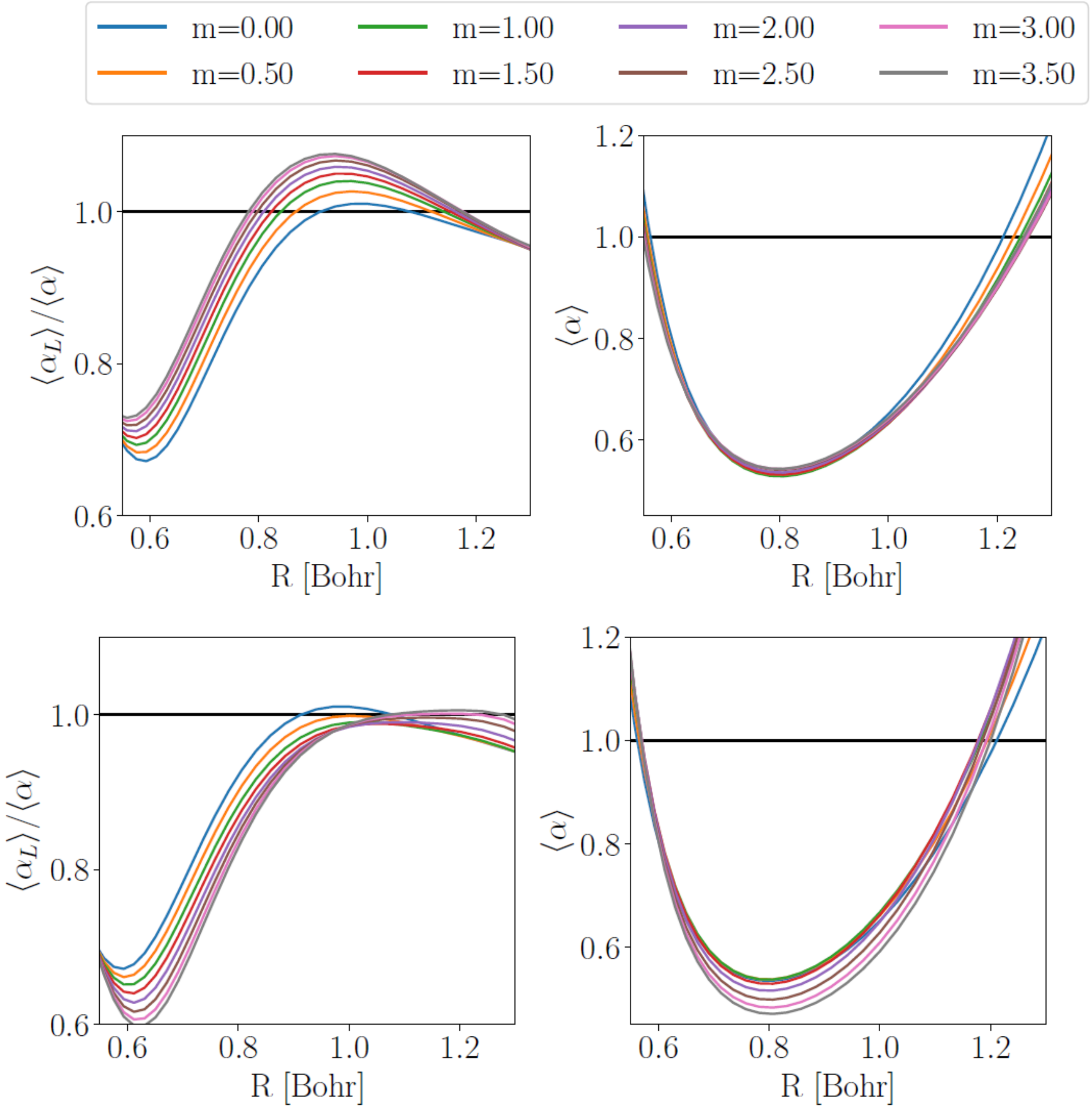


Angularly averaged enhancement factor

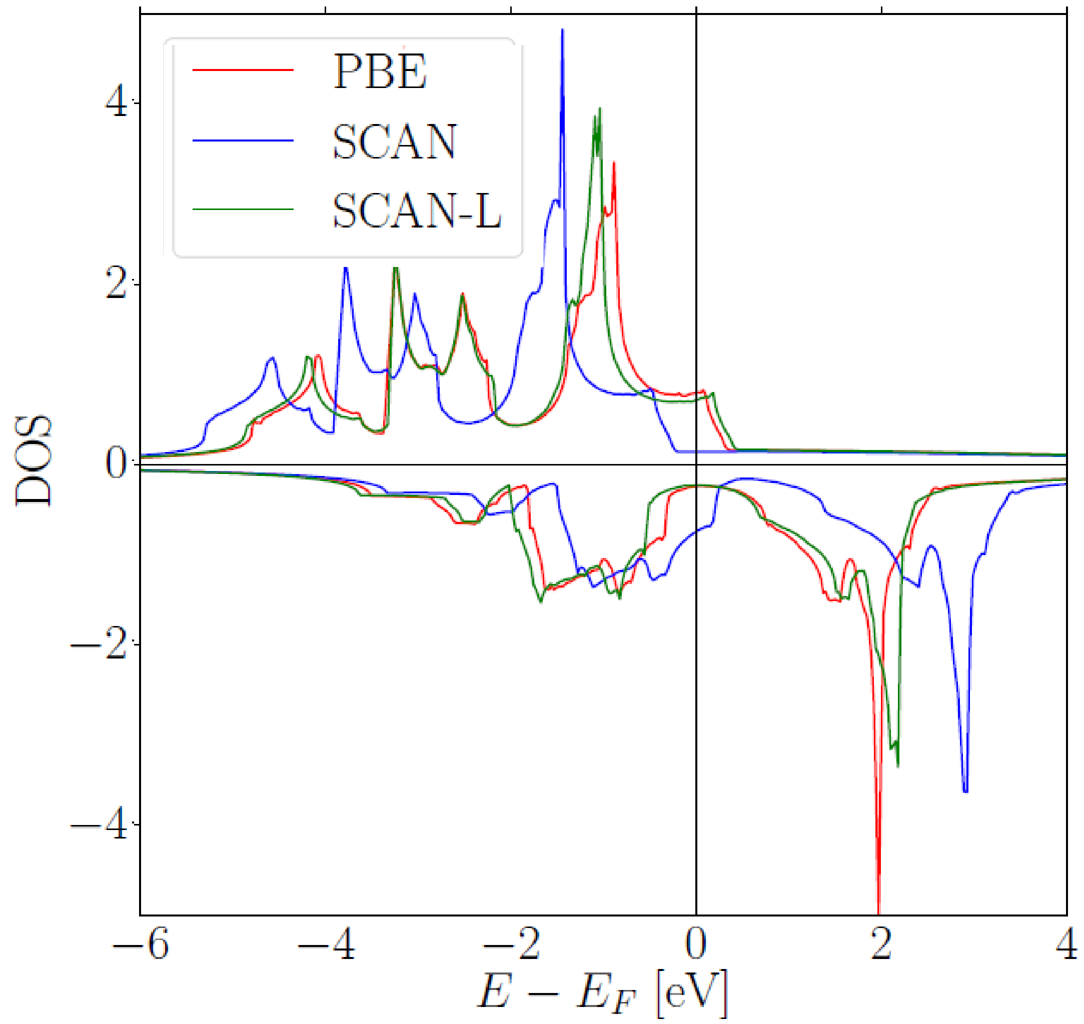
SCAN in BCC Fe

$$f_x(\alpha) = \theta(1-\alpha)e^{-c_{1x}\alpha/(1-\alpha)} - d_x\theta(\alpha-1)e^{-c_{2x}/(\alpha-1)}$$





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.