Spin Orbit coupling implementation in SIESTA

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• Motivation
• Relativistic approximations in SIESTA and magnetism
• Non-collinear magnetism
• Pseudopotential approximation
• Non-local pseudopotential operators and Spin-Orbit Coupling
  └─ Scalar Relativistic calculations
  └─ Fully Relativistic calculations
• Practical issues
• Some results
Motivation

Relativistic approximations in SIESTA and magnetism
Non-collinear magnetism
Pseudopotential approximation
Non-local pseudopotential operators and Spin-Orbit Coupling
  ➔ Scalar Relativistic calculations
  ➔ Fully Relativistic calculations

Practical issues

Some results
Nano-devices (DFT capabilities):

- Medical applications
- Catalytic reactions
- High density magnetic recording
- Biological sensors
- Optoelectronics, etc
Nano-devices (DFT capabilities):

- Medical applications
- Catalytic reactions
- High density magnetic recording
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Motivation

Nano-devices (DFT capabilities):
- Medical applications
- Catalytic reactions
- High density magnetic recording
- Biological sensors
- Optoelectronics, etc.

Multilayers, thin films

Magnetic nanoparticles onto a surface:

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Nano-devices (DFT capabilities):

- Medical applications
- Catalytic reactions
- High density magnetic recording
- Biological sensors
- Optoelectronics, etc

**Major obstacle:** Superparamagnetic limit

\[ \tau_N = \tau_0 \exp\left(\frac{K_u V}{k_B T}\right) \]

Neel relaxation law

\( K_u \): Anisotropy
\( V \): NP volume

Energy barrier
Motivation

Au fcc:

Topological Insulators

Dirac cone

Bi$_2$Se$_3$
Summary

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  - Scalar Relativistic calculations
  - Fully Relativistic calculations
- Practical issues
- Some results
Scalar Relativistic Hamiltonian:

$$H^{SR\ TOTAL} = H^{NR} + H^{SR} \iff H^{SR\ SIESTA} = H^{SR\ KS}$$

- magnetic systems
Scalar Relativistic Hamiltonian:

\[
H_{TOTAL}^{SR} = H_{NR} + H_{SR}
\]

- magnetic systems

Darwin and velocity corrections terms

\[
H_{SR}^{Siesta} = H_{KS}^{SR}
\]
Relativistic approximations in SIESTA and magnetism

\[
\begin{bmatrix}
\hat{T}_e + \hat{V}^{ps}_e + \hat{V}_H + \hat{V}^\sigma_{XC}
\end{bmatrix}
\]

Darwin and velocity corrections terms

- Scalar Relativistic Hamiltonian:

\[
H_{TOTAL}^{SR} = H_{NR} + H_{SR}
\]

\[
H_{TOTAL}^{SIESTA} = H_{KS}^{SR}
\]

- magnetic systems

• Fully relativistic Hamiltonian:

\[
H_{TOTAL} = H_{NR} + H_{SR} + H_{SO}
\]

\[
H_{TOTAL}^{FR} = H_{KS}^{SR} + H_{SO}
\]

- Spin – orbit coupling

\[
H_{KS}^{SR} = h_{\mu \nu}^{KS, \uparrow \downarrow}
\]

\[
h_{\mu \nu}^{KS, \uparrow \downarrow} = 0
\]

\[
H_{KS}^{SR} = 0
\]

\[
h_{\mu \nu}^{KS, \uparrow \downarrow} = 0
\]

\[
\alpha \mathbf{L} \cdot \mathbf{S}
\]

No relativistic KS Hamiltonian

Relativistic corrections

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Relativistic approximations in SIESTA and magnetism

- **Scalar Relativistic Hamiltonian:**
  \[ H_{TOTAL}^{SR} = H_{NR} + H_{SR} \]
  \[ H_{TOTAL}^{SIESTA} = H_{KS}^{SR} \]

- **Fully relativistic Hamiltonian:**
  \[ H_{TOTAL}^{FR} = H_{NR} + H_{SR} + H_{SO} \]
  \[ H_{TOTAL}^{SIESTA} = H_{KS}^{SR} + H_{SO} \]

