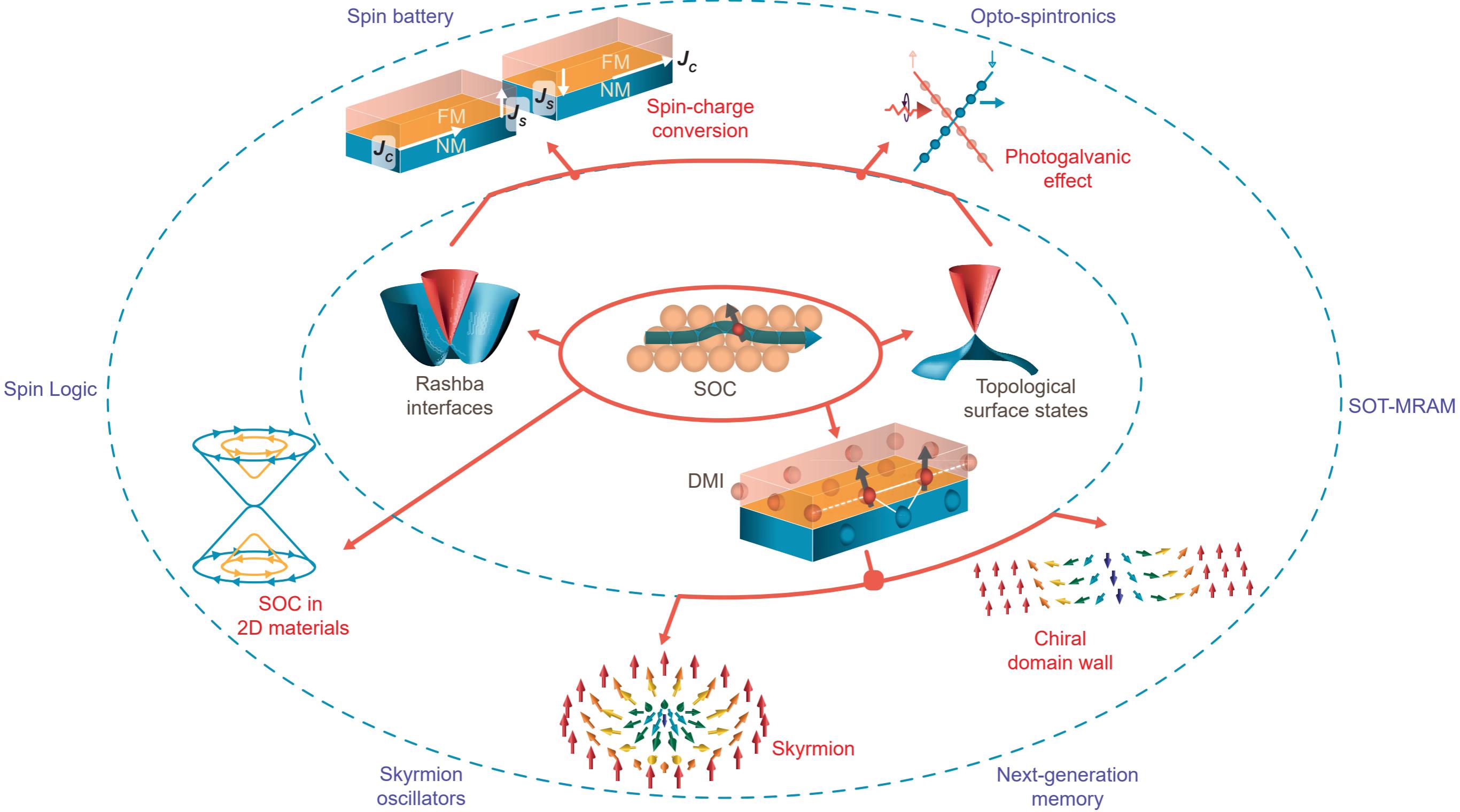


Gauge symmetries of density functionals: from first principles to practical approximations for magnetism

Stefano Pittalis
CNR-NANO S3 Modena, Italy



Motivation



Editorial: Altermagnetism—A New Punch Line of Fundamental Magnetism

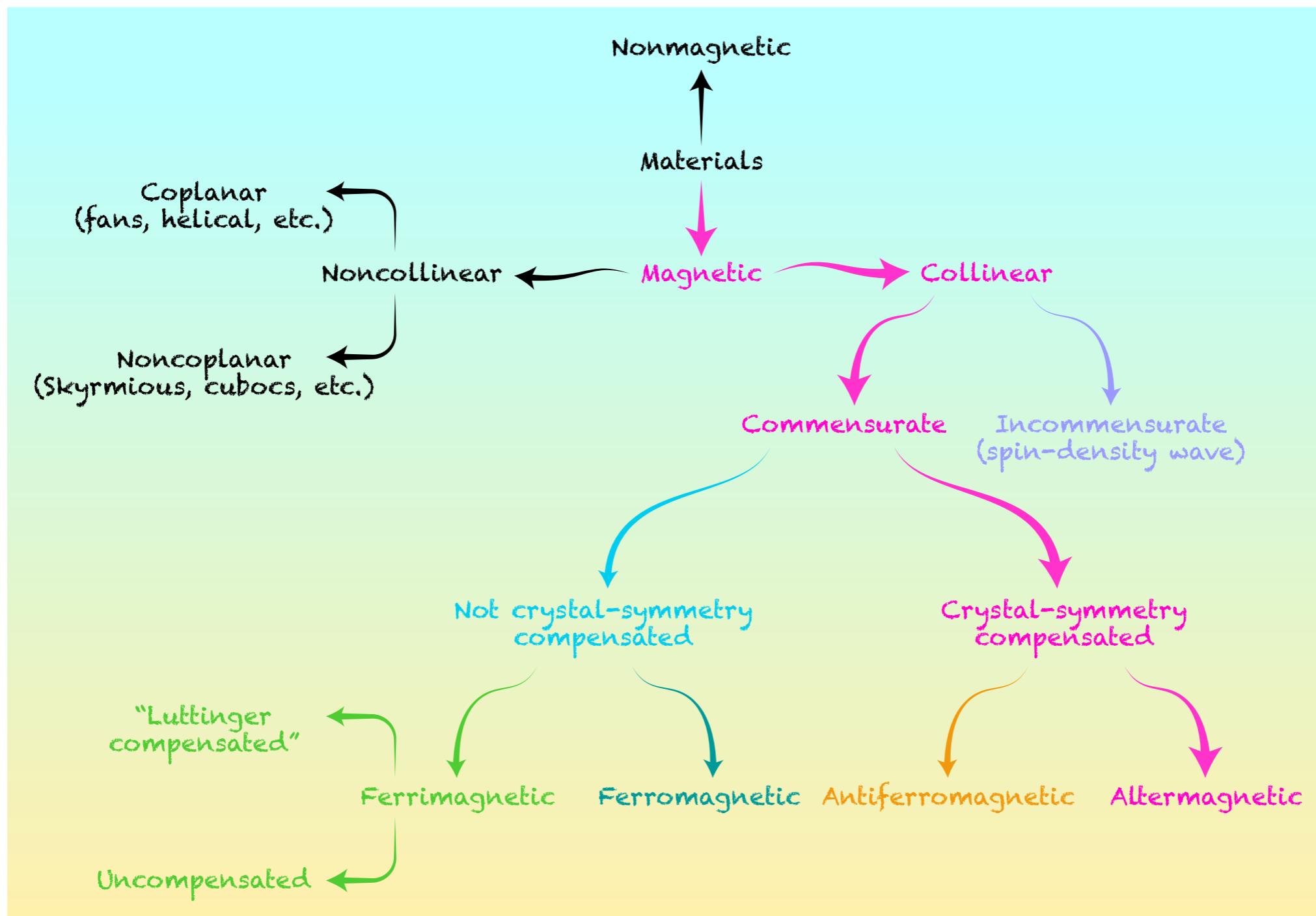


FIG. 1. A comprehensive classification scheme of different magnetic orders that shows altermagnetism as a fundamentally new class of magnetic order.

Outline

- Intro to SpinCurrent-DFT (SCDFT)
- SCDFT for the electron localization function for non-collinear spins
- SCDFT for the Rashba's band splittings
- SCDFT for collinear (anti-)ferromagnetism

SpinCurrent-DFT



G. Vignale



M. Rasolt

VOLUME 59, NUMBER 20

PHYSICAL REVIEW LETTERS

16 NOVEMBER 1987

Density-Functional Theory in Strong Magnetic Fields

PHYSICAL REVIEW B

VOLUME 37, NUMBER 18

15 JUNE 1988-II

**Current- and spin-density-functional theory for inhomogeneous electronic systems
in strong magnetic fields**



K. Bencheikh

INSTITUTE OF PHYSICS PUBLISHING

JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 11929–11936

PII: S0305-4470(03)64019-9

**Spin-orbit coupling in the
spin-current-density-functional theory**

From Spin-DFT to SpinCurrent-DFT

$$\hat{H}_{\text{SDFT}} = \int d^3r \ \hat{\Psi}^\dagger \left(-i \frac{\nabla}{2} \right)^2 \hat{\Psi} + \hat{W} + \int d^3r \ [\hat{n}v + \hat{m}^a B^a]$$

Two-component spinor!

$$\hat{\Psi} = \begin{bmatrix} \hat{\Psi}_\uparrow \\ \hat{\Psi}_\downarrow \end{bmatrix}$$

$$\hat{n} = \hat{\Psi}^\dagger \hat{\Psi}$$

$$\hat{m}^a = \hat{\Psi}^\dagger \sigma^a \hat{\Psi}$$



Pauli matrices

Perform the minimal substitution

$$-i\nabla \rightarrow -i\nabla + \frac{1}{c}\mathbf{A} + \frac{1}{c}\sigma^a \mathbf{A}^a$$

