2026-01-16 Fermi-Surfaces, DFT+U, Tensor-Moments, and the ELK-Code

Sebastian Kalhöfer
Lars Nordström

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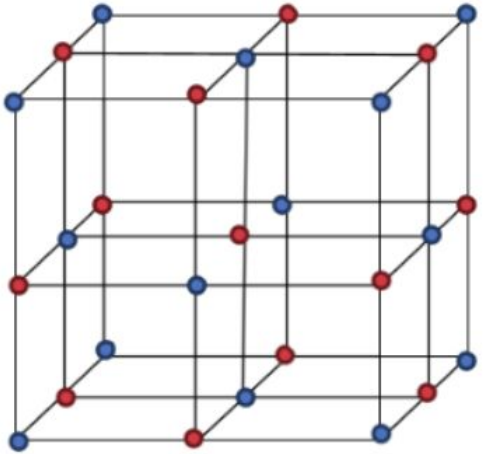
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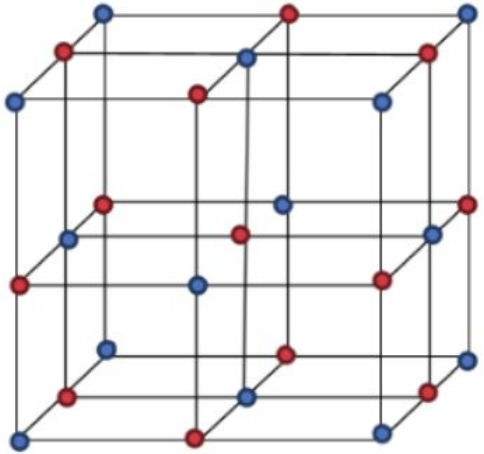
- topology
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Quick Repetition:



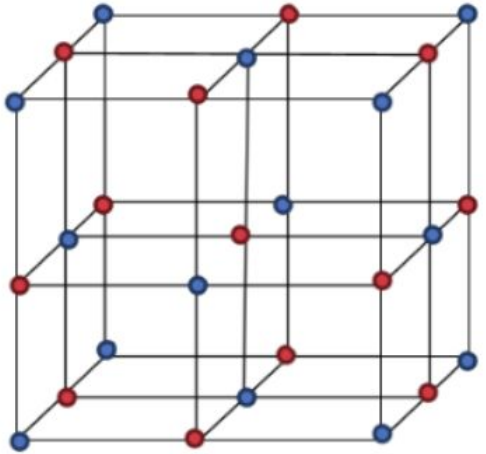
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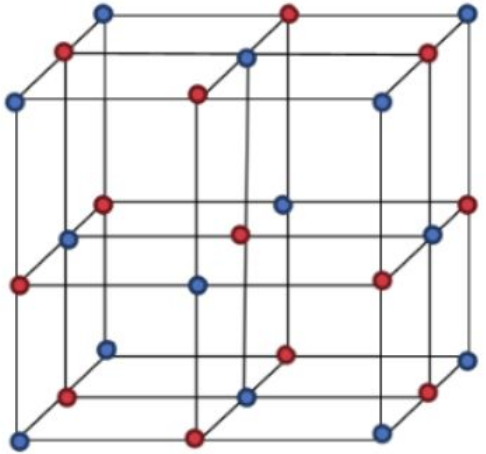
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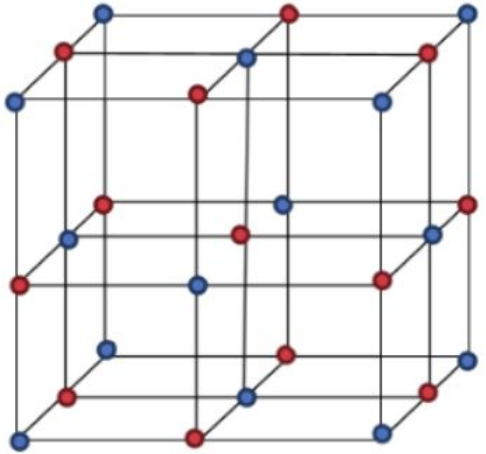