- **Spin – orbit coupling**

  ![Diagram](image)

  - Darwin and velocity corrections terms
  - Magnetic systems
  - No relativistic KS Hamiltonian
  - Relativistic corrections \( \propto \mathbf{L} \cdot \mathbf{S} \)
  - Degeneracy \( 2J + 1 \)

  - Magnetic systems

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- Relativistic approximations in SIESTA and magnetism
  - **Non-collinear magnetism**
  - Pseudopotential approximation
  - Non-local pseudopotential operators and Spin-Orbit Coupling
    - Scalar Relativistic calculations
    - Fully Relativistic calculations
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SIESTA non-collinear:

- LSDA: colineal (common quantization axis)

\[ H_{TOTAL}^\sigma = \hat{T}_e + \hat{V}_{ps}^\sigma + \hat{V}_H + \hat{V}_{XC}^\sigma \]
SIESTA non-collinear:

- LSDA: colineal (common quantization axis)

\[ H^\sigma_{TOTAL} = [\hat{T}_e + \hat{V}^\sigma_{ps} + \hat{V}_H + \hat{V}^\sigma_{XC}] \]

- SO: no-colineal (quantization axis varies with r)

\[ H^{\sigma\sigma'}_{TOTAL} = [\hat{T}_e + \hat{V}^{\sigma\sigma'}_{ps} + \hat{V}_H + \hat{V}^{\sigma\sigma'}_{XC}] \]
SIESTA non-collinear:

- LSDA: colineal (common quantization axis)
  \[ H_{TOTAL}^{\sigma} = \left[ \hat{T}_e + \hat{V}_{ps}^{\sigma} + \hat{V}_H + \hat{V}_{XC}^{\sigma} \right] \]

- SO: no-collinear (quantization axis varies with \( r \))
  \[ H_{TOTAL}^{\sigma\sigma'} = \left[ \hat{T}_e + \hat{V}_{ps}^{\sigma\sigma'} + \hat{V}_H + \hat{V}_{XC}^{\sigma\sigma'} \right] \]

\[ \rho = \begin{pmatrix} \uparrow & \downarrow \\ \downarrow & \uparrow \end{pmatrix} \xrightarrow{U\rho U^\dagger \text{ locally}} \tilde{\rho} = \begin{pmatrix} \uparrow \\ \downarrow \end{pmatrix} \]

\[ \tilde{V}_{XC}^{\sigma} \left[ \tilde{\rho}^{\sigma} \right] \xrightarrow{U^\dagger(r)\tilde{V}_{XC}(r)U(r)} \tilde{V}_{XC}^{\sigma\sigma'}(r) = \frac{1}{2} (\tilde{V}_{XC}^{\uparrow} + \tilde{V}_{XC}^{\downarrow}) \mathbf{1} + \frac{1}{2} (\tilde{V}_{XC}^{\uparrow} - \tilde{V}_{XC}^{\downarrow}) \sigma \cdot \mathbf{m}(r) \]
SIESTA non-collinear:

- LSDA: colineal (common quatization axis)
  \[ H^{\sigma}_{TOTAL} = \left[ \hat{T}_e + \hat{V}_{ps}^\sigma + \hat{V}_H + \hat{V}_{XC}^\sigma \right] \]
- SO: no-colineal (quatization axis varies with \( r \))
  \[ H^{\sigma\sigma'}_{TOTAL} = \left[ \hat{T}_e + \hat{V}_{ps}^{\sigma\sigma} + \hat{V}_H + \hat{V}_{XC}^{\sigma\sigma'} \right] \]

\[
\rho = \begin{pmatrix}
\uparrow & \uparrow \\
\downarrow & \downarrow
\end{pmatrix}
\xrightarrow{U\rho U^\dagger \text{ locally}}
\tilde{\rho} = \begin{pmatrix}
\uparrow \\
\downarrow
\end{pmatrix}
\]

\[
\tilde{V}_{XC}^\sigma \left[ \tilde{\rho}^\sigma \right] \rightarrow \tilde{V}_{XC}^{\sigma\sigma'}(r) = \frac{1}{2}(\tilde{V}_{XC}^\uparrow + \tilde{V}_{XC}^\downarrow) + \frac{1}{2}(\tilde{V}_{XC}^\uparrow - \tilde{V}_{XC}^\downarrow) \sigma \cdot \mathbf{m}(r)
\]