SpinCurrent-DFT

$$\hat{H}_{\text{SCDFT}} = \hat{T} + \hat{W} + \int d^3r \hat{n}\tilde{v} + \int d^3r \hat{m}^a \tilde{B}^a$$

$$+ \frac{1}{c} \int d^3r \hat{\mathbf{j}} \cdot \mathbf{A} + \frac{1}{c} \int d^3r \hat{\mathbf{J}}^a \cdot \mathbf{A}^a$$

$$\hat{\mathbf{j}} = \frac{1}{2i} \left[\hat{\Psi}^\dagger \nabla \hat{\Psi} - (\nabla \hat{\Psi}^\dagger) \hat{\Psi} \right]$$

$$\hat{\mathbf{J}}^a = \frac{1}{2i} \left[\hat{\Psi}^\dagger \sigma^a \nabla \hat{\Psi} - (\nabla \hat{\Psi}^\dagger) \sigma^a \hat{\Psi} \right]$$

$$\tilde{v} = v + \frac{1}{2c^2} [\mathbf{A} \cdot \mathbf{A} + \mathbf{A}^a \cdot \mathbf{A}^a]$$

$$\tilde{B}^a = B^a + \frac{1}{2c^2} \mathbf{A} \cdot \mathbf{A}^a$$

Kohn-Sham formulation

$$\begin{aligned} E &= \min_{\Psi} \langle \Psi | \hat{H}_{\text{SCDFT}} | \Psi \rangle \\ &= \min_{(n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}})} \left\{ \min_{\Phi \rightarrow (n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}})} \langle \Phi | \hat{T} | \Phi \rangle + E_{\text{Hxc}}[n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}}] \right. \\ &\quad \left. + \int d^3r \ n(\mathbf{r}) \tilde{v}(\mathbf{r}) + \int d^3r \ m^a \tilde{B}^a + \frac{1}{c} \int d^3r \ \mathbf{j} \cdot \mathbf{A} + \frac{1}{c} \int d^3r \ \mathbf{J}^a \cdot \mathbf{A}^a \right\} \end{aligned}$$

Kohn-Sham system in SCDFT

$$\left[\frac{1}{2} \left(-i\nabla + \frac{1}{c} \mathcal{A}_{\text{KS}} \right)^2 + \mathcal{V}_{\text{KS}} \right] \begin{bmatrix} \Phi_{\uparrow} \\ \Phi_{\downarrow} \end{bmatrix} = \varepsilon \begin{bmatrix} \Phi_{\uparrow} \\ \Phi_{\downarrow} \end{bmatrix}$$

$$\mathcal{A}_{\text{KS}} = \mathbf{A}_{\text{KS}} + \sigma^a \mathbf{A}_{\text{KS}}^a$$

$$\mathcal{V}_{\text{KS}} = v_{\text{KS}} + \sigma^a B_{\text{KS}}^a + \frac{1}{2c^2} [\mathcal{A}^2 - \mathcal{A}_{\text{KS}}^2]$$

$$\mathbf{A}_{\text{KS}} = \mathbf{A} + \mathbf{A}_{\text{xc}}$$

$$v_{\text{KS}} = v + v_{\text{H}} + v_{\text{xc}}$$

$$\frac{1}{c} \mathbf{A}_{\text{xc}} = \frac{\delta E_{\text{xc}}}{\delta \mathbf{j}}$$

$$v_{\text{xc}} = \frac{\delta E_{\text{xc}}}{\delta n}$$

$$\mathbf{A}_{\text{KS}}^a = \mathbf{A}^a + \mathbf{A}_{\text{xc}}^a$$

$$B_{\text{KS}}^a = B^a + B_{\text{xc}}^a$$

$$\frac{1}{c} \mathbf{A}_{\text{xc}}^a = \frac{\delta E_{\text{xc}}}{\delta \mathbf{J}^a}$$

$$B_{\text{xc}}^a = \frac{\delta E_{\text{xc}}}{\delta m^a}$$

Gauge transformations

$$\begin{aligned} U(1) : \quad \hat{\Psi}(\mathbf{r}) \rightarrow \hat{\Psi}(\mathbf{r}) &= \exp \left[\frac{i}{c} \Lambda_0(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) \\ &= U(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \end{aligned}$$

$$\begin{aligned} SU(2) : \quad \hat{\Psi}(\mathbf{r}) \rightarrow \hat{\Psi}'(\mathbf{r}) &= \exp \left[\frac{i}{c} \vec{\Lambda}(\mathbf{r}) \circ \vec{\sigma} \right] \hat{\Psi}(\mathbf{r}) \\ &= U_{\text{S}}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \end{aligned}$$

$U(1) \times SU(2)$ Gauge Invariance of x_c

$$E_{xc}[n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}}] = E_{xc}[n', \vec{m}', \mathbf{j}', \vec{\mathbf{J}}']$$

$$n(\mathbf{r}) \rightarrow n'(\mathbf{r}) = n(\mathbf{r})$$

$$\mathbf{j} \rightarrow \mathbf{j}' = \mathbf{j} + \frac{1}{c} n \nabla \Lambda_0 + \frac{i}{2} \vec{m} \circ \text{Tr} (\vec{\sigma} U_S \nabla U_S^{-1})$$

$$\vec{m} \rightarrow \vec{m}' = R(\vec{\Lambda}) \vec{m}$$

$$\vec{\mathbf{J}} \rightarrow \vec{\mathbf{J}}' = R(\vec{\Lambda}) \left[\vec{\mathbf{J}} - \frac{1}{c} (\nabla \Lambda_0) \vec{m} - \frac{i}{2} n \text{Tr} (\vec{\sigma} U_S \nabla U_S^{-1}) \right]$$

$U(1) \times SU(2)$ Gauge Invariance of E_{xc}

$$E_{xc}[n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}}] = E_{xc}[n', \vec{m}', \mathbf{j}', \vec{\mathbf{J}}']$$

We must approximate the xc-energy
via practical
 $U(1) \times SU(2)$ gauge-invariant quantities

xc-energy approximations



MBP-diagrams: unoccupied orbitals /eigenvalues

Hybrids:

Meta-GGAs:

GGAs:

LDA

$$E_{\text{xc}} \approx \alpha E_{\text{x}}^{\text{Fock}} + (1 - \alpha) E_{\text{x}}^{\text{DFA}} + E_{\text{c}}^{\text{DFA}}$$

$$E_{\text{xc}}[n] \approx \int d^3r \ \epsilon(n(\mathbf{r}), \nabla n(\mathbf{r}), \tau(\mathbf{r}))$$

$$E_{\text{xc}}[n] \approx \int d^3r \ \epsilon(n(\mathbf{r}), \nabla n(\mathbf{r}))$$

$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

$$E_{\text{x}}^{\text{Fock}} = \sum_{\sigma} \int \int \frac{d^3r d^3r'}{2} \ \frac{|\sum_i^{\text{occ}} \varphi_{i,\sigma}^*(\mathbf{r}) \varphi_{i,\sigma}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}$$

Exact-Exchange Spin-Current Density-Functional Theory

Stefan Rohra and Andreas Görting

Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Egerlandstrasse 3, D-91058 Erlangen, Germany
(Received 4 November 2005; published 7 July 2006)**Spin-Potential Functional Formalism for Current-Carrying Noncollinear Magnetic Systems**Tim Heaton-Burgess,¹ Paul Ayers,² and Weitao Yang¹¹*Department of Chemistry, Duke University, Durham, North Carolina 27708, USA*²*Department of Chemistry, McMaster University, Hamilton, Ontario, Canada L8S 4M1*

(Received 19 July 2006; published 18 January 2007)

Optimized effective potential method for current-spin-density-functional theoryS. Pittalis, S. Kurth,¹ N. Helbig,¹*Institut für Theoretische Physik, Humboldt-Universität Berlin, Unter den Linden 14, D-14195 Berlin, Germany*

(Received 26 September 2006; published 1 December 2006)

Comparison of exact-exchange calculations for solids in current-spin-density-functional theory and spin-density-functional theoryA. Sharma,^{1,2,*} S. Pittalis,¹ S. Kurth,² S. Shallcross,³ J. K. Dewhurst,⁴ and E. K. U. Gross²**Exact-exchange-correlation orbital functionals in current-density functional theory: Application to a quantum dot in magnetic fields**N. Helbig,^{1,2,3} S. Kurth,^{2,3} S. Pittalis,^{2,3} E. Räsänen,^{2,3} and E. K. U. Gross^{2,3}**Spin-current density-functional theory for a correct treatment of spin-orbit interactions and its application to topological phase transitions**

Egor Trushin and Andreas Görling*

Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen, Germany

Generalize KS in SpinCurrent-DFT

PHYSICAL REVIEW MATERIALS **8**, 013802 (2024)

Generalized Kohn-Sham approach for the electronic band structure of spin-orbit coupled materials

Jacques K. Desmarais^{ID, 1,*} Giacomo Ambrogio^{ID, 1} Giovanni Vignale^{ID, 2} Alessandro Erba^{ID, 1} and Stefano Pittalis^{ID, 3,†}

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²*Institute for Functional Intelligent Materials, National University of Singapore, 4 Science Drive 2, 117544 Singapore*

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(Received 19 September 2023; accepted 7 December 2023; published 16 January 2024)