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- Born-Oppenheimer-Approximation (...)
- Focusing on the electronic Problem (...) (reliable for “many” observables & materials)
- Mean Field Approximation (...) (reliable for “many” observables & materials)

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$$\left(\left[\mathrm{T}_e + \mathrm{V}_{e-e} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a}\right]\phi_{\alpha,\tau}\right)(\mathbf{r}) = \epsilon_{\alpha,\tau}\phi_{\alpha,\tau}(\mathbf{r}) \quad \overset{\text{Approximation}}{\Longleftrightarrow} \quad \left(\left[\mathrm{T}_e + \mathrm{V}_{\text{eff}} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a}\right]\phi_{\alpha,\tau}\right)(\mathbf{r}) = \epsilon_{\alpha,\tau}\phi_{\alpha,\tau}(\mathbf{r}) \tag{2.33}$$

whereas the effective one-particle-potentials

$$\mathrm{V}_{\text{eff}}(\mathbf{r}) \equiv \sum_{i=1}^{N_e} \mathrm{V}_{\text{eff}}(\mathbf{r}_i) \equiv \sum_{i=1}^{N_e} \mathrm{V}_{\mathrm{H}}(\mathbf{r}_i) + \mathrm{V}_{\mathrm{XC}}(\mathbf{r}_i) \tag{2.34}$$

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- Born von Karman boundary conditions (...)
- Bloch-Theorem (...)

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$$\left(H\Psi_{\mathrm{sv}}\right)(\mathbf{r},s) = E_{\mathrm{sv}}\Psi_{\mathrm{sv}}(\mathbf{r},s), \tag{4.16}$$

whereas $s \in \{\uparrow,\downarrow\}$ and the Hamiltonian is given by

$$\begin{aligned} H &= \frac{\hat{\mathbf{p}}^2}{2m} + V_{\mathrm{fv}}(\mathbf{r}) \quad + H_{\mathrm{SO}}(\mathbf{r}) + \mathbf{V}_{\mathrm{xc}}(\mathbf{r})\cdot\boldsymbol{\sigma}, \\ &\equiv \qquad H_0 \qquad + H_{\mathrm{SO}}(\mathbf{r}) + \mathbf{V}_{\mathrm{xc}}(\mathbf{r})\cdot\boldsymbol{\sigma}, \end{aligned} \tag{4.17}$$

and the spin-orbit interaction term reads

$$H_{\mathrm{SO}}(\mathbf{r}) = \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\left(\boldsymbol{\nabla}V_{\mathrm{fv}}(\mathbf{r})\times\hat{\mathbf{p}}\right), \tag{4.18}$$

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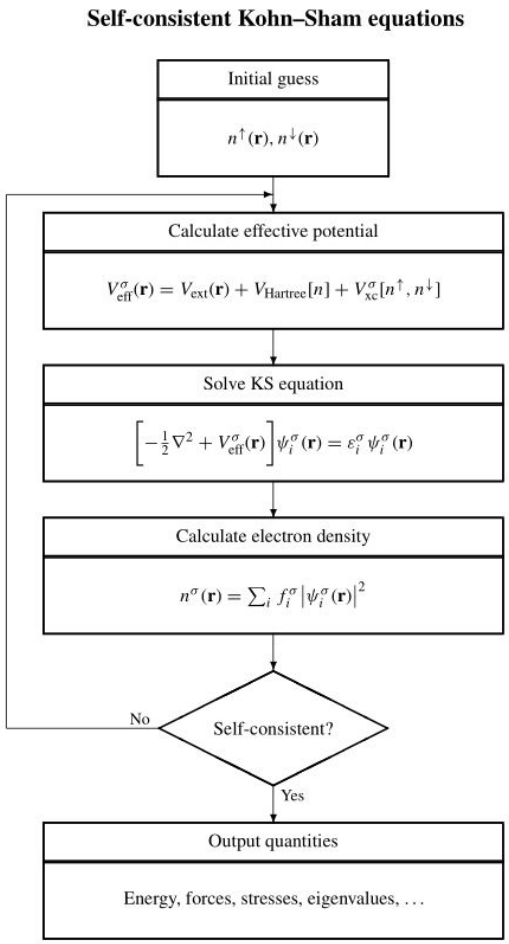
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Definition 9.1 The *[F]ermi-[S]urface of a non-interacting metallic system* is defined as the set