\[
|\mathbf{m}| = \sqrt{(\rho^{\uparrow\uparrow} - \rho^{\downarrow\downarrow})^2 + 4(Re\{\rho^{\uparrow\downarrow}\})^2 + Im\{\rho^{\uparrow\downarrow}\}^2}
\]

\[
\tan \theta(r) = \frac{2[[Re \rho^{\uparrow\downarrow}]^2 + [Im \rho^{\uparrow\downarrow}]^2]^{1/2}}{[\rho^{\uparrow\uparrow} - \rho^{\downarrow\downarrow}]}
\]

\[
\tan \phi(r) = -\frac{Im \rho^{\uparrow\downarrow}}{Re \rho^{\uparrow\downarrow}}
\]
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Pseudopotential approximation

Bond between atoms

- Core e\(^{-}\) are independent

Join the effect of nucleus + inner e\(^{-}\)

\[ \psi_{i}^{KS, \sigma} = \epsilon_{i}^{KS, \sigma} \psi_{i}^{KS, \sigma} \]

\[ \hat{V}_{el}^{ps}(r) = \sum_{lm} V_{lm}^{ps}(r) |lm\rangle \langle lm| \]

Depend of each \( l \)
Pseudopotential approximation

Bond between atoms

- Core e\(^{-}\) are independent

Valence orbitals

Nucleus + core e

Join the effect of nucleus + inner e\(^{-}\)

\[
\hat{T}_e + \hat{V}_{el}^{\text{PS}} + \hat{V}_H + \hat{V}_{XC}^{\sigma} \psi_i^{KS,\sigma} = \varepsilon_i^{KS,\sigma} \psi_i^{KS,\sigma}
\]

\[
\hat{V}_{el}^{\text{PS}}(r) = \sum_{lm} V_{lm}^{\text{PS}}(r) |lm\rangle \langle lm| 
\]

- Exact potential from a radius
- PPs must be smooth \(\rightarrow\) Simplify the integrals
- Are generated for each atom using different XC functionals
- Troullier-Martins scheme
- Reduction of the matrix elements \(N_c+N_v\) to \(N_v\)
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Spin - orbit coupling (SO): Non-local Pseudopotential operators

\[ V_{dn} = V_{i}^{\text{ion}} = \frac{1}{2l+1} \left[ (l+1)V_{l+1/2} + lV_{l-1/2} \right] \]

\[ V_{up} = V_{i}^{\text{so}} = \frac{2}{2l+1} \left[ V_{l+1/2} - V_{l-1/2} \right] \]
Spin - orbit coupling (SO): Non-local Pseudopotential operators

ATOM (PPs generator)  
Spin Polarized: Schrödinger eq.

Fully Relativistic: Dirac: $V_{l+1/2}(r), V_{l-1/2}(r)$

$V_{dn} = V_{l}^{\text{ion}} = \frac{1}{2l+1} [(l+1)V_{l+1/2} + lV_{l-1/2}]$

$V_{up} = V_{l}^{\text{so}} = \frac{2}{2l+1} [V_{l+1/2} - V_{l-1/2}]$

• Scalar-relativistic (SR), SP ($V^{\text{ion}} = V^{\text{ps}}$), NC ($V^{\text{ion}} = V^{\text{ps}}$):

$$\hat{V}^{\text{ps}}_I = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} V^{\text{ps}}_{l,I}(r) |lm\rangle \langle lm| = \sum_{l=0}^{\infty} V^{\text{ps}}_{l,I}(r) \hat{P}_l,$$

Semi-local op.: Acts in different way on each I but in the same fashion on the radial parts.
Spin - orbit coupling (SO): Non-local Pseudopotential operators

**ATOM (PPs generator)**

Spin Polarized: Schrödinger eq.