Jacques



Giacomo

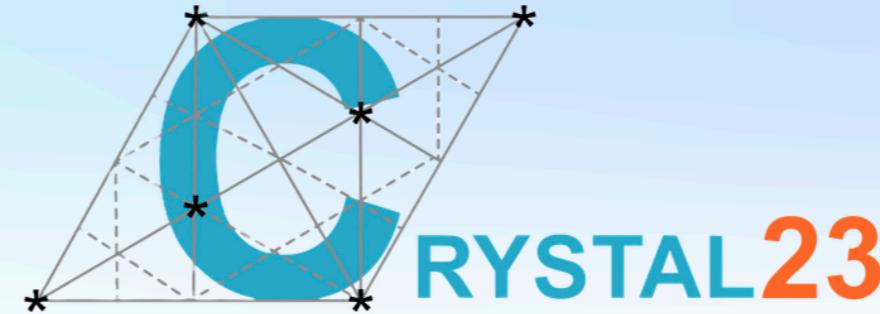
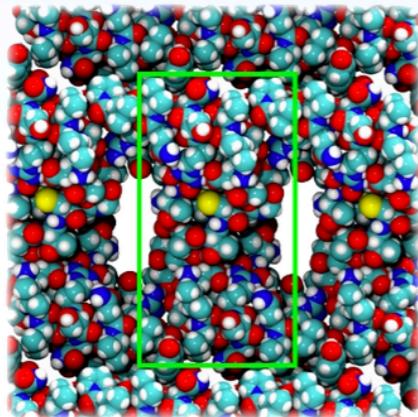
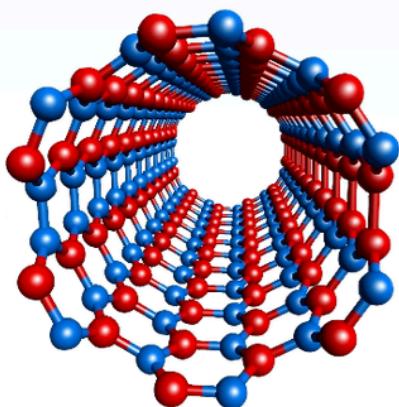
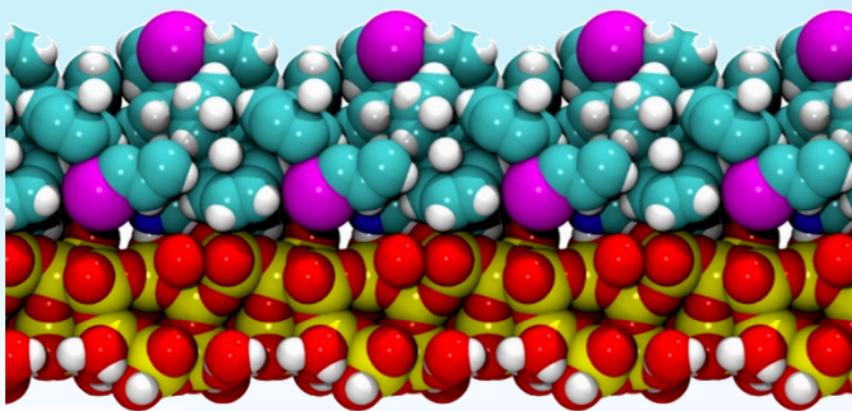


Giovanni



Alessandro

Implementation



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Generalized-KS in SpinCurrent-DFT

$$\begin{aligned}
E &= \min_{\Psi} \langle \Psi | \hat{H}_{\text{SCDFT}} | \Psi \rangle \\
&= \min_{(n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}})} \left\{ \min_{\Phi \rightarrow (n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}})} \langle \Phi | \hat{T} + \hat{W} | \Phi \rangle + E_c[n, \vec{m}, \mathbf{j}, \vec{\mathbf{J}}] \right. \\
&\quad \left. + \int d^3r n \tilde{v} + \int d^3r m^a \tilde{B}^a + \frac{1}{c} \int d^3r \mathbf{j} \cdot \mathbf{A} + \frac{1}{c} \int d^3r \mathbf{J}^a \cdot \mathbf{A}^a \right\}
\end{aligned}$$



$$\begin{aligned}
E &= \min_{\Phi} \left\{ \langle \Phi | \hat{T} + \hat{W} | \Phi \rangle + E_c^{\text{GKS}}[n[\Phi], \vec{m}[\Phi], \mathbf{j}[\Phi], \vec{\mathbf{J}}[\Phi]] \right. \\
&\quad \left. + \int d^3r n[\Phi](\mathbf{r}) \tilde{v}(\mathbf{r}) + \int d^3r m^a[\Phi](\mathbf{r}) \tilde{B}^a(\mathbf{r}) + \frac{1}{c} \int d^3r \mathbf{j}[\Phi](\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) + \frac{1}{c} \int d^3r \mathbf{J}^a[\Phi](\mathbf{r}) \cdot \mathbf{A}^a(\mathbf{r}) \right\}
\end{aligned}$$

Let's consider the most popular MGGA

The screenshot shows the homepage of **nature chemistry**. The header includes a navigation bar with links: Home, Current issue, Comment, Research, Archive, Authors & referees, and About the journal. Below the header, a breadcrumb trail shows the path: home > current issue > article > abstract. The main title of the article is "NATURE CHEMISTRY | ARTICLE". The title of the paper is "Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional". The authors listed are Jianwei Sun, Richard C. Remsing, Yubo Zhang, Zhaoru Sun, Adrienn Ruzsinszky, Haowei Peng, Zenghui Yang, Arpita Paul, Umesh Waghmare, Xifan Wu, Michael L. Klein & John P. Perdew.

**nature
chemistry**

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home > current issue > article > abstract

NATURE CHEMISTRY | ARTICLE

Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional

Jianwei Sun, Richard C. Remsing, Yubo Zhang, Zhaoru Sun, Adrienn Ruzsinszky, Haowei Peng, Zenghui Yang, Arpita Paul, Umesh Waghmare, Xifan Wu, Michael L. Klein & John P. Perdew

Strongly Constrained and Appropriately Normed Semilocal Density Functional

Jianwei Sun,^{1,*} Adrienn Ruzsinszky,¹ and John P. Perdew^{1,2}

¹*Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA*

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(Received 12 April 2015; published 14 July 2015)

The ground-state energy, electron density, and related properties of ordinary matter can be computed efficiently when the exchange-correlation energy as a functional of the density is approximated semilocally. We propose the first meta-generalized-gradient approximation (meta-GGA) that is fully constrained, obeying all 17 known exact constraints that a meta-GGA can. It is also exact or nearly exact for a set of “appropriate norms,” including rare-gas atoms and nonbonded interactions. This strongly constrained and appropriately normed meta-GGA achieves remarkable accuracy for systems where the exact exchange-correlation hole is localized near its electron, and especially for lattice constants and weak interactions.

Editors' Suggestion

Applicability of the Strongly Constrained and Appropriately Normed Density Functional to Transition-Metal Magnetism



Yuhao Fu and David J. Singh
Phys. Rev. Lett. **121**, 207201 – Published 14 November 2018



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PHYSICAL REVIEW B

covering condensed matter and materials physics

Shortcomings of meta-GGA functionals when describing magnetism



Fabien Tran, Guillaume Baudesson, Jesús Carrete, Georg K. H. Madsen, Peter Blaha, Karlheinz Schwarz, and David J. Singh
Phys. Rev. B **102**, 024407 – Published 6 July 2020



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Generalized Gradient Approximation Made Simple

John P. Perdew, Kieron Burke,* Matthias Ernzerhof

Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118

(Received 21 May 1996)

We begin with the GGA for correlation in the form

$$E_C^{\text{GGA}}[n_{\uparrow}, n_{\downarrow}] = \int d^3r n [\epsilon_C^{\text{unif}}(r_s, \zeta) + H(r_s, \zeta, t)], \quad (3)$$

$\nabla \zeta$ corrections to Eq. (3), which are small for most purposes, will be derived in later work. We construct the

Gradients of spin polarization are **NOT** included!

SCAN functional

PRL 115, 036402 (2015)

PHYSICAL REVIEW LETTERS

week ending
17 JULY 2015

Strongly Constrained and Appropriately Normalized Density Functional

Jianwei Sun,^{1,*} Adrienn Ruzsinszky,¹ and J. P. Perdew^{1,2}

¹*Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA*

²*Department of Chemistry, Temple University, Philadelphia, Pennsylvania 19122, USA*

(Received 17 June 2015; revised 14 July 2015)

The ground-state energy, electronic structure, and related properties of ordinary matter can be computed efficiently when the exchange-correlation energy as a functional of the density is approximated semilocally. We propose the first density-gradient approximation (meta-GGA) that is fully constrained, obeying all 17 constraints that a meta-GGA can. It is also exact or nearly exact for a set of “appropriate” rare-gas atoms and nonbonded interactions. This strongly constrained and appropriate meta-GGA achieves remarkable accuracy for systems where the exact exchange-correlation is localized near its electron, and especially for lattice constants and weak interactions.

Not $U(1) \times SU(2)$ Gauge invariant!

Bird's-eye view of SCAN (closed shell case)

$$E_{\text{xc}} = \int d^3r \ n(\mathbf{r}) \epsilon_{\text{xc}}^{\text{SCAN}}(\mathbf{r})$$

$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

$$\epsilon_{\text{xc}}^{\text{SCAN}} = \epsilon_{\text{xc}}^1 + (\epsilon_{\text{xc}}^0 - \epsilon_{\text{xc}}^1) f_{\text{xc}}(\alpha)$$

$$\alpha = (\tau - \tau_W)/\tau_{\text{unif}}$$

$$\text{ELF} = 1/(1 + \alpha^2)$$

Electron Localization Function for Noncollinear Spins

Jacques K. Desmarais^{1,*} Giovanni Vignale² Kamel Bencheikh,³ Alessandro Erba¹ and Stefano Pittalis^{4,†}

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²*Institute for Functional Intelligent Materials, National University of Singapore, 4 Science Drive 2, Singapore 117544, Singapore*

³*Setif 1 University-Ferhat Abbas, Faculty of Sciences, Department of Physics and Laboratory of Quantum Physics
and Dynamical Systems, Setif, Algeria*

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(Received 24 May 2024; revised 14 July 2024; accepted 22 August 2024; published 25 September 2024)



Jacques



Giovanni



Kamel



Alessandro

Electron localization function (ELF)

$$\text{ELF}(\mathbf{r}) \equiv \frac{1}{1 + [D(\mathbf{r})/D^{\text{unif}}(\mathbf{r})]^2}$$