$$\mathrm{FS} = \left\{\mathbf{k} \in \mathrm{Q} \mid \exists n \in \mathbb{N} : \epsilon_{n\mathbf{k}} = \mu(T = 0\,\mathrm{K}) \equiv E_{\mathrm{F}}\right\}.$$

Example-System:

- Sr_2RhO_4 (Strontium rhodate)

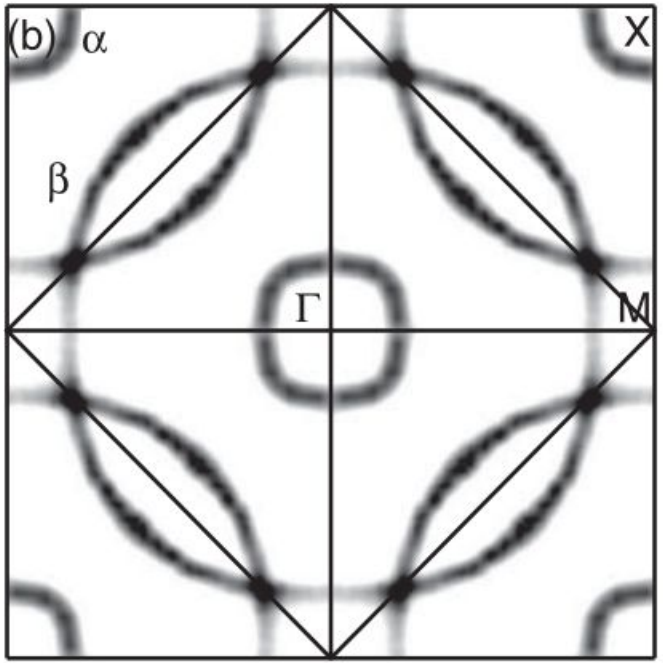
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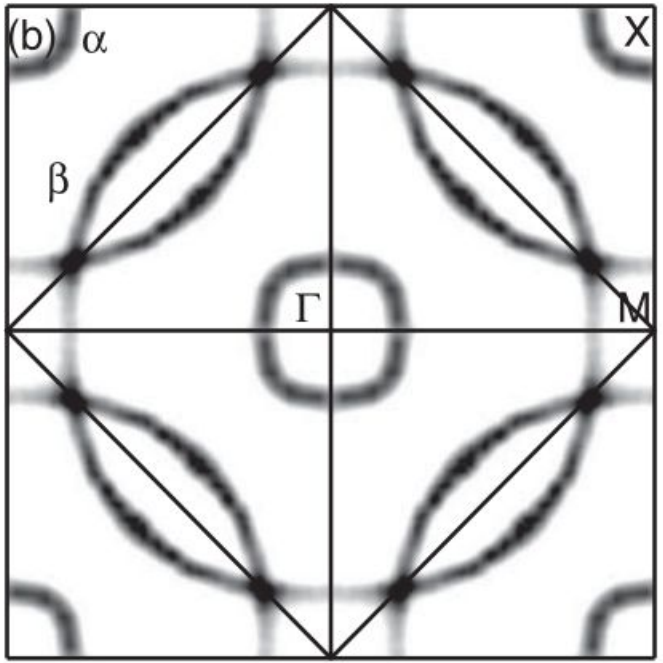
Missing xy-Band Fermi Surface in 4d Transition-Metal Oxide Sr_2RhO_4: Effect of the Octahedra Rotation on the Electronic Structure