Fully Relativistic: Dirac: \( V_{l+1/2}(r), V_{l-1/2}(r) \)

\[
\begin{align*}
V_{dn} &= V_{l}^{\text{ion}} = \frac{1}{2l+1} \left[ (l+1)V_{l+1/2} + lV_{l-1/2} \right] \\
V_{up} &= V_{l}^{\text{so}} = \frac{2}{2l+1} \left[ V_{l+1/2} - V_{l-1/2} \right]
\end{align*}
\]

- **Scalar-relativistic (SR), SP \( V^{\text{ion}} = V^{\text{ps}} \), NC \( V^{\text{ion}} = V^{\text{ps}} \):**

\[
\hat{V}_{I}^{\text{ps}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} V_{l,I}^{\text{ps}}(r)|lm\rangle\langle lm| = \sum_{l=0}^{\infty} V_{l,I}^{\text{ps}}(r)\hat{P}_{l}, \quad \leftrightarrow
\]

Matrix elements: \( M \times N^2 \)

\[
V_{I,\mu\nu}^{\text{ps}} = \langle \phi_{\mu} | \hat{V}_{I}^{\text{ps}} | \phi_{\nu} \rangle = \sum_{l,m} \int \phi_{\mu}^{*}(r)V_{l,I}^{\text{ps}}(r)\phi_{\nu}(r)d^3r
\]

Semi-local op.: Acts in different way on each \( I \) but in the same fashion on the radial parts.

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Spin - orbit coupling (SO): Non-local Pseudopotential operators

**ATOM** (PPs generator)

Spin Polarized: Schrödinger eq.

Fully Relativistic: Dirac: $V_{l+1/2}(r), V_{l-1/2}(r)$

\[
V_{dn} = V^\text{ion}_l = \frac{1}{2l+1} [(l+1)V_{l+1/2} + lV_{l-1/2}]
\]

\[
V_{up} = V^\text{so}_l = \frac{2}{2l+1} [V_{l+1/2} - V_{l-1/2}]
\]

- **Scalar-relativistic** (SR), SP ($V^\text{ion} = V^{ps}$), NC ($V^\text{ion} = V^{ps}$):  

  \[
  \hat{V}^{ps}_l = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} V^{ps}_{l,I}(r) |lm\rangle \langle lm| = \sum_{l=0}^{\infty} V^{ps}_{l,I}(r) \hat{P}_l,
  \]

  Matrix elements: M x $N^2$

  \[
  V^{ps}_{l,I,\mu\nu} = \langle \phi_\mu | \hat{V}^{ps}_l | \phi_\nu \rangle = \sum_{l,m} \int \phi^*_\mu(r)V^{ps}_{l,I}(r)\phi_\nu(r) d^3r
  \]

  Three center integrals

  Fully non-local Kleinman-Bylander (KB) op.

- **Matrix elements**: M x N elements

  - Products of two center integrals

  - $H^{Total} = \begin{pmatrix}
  \uparrow & \uparrow & 0 \\
  0 & \downarrow & \downarrow 
  \end{pmatrix}$

  $\delta \hat{V}^{ps} \approx \hat{V}^{KB} = \sum_{l=0}^{K_B} \sum_{m=-l}^{l} \sum_{n=1}^{K_B} |\chi^{KB}_{lnn}\rangle v^{KB}_{ln} \langle \chi^{KB}_{lnn}|$

  \[
  v^{KB}_{ln} = \langle \phi_{ln} | \delta V_l(r) | \phi_{ln} \rangle^{-1}
  \]

  \[
  \chi^{KB}_{lnn}(r) = \delta V_l(r) \phi_{ln}(r) Y_{lm}(\hat{r})
  \]
**On-Site Spin Orbit Coupling**

**ATOM** (PPs generator)

- Spin Polarized: Schrödinger eq.
- Fully Relativistic: Dirac: $V_{l+1/2}^i(r), V_{l-1/2}^i(r)$

\[
\begin{align*}
V_{dn} &= \frac{1}{2l+1} \left[ (l+1)V_{l+1/2} + lV_{l-1/2} \right] \\
V_{up} &= \frac{2}{2l+1} \left[ V_{l+1/2} - V_{l-1/2} \right]
\end{align*}
\]