$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

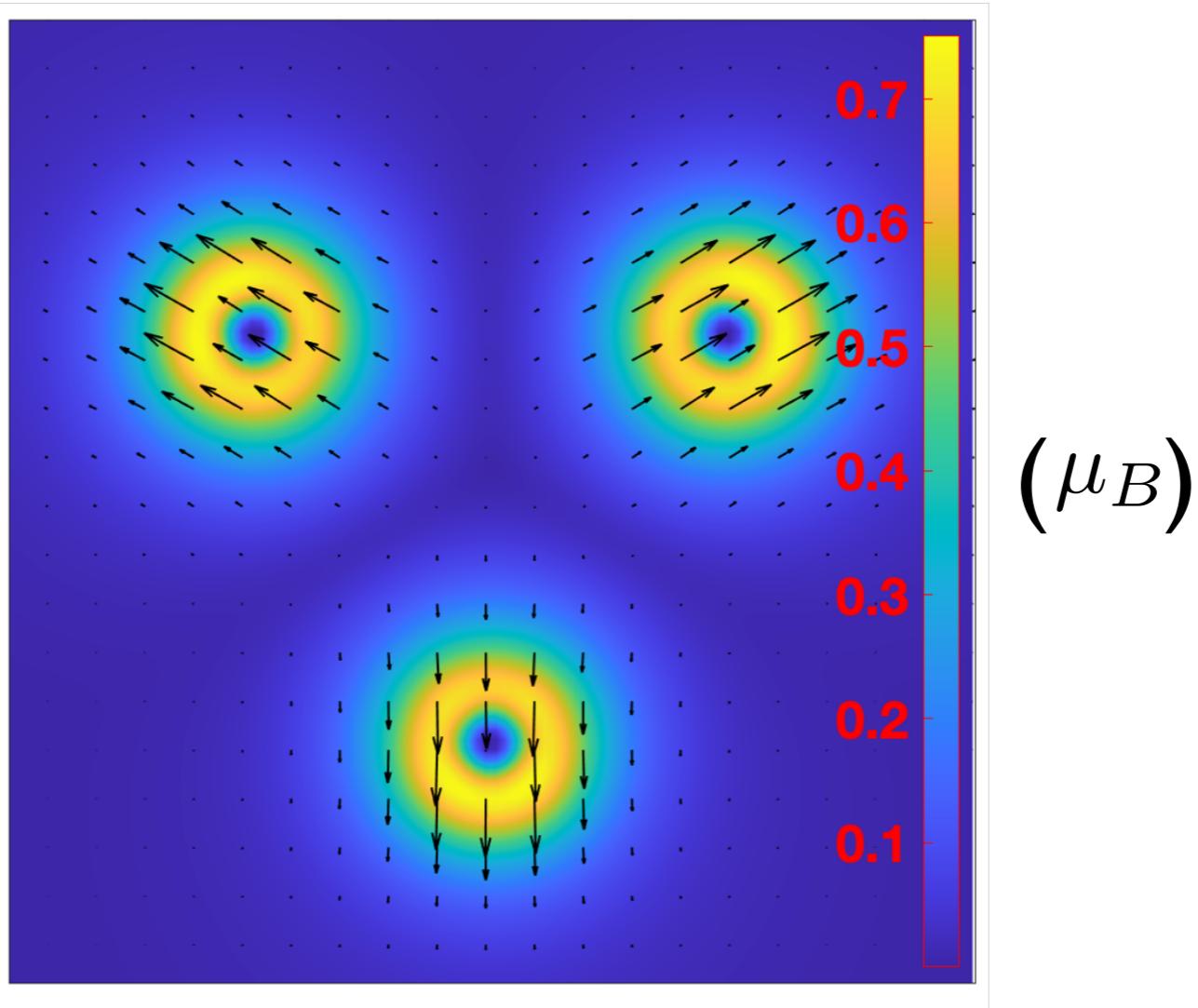
$$D(\mathbf{r}) = \tau(\mathbf{r}) - \frac{\nabla n(\mathbf{r}) \cdot \nabla n(\mathbf{r})}{8n(\mathbf{r})}$$

Measure difference of Fermionic kinetic energy w.r.t. Bosonic kinetic energy

$$D^{\text{unif}}(\mathbf{r}) = \frac{3}{10} (3\pi^2)^{2/3} n^{5/3}(\mathbf{r})$$

Normalization relative to the uniform gas

Magnetization in Cr3



Magnetization in Cr3 from 2c-HF+SOC

ELF: Näive extension to non-coll. Spins

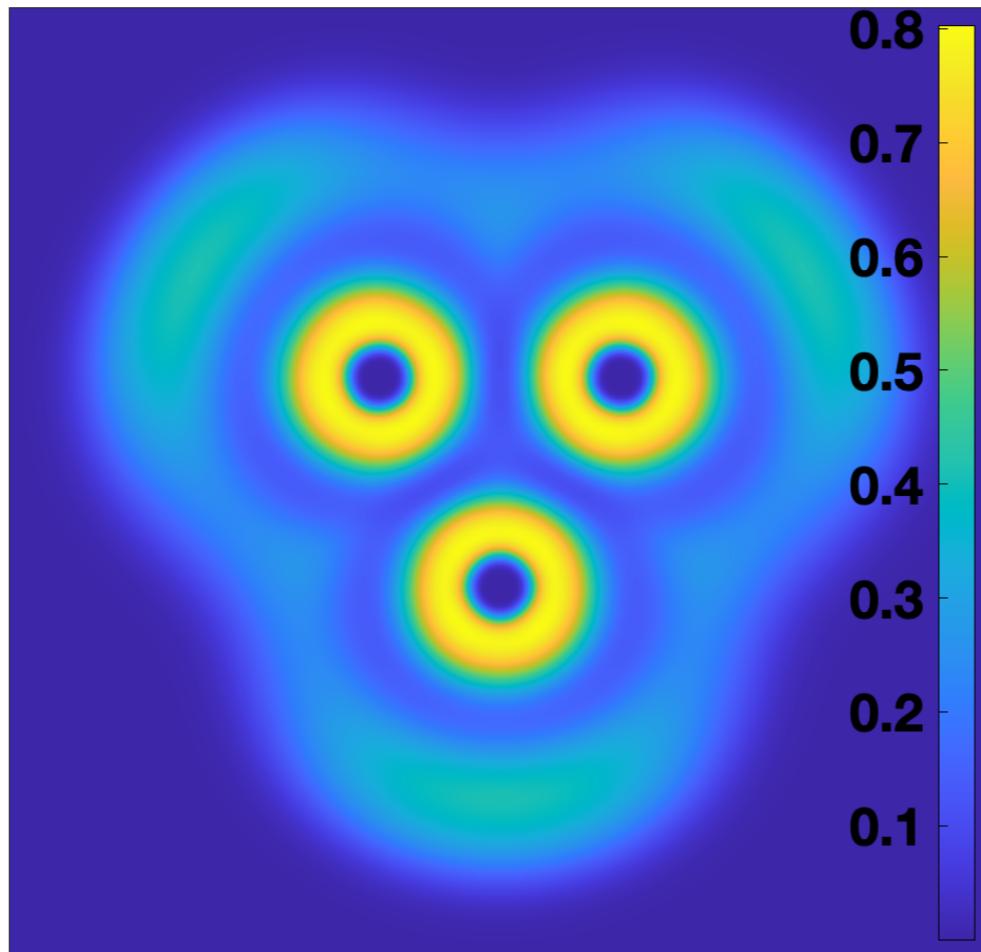
$$\text{ELF}(\mathbf{r}) \equiv \frac{1}{1 + [D(\mathbf{r})/D^{\text{unif}}(\mathbf{r})]^2}$$

$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

$$D(\mathbf{r}) = \boxed{\tau(\mathbf{r})} - \frac{\nabla n(\mathbf{r}) \cdot \nabla n(\mathbf{r})}{8n(\mathbf{r})}$$

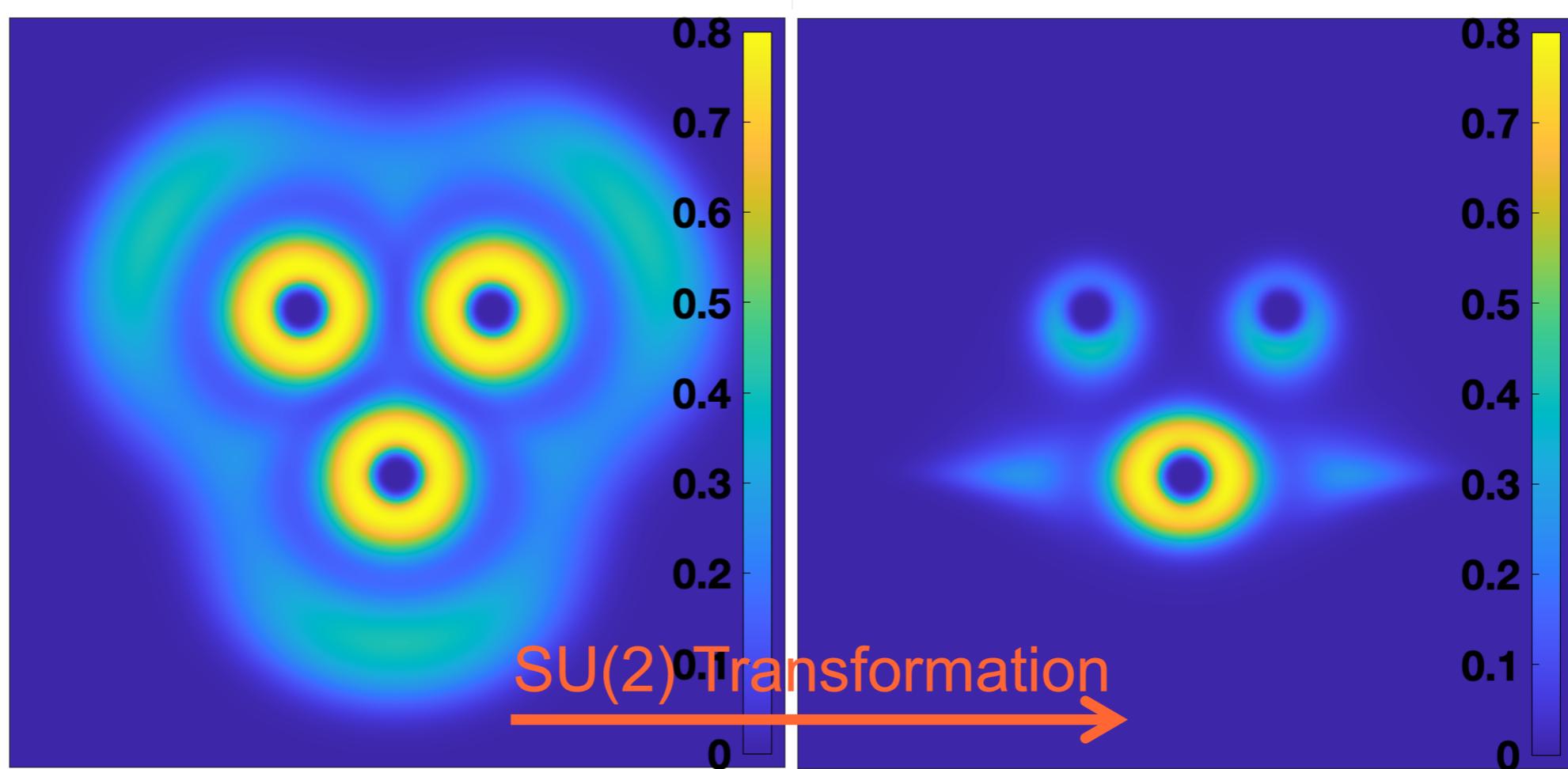
$$\tau(\mathbf{r}) \rightarrow \tau_{\text{nc}}(\mathbf{r}) = \frac{1}{2} \sum_k^{\text{occ}} [\nabla \Phi_k(\mathbf{r})]^\dagger \cdot \nabla \Phi_k(\mathbf{r})$$

ELF: Näive extension to non-coll. Spins



Plot for Cr3

ELF: Näive extension to non-coll. Spins



$$\begin{aligned} SU(2) : \quad \hat{\Psi}(\mathbf{r}) \rightarrow \hat{\Psi}'(\mathbf{r}) &= \exp \left[\frac{i}{c} \vec{\Lambda}(\mathbf{r}) \circ \vec{\sigma} \right] \hat{\Psi}(\mathbf{r}) \\ &= U_S(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \end{aligned}$$

$U(1) \times SU(2)$ Gauge Invariant ELF

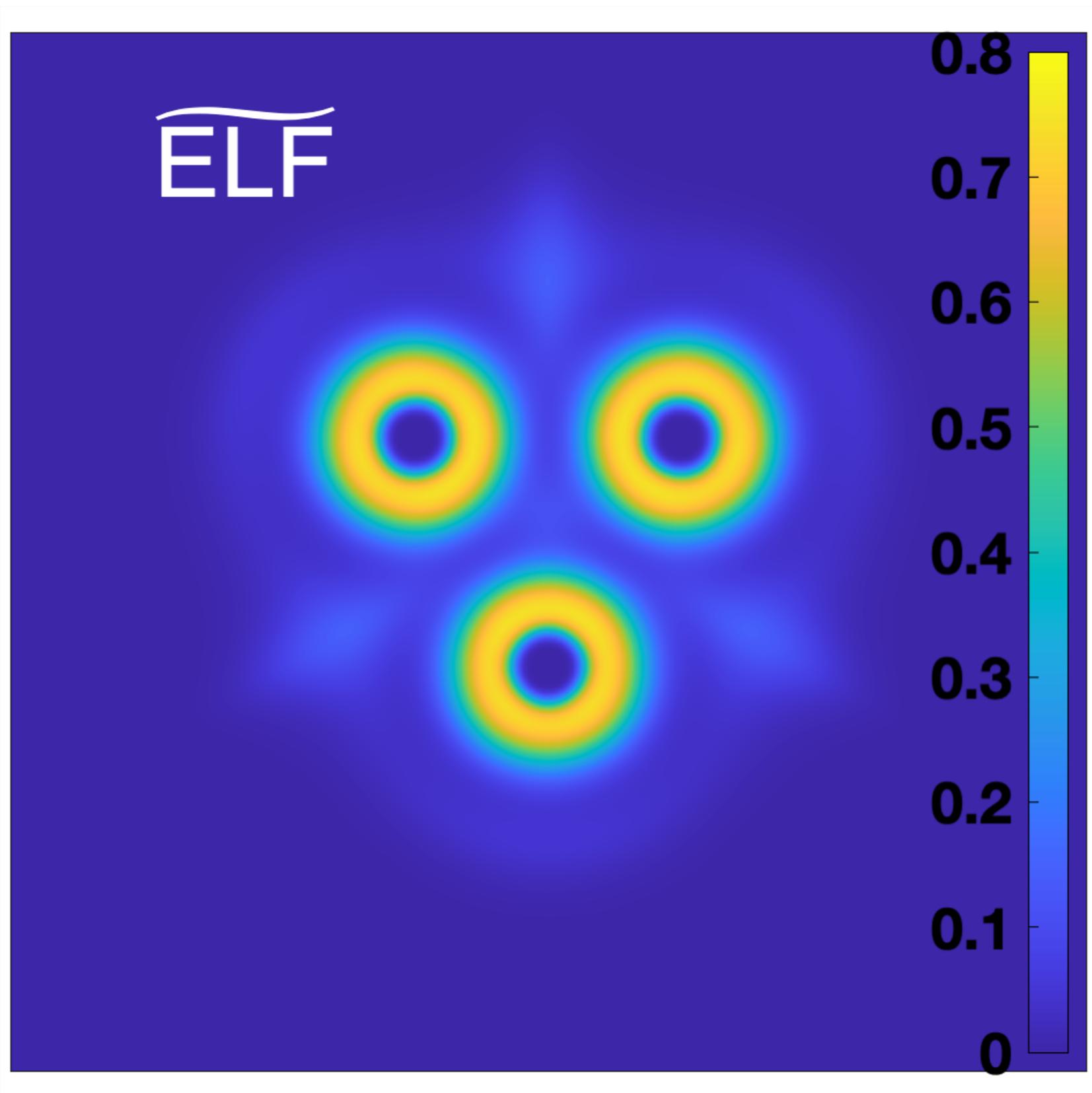
$$\text{ELF}(\mathbf{r}) \equiv \frac{1}{1 + [D(\mathbf{r})/D^{\text{unif}}(\mathbf{r})]^2}$$

$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

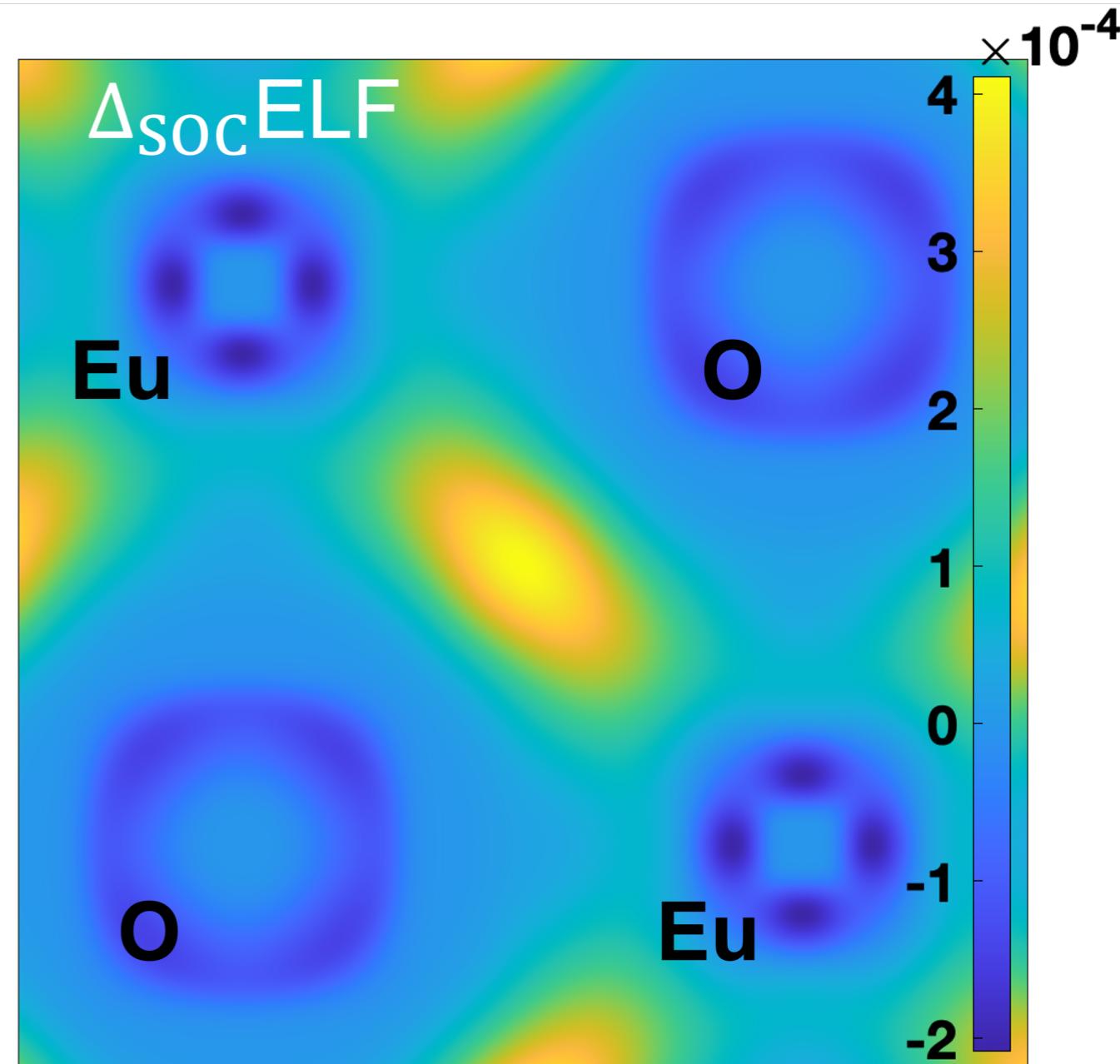
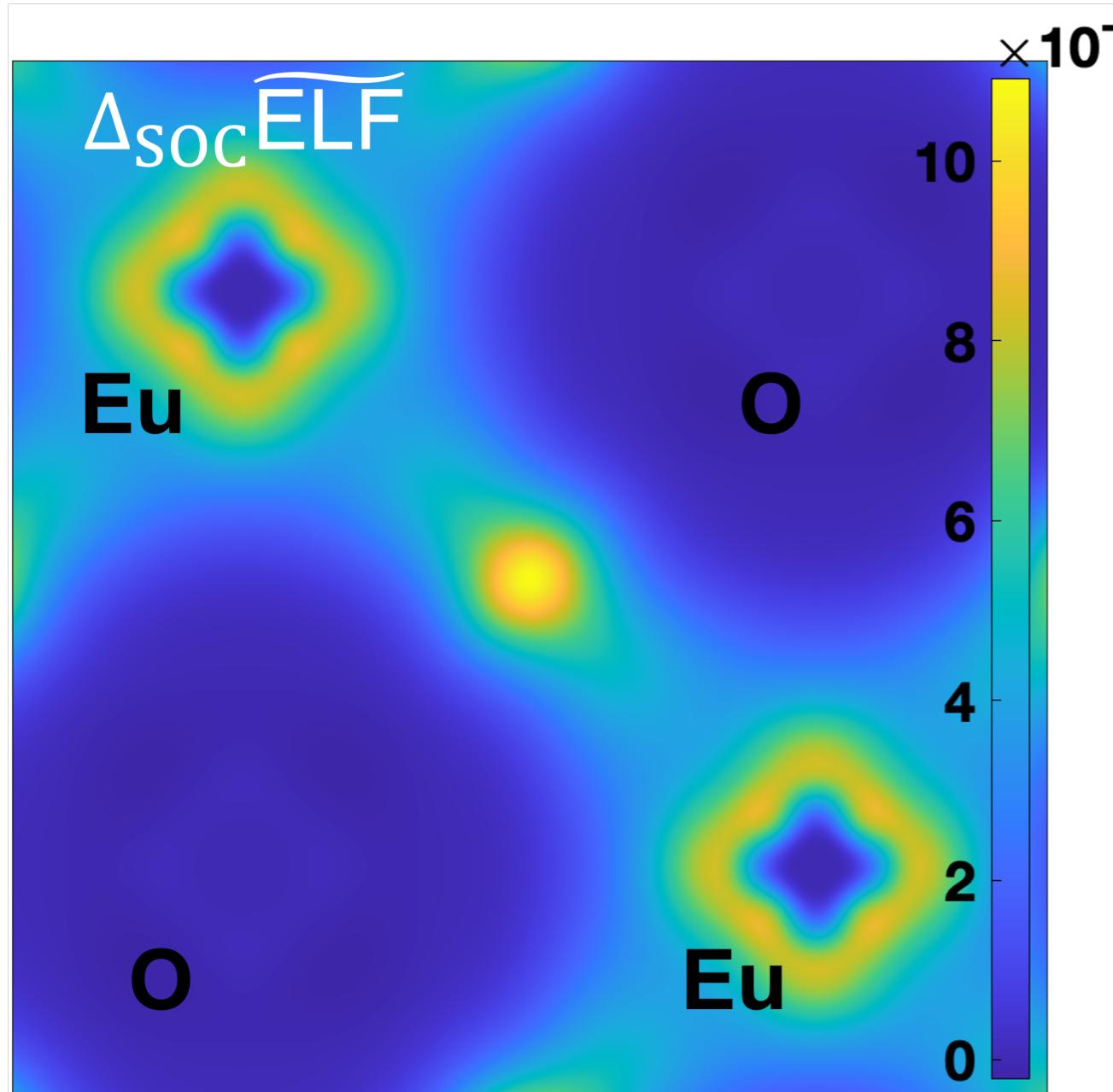
$$D(\mathbf{r}) = \boxed{\tau(\mathbf{r})} - \frac{\nabla n(\mathbf{r}) \cdot \nabla n(\mathbf{r})}{8n(\mathbf{r})}$$