- Fully relativistic on-site Spin-Orbit (semi-local): **ON-SITE**

\[
\hat{V}_{ps}^I = \sum_{l,J} V_{l,J}^{ps}(r) \hat{P}_J = \sum_{l,J,m_J} |Jm_J\rangle V_{l,J}^{ps}(r) \langle Jm_J|
\]
Spin Polarized: Schrödinger eq.

\[ \hat{V}_I^{ps} = \sum_{l,J} V_{l,J}^{ps}(r) \hat{P}_J = \sum_{l,J,m_J} |Jm_J \rangle V_{l,J}^{ps}(r) \langle Jm_J| \]

Changing basis from \((J,m_J)\) to \((l,m)\)

\[ \hat{V}_I^{ps}(r) = \sum_{l,m} |lm \rangle [V_{l}^{SR}(r) + V_{l}^{SO}(r) L \cdot S] \langle lm| \]

On-site SO approximation if only terms involving orbitals of the same atom are included

On-site approximation for spin–orbit coupling in linear combination of atomic orbitals density functional methods

L Fernández-Seivane, M A Oliveira, S Sanvito, and J Ferrer

### Fully relativistic on-site Spin-Orbit (semi-local): ON-SITE

\[ V_{dn} = V_{i}^{ion} = \frac{1}{2l+1} [(l+1)V_{l+1/2} + lV_{l-1/2}] \]

\[ V_{up} = V_{i}^{so} = \frac{2}{2l+1} [V_{l+1/2} - V_{l-1/2}] \]
ATOM (PPs generator)  

Spin Polarized: Schrödinger eq.

Fully Relativistic: Dirac:  

\[
V_{i+1/2}(r), V_{i-1/2}(r) \Rightarrow \begin{cases} 
V_{dn} = V_{i}^{\text{ion}} = \frac{1}{2l+1} [(l+1)\nu_{l+1/2} + l\nu_{l-1/2}] \\
V_{up} = V_{i}^{\text{so}} = \frac{2}{2l+1} [\nu_{l+1/2} - \nu_{l-1/2}] 
\end{cases}
\]

- Fully relativistic and fully non-local Off-Site Spin-Orbit implementation: OFF-SITE

\[
\begin{align*}
V_{i+1/2}(r) &= V_{dn,i}(r) + \frac{l}{2} V_{up,i}(r) \\
V_{i-1/2}(r) &= V_{dn,i}(r) - \frac{(l+1)}{2} V_{up,i}(r)
\end{align*}
\]
**ATOM** (PPs generator)  
Spin Polarized: Schrödinger eq.

Fully Relativistic: Dirac: \( V_{l+1/2}(r), V_{l-1/2}(r) \)

\[
V_{dn} = V_i^{\text{ion}} = \frac{1}{2l+1} \left( (l+1)V_{l+1/2} + lV_{l-1/2} \right)
\]

\[
V_{up} = V_i^{\text{so}} = \frac{2}{2l+1} \left( V_{l+1/2} - V_{l-1/2} \right)
\]

- Fully relativistic and fully non-local **Off-Site Spin-Orbit** implementation: OFF-SITE

\[
V_{l+1/2}(r) = V_{dn,l}(r) + \frac{l}{2} V_{up,l}(r)
\]

\[
V_{l-1/2}(r) = V_{dn,l}(r) - \frac{(l+1)}{2} V_{up,l}(r)
\]

\[
\hat{V}_l^{\text{ps}} = \sum_{l,j} V_{l,j}^{\text{ps}}(r) \hat{P}_j = \sum_{l,j,m} |Jm,j\rangle V_{l,j}^{\text{ps}}(r) \langle Jm,j|
\]
\textbf{ATOM (PPs generator)}

Spin Polarized: Schrödinger eq.

\begin{align*}
V_{dn} &= V_{i}^{\text{ion}} = \frac{1}{2l+1} [(l+1)V_{l+1/2} + lV_{l-1/2}] \\
V_{up} &= V_{i}^{\text{so}} = \frac{2}{2l+1} [V_{l+1/2} - V_{l-1/2}]
\end{align*}