$$\tilde{\tau}_{\text{nc}}(\mathbf{r}) = \left(\tau_{\text{nc}}(\mathbf{r}) - \frac{\mathbf{j}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r})}{2n(\mathbf{r})} + \frac{\nabla m^a(\mathbf{r}) \cdot \nabla m^a(\mathbf{r})}{8n(\mathbf{r})} \right) + \left(\frac{m^a(\mathbf{r}) \tau_{\text{nc}}^a(\mathbf{r})}{n(\mathbf{r})} - \frac{\mathbf{J}^a(\mathbf{r}) \cdot \mathbf{J}^a(\mathbf{r})}{2n(\mathbf{r})} \right)$$

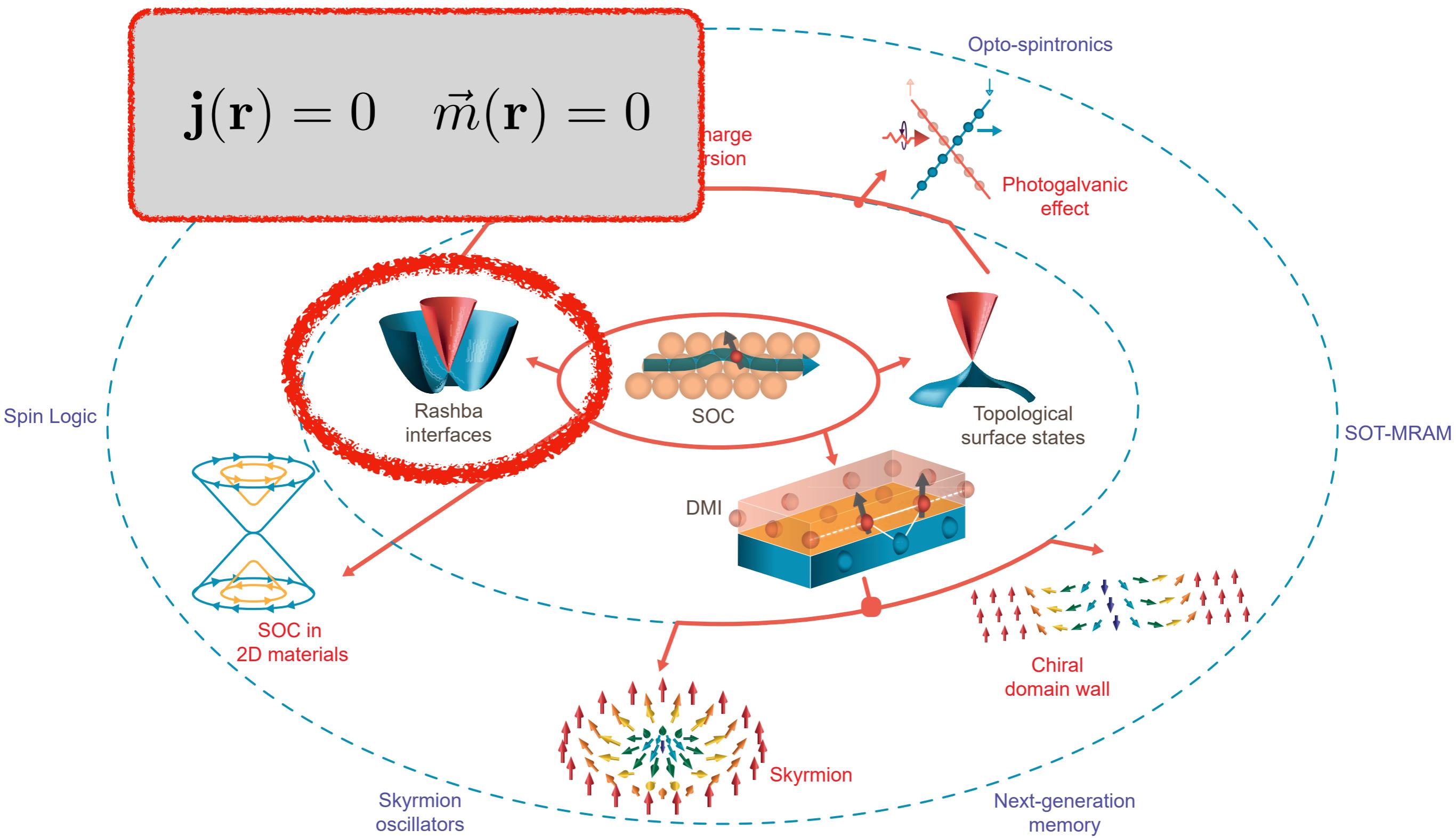
Gauge invariant ELF for Cr₃



SOC effect in EuO



Let's consider Rashba's splittings



Spin Currents via the Gauge Principle for Meta-Generalized Gradient Exchange-Correlation Functionals

Jacques K. Desmarais^{1,*}, Jefferson Maul¹, Bartolomeo Civalleri¹, Alessandro Erba¹,
Giovanni Vignale², and Stefano Pittalis^{1,†}

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²*Institute for Functional Intelligent Materials, National University of Singapore, 4 Science Drive 2, Singapore 117544*

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(Received 14 November 2023; accepted 15 May 2024; published 21 June 2024)



Jacques



Jeff



Mimmo



Giovanni



Alessandro

From SCAN to JSCAN 1/2

$$E_{\text{xc}} = \int d^3r \ n(\mathbf{r}) \epsilon_{\text{xc}}^{\text{SCAN}}(\mathbf{r})$$

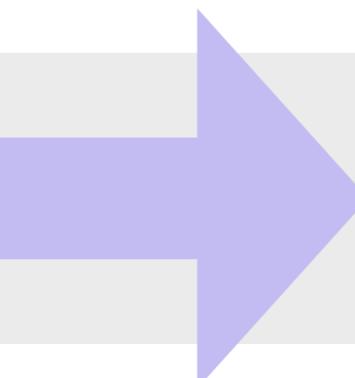
$$\tau = \frac{1}{2} \sum_j^{\text{occ}} |\nabla \varphi_j|^2$$

$$\epsilon_{\text{xc}}^{\text{SCAN}} = \epsilon_{\text{xc}}^1 + (\epsilon_{\text{xc}}^0 - \epsilon_{\text{xc}}^1) f_{\text{xc}}(\alpha)$$

$$\alpha = (\tau - \tau_W)/\tau_{\text{unif}}$$

$$\text{ELF} = 1/(1 + \alpha^2)$$

$$\tau \rightarrow \tilde{\tau} = \tau_{\text{nc}} - \frac{\vec{\mathbf{J}} \odot \vec{\mathbf{J}}}{2n}$$



$$\alpha \rightarrow \tilde{\alpha} = \alpha - \frac{\vec{\mathbf{J}} \odot \vec{\mathbf{J}}}{2n\tau_{\text{unif}}}$$

**To enforce SU(2) invariance
(time reversal symmetric states)**

From SCAN to JSCAN 2/2

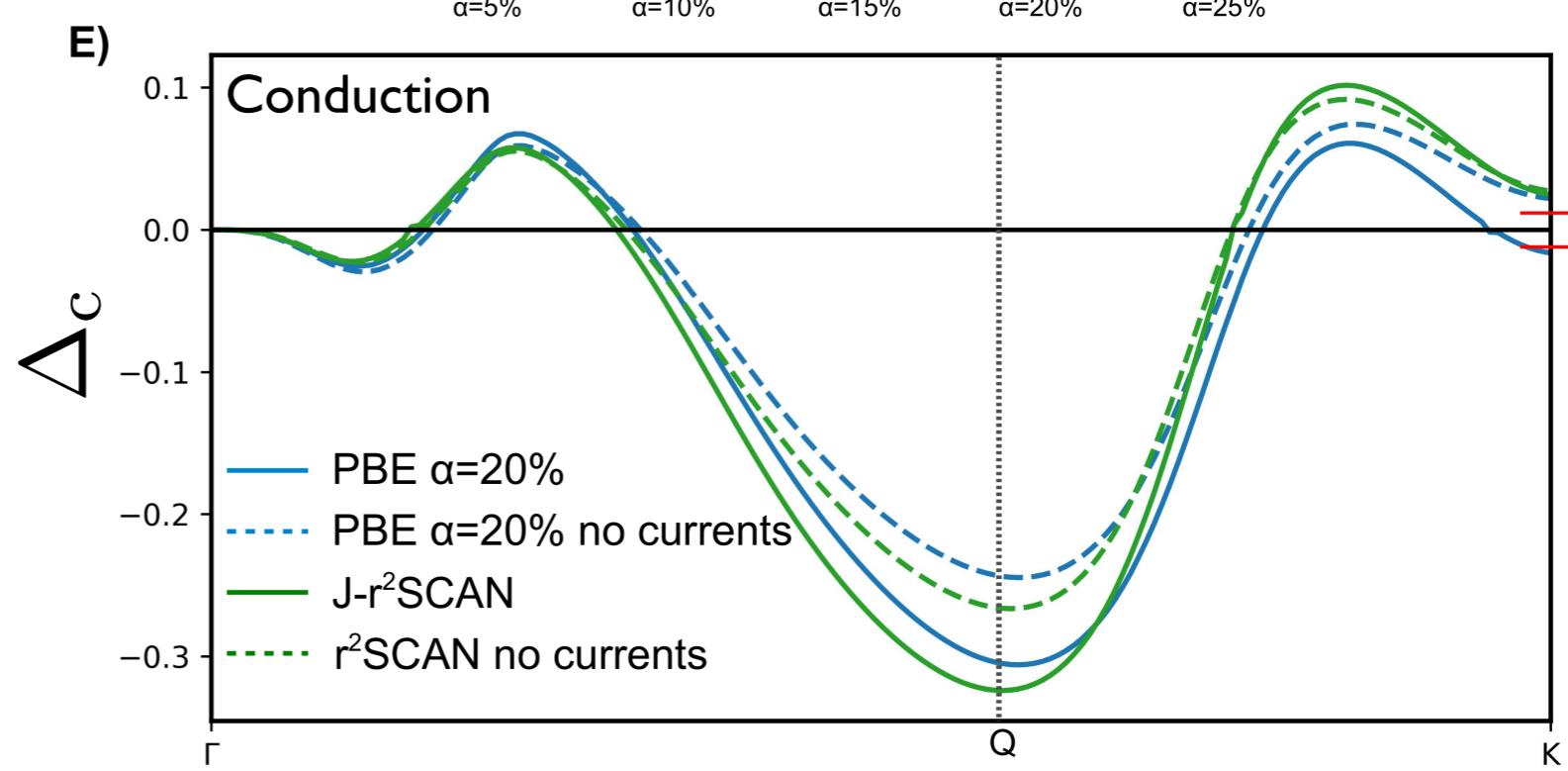
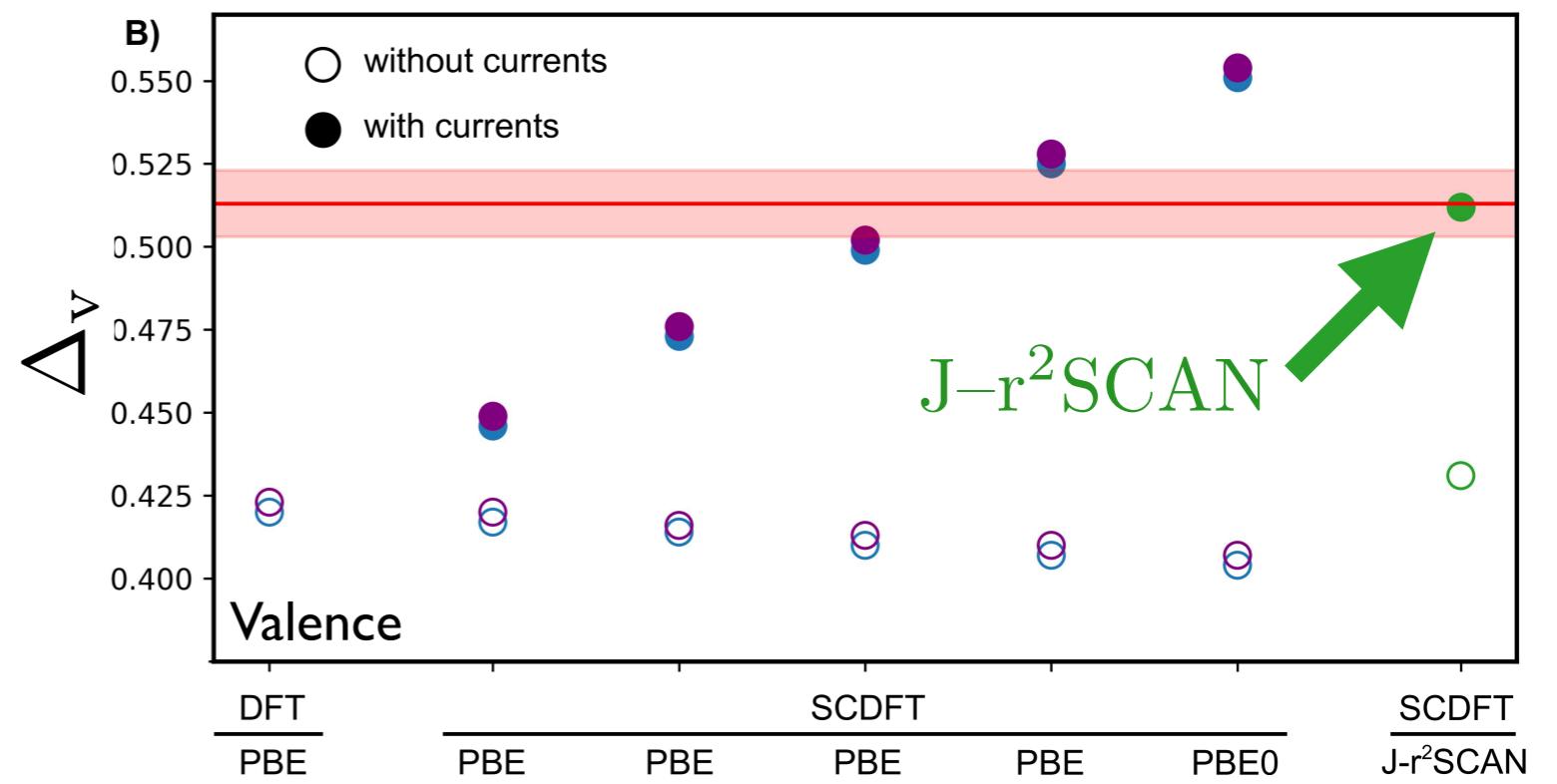
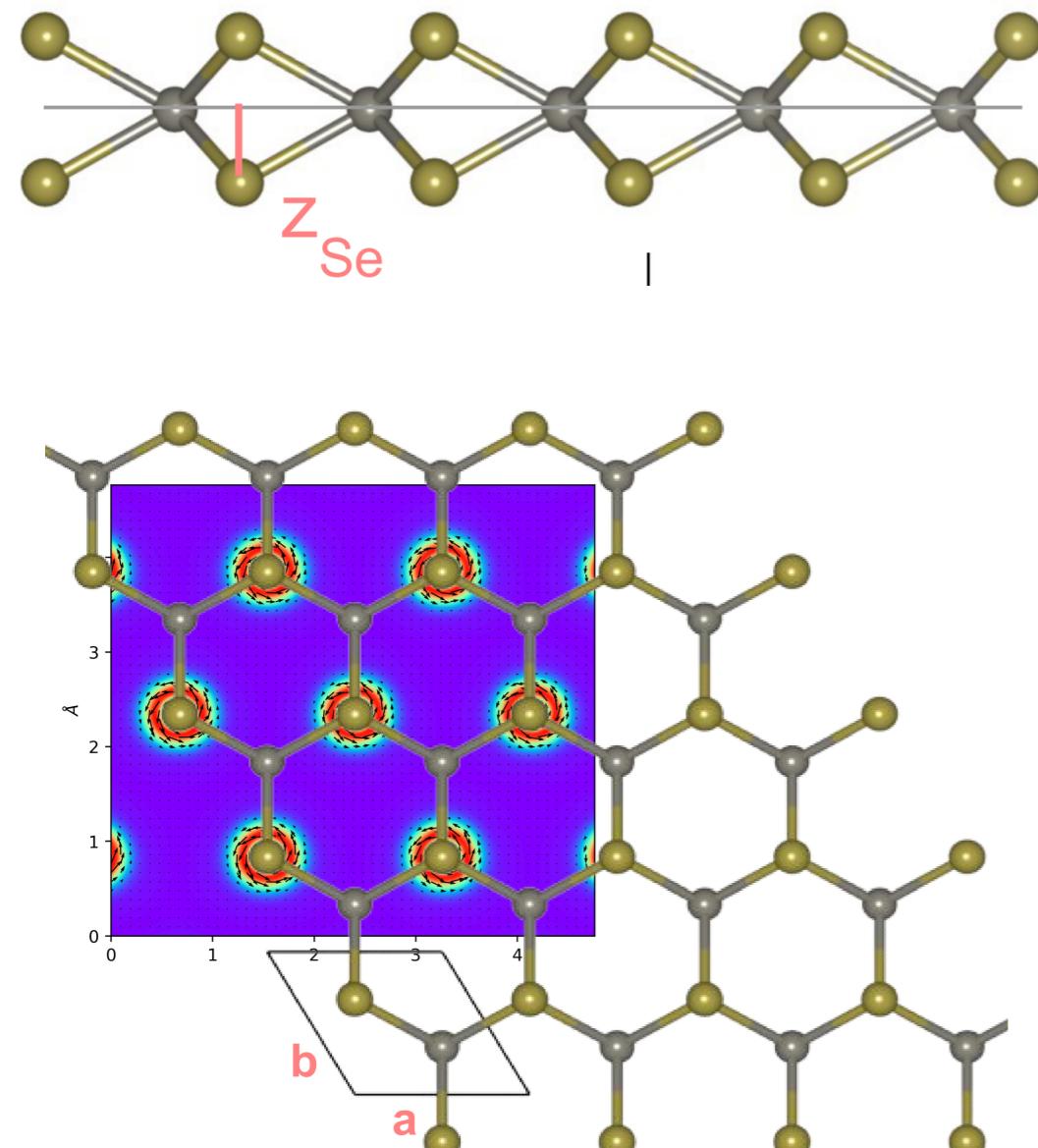
Self-consistent solutions involve a non-Abelian xc vector potential