Fully Relativistic: Dirac:

\begin{align*}
V_{l+1/2}(r), V_{l-1/2}(r) &\to \begin{cases}
V_{dn,l}(r) + \frac{l}{2} V_{up,l}(r) \\
V_{dn,l}(r) - \frac{(l+1)}{2} V_{up,l}(r)
\end{cases}
\end{align*}

\textbf{Fully relativistic and fully non-local \textbf{Off-Site Spin-Orbit} implementation: OFF-SITE}

\begin{align*}
\hat{V}_{i}^{\text{ps}} &= \sum_{l,J} V_{i,l}^{\text{ps}}(r) \hat{P}_{J} = \sum_{l,J,m_J} |Jm_J\rangle V_{i,l}^{\text{ps}}(r) \langle Jm_J|
\end{align*}

\textbf{Fully non-local Kleinman-Bylander (KB) op.}

\begin{align*}
\delta \hat{V}_{i}^{\text{ps}} &\approx \hat{V}_{i}^{\text{KB}} = \sum_{lJm_J} |v_{l\pm} ; lJ \pm , m_J \pm \rangle \langle v_{l\pm} ; lJ \pm , m_J \pm |
\end{align*}

\begin{align*}
v_{l\pm}(r) &= \frac{\delta V_{i,l}^{\text{ps}}(r) R_{lJ}^{\text{ps}}(r)}{\langle R_{lJ}^{\text{ps}} | \delta V_{i,l}^{\text{ps}} | R_{lJ}^{\text{ps}} \rangle^{1/2}}
\end{align*}
Off-Site Spin Orbit Coupling

**ATOM** (PPs generator)

- Spin Polarized: Schrödinger eq.
- Fully Relativistic: Dirac:
  \[
  V_{l+1/2}(r), V_{l-1/2}(r)
  \]

- Fully relativistic and fully non-local Off-Site Spin-Orbit implementation: OFF-SITE

\[
V_{l+1/2}(r) = V_{dn,l}(r) + \frac{l}{2} V_{up,l}(r)
\]

\[
V_{l-1/2}(r) = V_{dn,l}(r) - \frac{(l+1)}{2} V_{up,l}(r)
\]

\[
\hat{V}^\text{ps}_I(r) = \hat{V}^\text{SR}(r) + \hat{V}^\text{SO}(r)
\]

\[
\hat{V}^\text{SR}(r) = \sum_{lm} \left[ v_{lm}^{SR} |v_{lm}^{SR} \right]
\]

\[
\hat{V}^\text{SO}(r) = \sum_{lm} \left[ \frac{1}{4} l(l+1) - \frac{1}{2} L \cdot S \right] |v_{lm}^{SO} \langle v_{lm}^{SO} | + \sum_{lm} L \cdot S \left[ |v_{lm}^{SR} \rangle \langle v_{lm}^{SR} | + |v_{lm}^{SO} \rangle \langle v_{lm}^{SO} | \right]
\]

\[
v_{lm}^{SR}(r) = \frac{l+1}{2l+1} v_{lm}^{J+}(r) + \frac{l}{2l+1} v_{lm}^{J-}(r)
\]

\[
v_{lm}^{SO}(r) = \frac{2}{2l+1} [v_{lm}^{J+}(r) - v_{lm}^{J-}(r)].
\]

\[
\delta \hat{V}^\text{ps} \approx \hat{V}^{KB} = \sum_{IJmJmJ} |v_{IJmJmJ} \langle v_{IJmJmJ} |
\]

\[
v_{IJmJmJ}(r) = \frac{\delta V^\text{ps}_{IJm} (r) R^\text{ps}_{IJm} (r)}{\left( \langle R^\text{ps}_{IJm} | \delta V^\text{ps}_{IJm} | R^\text{ps}_{IJm} \rangle \right)^{1/2}}
\]

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- Total Energy calculations including $E_{SO}$:

$$E^{SO} = \text{Tr}(\hat{\rho} \hat{V}^{SO}) = \sum_{\mu \nu \sigma \sigma'} \rho_{\mu \nu}^{\sigma \sigma'} V_{\nu \mu}^{SO, \sigma' \sigma}$$

- Forces: 

$$F^S_O = - \sum_{\sigma \sigma'} \frac{\partial E^{SO, \sigma \sigma'}}{\partial R_i}$$

- Calculation of band structures

- Mulliken analysis population. Magnetic moments, magnetization ($S_x, S_y, S_z$), etc.