$$\frac{1}{c} \vec{A}_{\text{xc}}^{\text{JSCAN}} = -\vec{J} \left[\frac{(\epsilon_{\text{xc}}^0 - \epsilon_{\text{xc}}^1) f'_{\text{xc}}(\tilde{\alpha})}{n\tau_{\text{unif}}} \right]$$

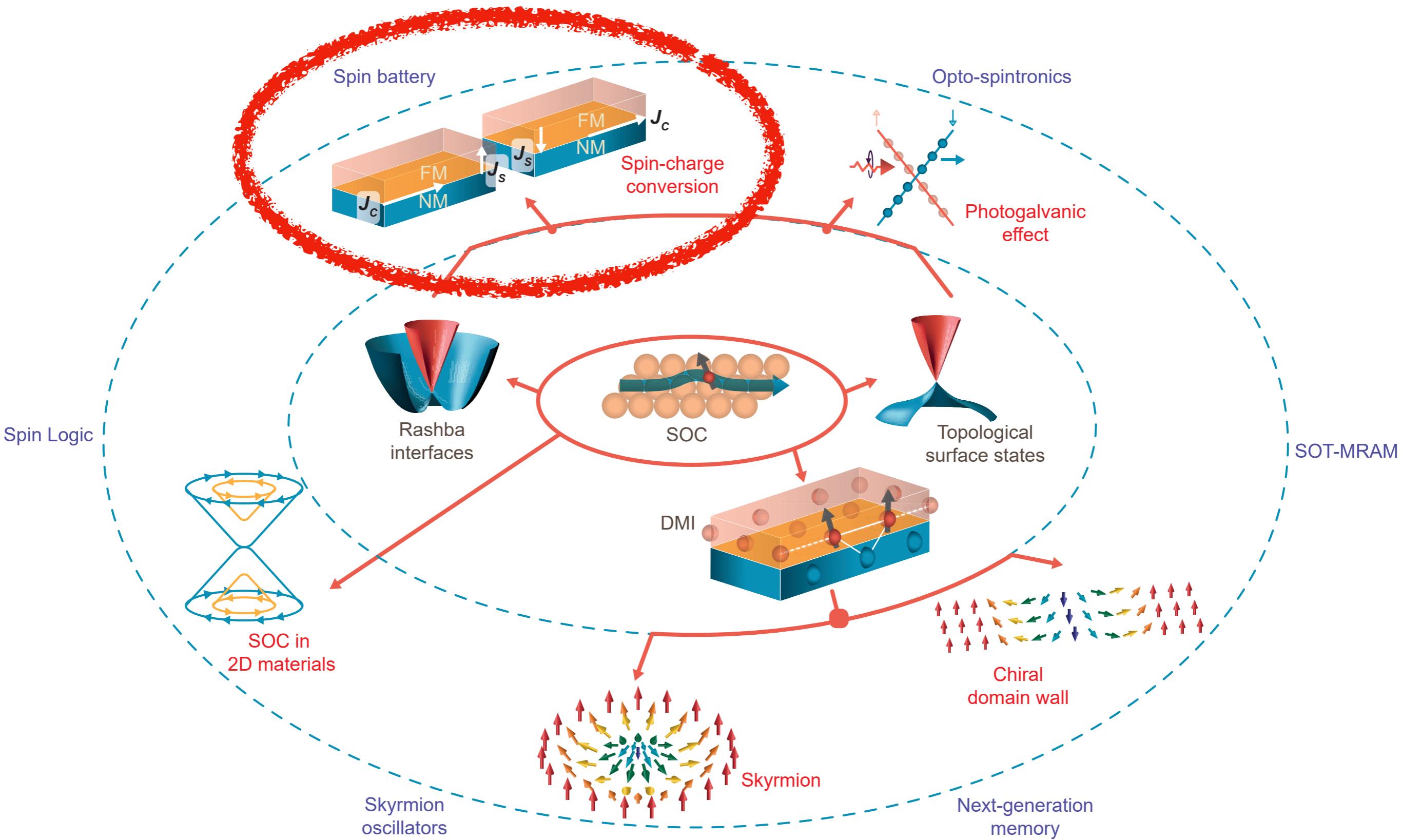
Splitting of the valence band at \mathbf{K} and band gap of molybdenum dichalcogenide Rashba systems (eV).

	2D MoSe ₂		3D α -MoTe ₂	
r ² SCAN	split 0.14	gap 1.57	split 0.28	gap 0.82
J-r ² SCAN	0.20	1.53	0.32	0.81
Exp.	0.18	1.6-2.3	0.3-0.34	1.03

WSe₂



Motivation



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Editors' Suggestion

Applicability of the Strongly Constrained and Appropriately Normed Density Functional to Transition-Metal Magnetism

Yuhao Fu and David J. Singh
Phys. Rev. Lett. **121**, 207201 – Published 14 November 2018



Article References Citing Articles (68)

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PHYSICAL REVIEW B

covering condensed matter and materials physics

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Shortcomings of meta-GGA functionals when describing magnetism



Fabien Tran, Guillaume Baudesson, Jesús Carrete, Georg K. H. Madsen, Peter Blaha, Karlheinz Schwarz, and David J. Singh
Phys. Rev. B **102**, 024407 – Published 6 July 2020



Article References Citing Articles (29)

Meta-Generalized-Gradient Approximation made Magnetic

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arXiv:2409.15201



Jacques



Alessandro



Giovanni

Modified SCAN for collinear solutions

$$E_x^{\text{mSCAN}}[n_{\uparrow}, n_{\downarrow}] = \int d^3r \ n \ \epsilon_x^{\text{unif}}(n_{\uparrow}, n_{\downarrow}) \ F_x^{\text{SCAN}}(n, s, \tilde{\alpha})$$

$$E_c^{\text{mSCAN}}[n_{\uparrow}, n_{\downarrow}] = \int d^3r \ n \ \epsilon_c^{\text{unif}}(n_{\uparrow}, n_{\downarrow}) \ F_c^{\text{SCAN}}(n, \zeta, s, \tilde{\alpha})$$

$$\tilde{\alpha} := \frac{n^{\uparrow}\tau^{\uparrow} + n^{\downarrow}\tau^{\downarrow} - \frac{(\nabla n^{\uparrow}) \cdot (\nabla n^{\downarrow})}{4}}{\frac{n^{\uparrow}}{2}\tau_{\text{unif}}^{\uparrow} + \frac{n^{\downarrow}}{2}\tau_{\text{unif}}^{\downarrow}}$$

Ferromagnetic metals

Spin moments (in μ_b /atom) and, within parentheses, magnetic energies (in meV) of FM metals as calculated with DFAs and compared against experiments.

	Fe	Co	Ni
LDA	2.23 (467)	1.57 (396)	0.56 (40.8)
PBE	2.26 (581)	1.59 (504)	0.56 (49.0)
SCAN	2.62 (1177)	1.74 (1175)	0.66 (113)
mSCAN	2.15 (461)	1.58 (447)	0.56 (47.3)
EXP	1.98-2.08	1.52-1.62	0.52-0.55

Non-magnetic systems

Spin moments (in μ_b /atom) and, within parentheses, magnetic energies (in meV) of FM metals as calculated with DFAs and compared against experiments.

	V	Pd	Cr ₂
LDA	0.00 (0.00)	0.00 (0.00)	2.69 (0.30)*
PBE	0.00 (0.00)	0.20 (0.70)	5.32 (0.87)*
SCAN	0.57 (6.27)	0.44 (17.2)	5.62 (10.3)*
mSCAN	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
EXP	0.00	0.00	0.00

* Values in eV.

Calculations from a ferromagnetic guess density matrix and the spin-moments were relaxed along the self-consistent procedure.

Anti-ferromagnetic Mott insulators

Spin moments (in μ_b /atom) and, within parenthesis, band gaps (in eV) of AFM Mott insulators as calculated with DFAs and compared against the experiments.

	FeO	CoO	NiO
LDA	3.51 (0.000)	2.40 (0.000)	1.20 (0.452)
PBE	3.57 (0.000)	2.48 (0.000)	1.37 (0.986)
SCAN	3.67 (0.635)	2.65 (1.29)	1.62 (2.66)
mSCAN	3.57 (0.224)	2.52 (0.440)	1.44 (1.29)
EXP*	2.32-4.00	1.75-2.98	1.45-1.90
EXP	(2.40)	(3.10-4.10)	(3.7)

*We remove the orbital contributions provided in Tran *et. al.* PRB **102** 024407.

**SpinCurrent-DFT can solve old and new problems
in nanomagnetism**



**Also relevant for simulating
quantum materials**

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in many
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