- Projected density of states

- LSDA + U

- Different vdW schemes.
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6.7 Spin polarization

Spin non-polarized

Choose the spin-components in the simulation.

NOTE: this flag has precedence over SpinOrbit, NonCollinearSpin and SpinPolarized while these older flags may still be used.

non-polarized Perform a calculation with spin-degeneracy (only one component).

polarized Perform a calculation with collinear spin (two spin components).

non-collinear Perform a calculation with non-collinear spin (4 spin components), up-down and angles.


spin-orbit Performs calculations including the spin-orbit coupling. By default the off-site SO option is set up to true. To perform an on-site SO calculations this option has to be spin-orbit+onsite.

6.8 Spin–Orbit coupling

Note: Due to the small SO energy value contribution to the total energy, the level of precision required to perform a proper fully relativistic calculation during the selfconsistent process is quite demanding. The following values must be carefully converged and checked for each specific system to assure that the results are accurate enough: SCF.H.Tolerance during the selfconsistency (typically between 10^{-3} eV – 10^{-4} eV), ElectronicTemperature, k-point sampling and high values of MeshCutoff (specifically for extended solids). In general, one can say that a good calculation will have high number of k-points, low ElectronicTemperature, extremely small SCF.DM.Tolerance and high values of MeshCutoff. We encourage the user to test carefully these options for each system. An additional point to take into account is the mixing scheme employed. You are encouraged to use SCF.Mix hamiltonian (currently is set up by default) instead of the density matrix, due to that speeds up the convergence. The pseudopotentials have to be properly generated and tested for each specific system and they have to be in their fully relativistic form together with the non-linear core corrections. Finally, it is worth to mention that the selfconsistent convergence for some non–high symmetric magnetizations directions with respect to the physical symmetry axis could be troublesome, however.
FePt – L1₀

MAE = E₉₀ – E₀ [meV]

Mesh cutoff [Ry]

MAE = E₉₀ – E₀ [meV]

K-points sampling

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Electronic and magnetic properties of bimetallic $L_1_0$ cuboctahedral clusters by means of fully relativistic density-functional-based calculations

R. Cuadrado and R. W. Chantrell
Department of Physics, University of York, York Y010 5DD, United Kingdom
(Received 25 July 2012; revised manuscript received 6 November 2012; published 18 December 2012)

Total energy vs. magnetizations angles

\[ \varphi = 0^\circ \]
\[ 0^\circ \leq \theta \leq 180^\circ \]
Some results

Electronic and magnetic properties of bimetallic $L1_0$ cuboctahedral clusters by means of fully relativistic density-functional-based calculations

R. Cuadrado and R. W. Chantrell

Department of Physics, University of York, York YO10 5DD, United Kingdom

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Total energy vs. magnetizations angles
Some results

Electronic and magnetic properties of bimetallic $L1_0$ cuboctahedral clusters by means of fully relativistic density-functional-based calculations

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Total energy vs. magnetizations angles

In-plane anisotropy
Some results

Metallic alloys \( L_{10} \)

A: M
B: NM
Some results

Topological Insulators

\( \text{Bi}_2 \text{Se}_3 \)
Thank you very much!
Spin - orbit coupling (SO): Relativistic Pseudopotentials

**ATOM** (PPs generator)

- Spin Polarized: Schrödinger eq.
- Fully Relativistic: Dirac: \( V_{l+1/2}(r), V_{l-1/2}(r) \)

\[
V_{dn} = V_{l}^{\text{ion}} = \frac{1}{2l+1} [(l+1)V_{l+1/2} + lV_{l-1/2}]
\]

\[
V_{up} = V_{l}^{\text{so}} = \frac{2}{2l+1} [V_{l+1/2} - V_{l-1/2}]
\]
Some results

$\text{Bi}_2\text{Se}_3$

GREEN geometry, SOC

$E - E_F$ (eV)