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[1]*School of Physics and Center for Strongly Correlated Materials Research, Seoul National University, Seoul, Korea*
[2]*Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[3]*National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan*
[4]*Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea*
(Received 6 September 2005; published 7 September 2006)



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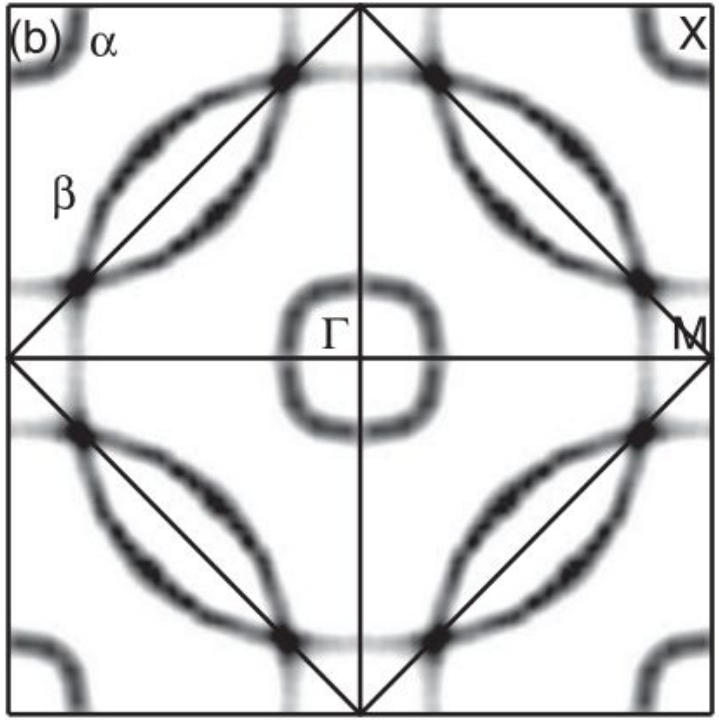
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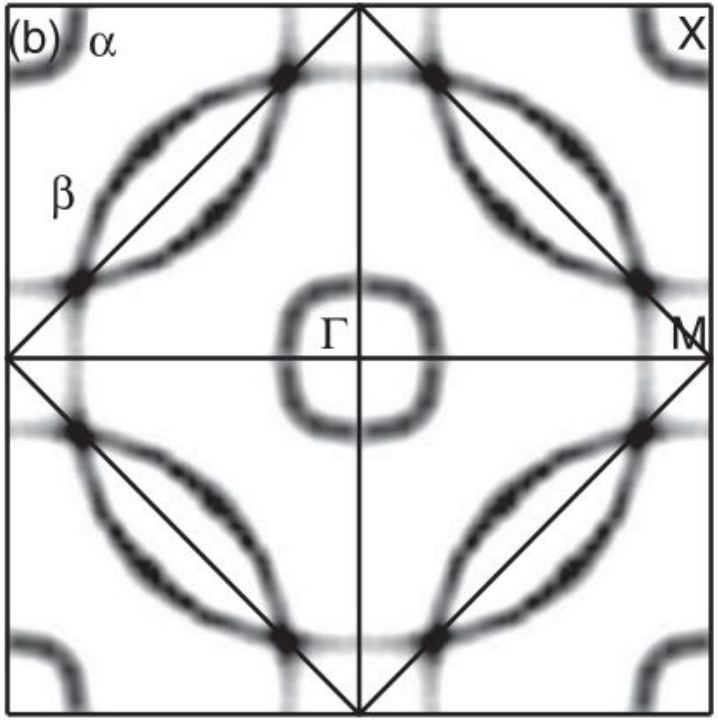
Fermi Surface and Quasiparticle Excitations of Sr_2RhO_4

F. Baumberger,[1] N. J. C. Ingle,[1,*] W. Meevasana,[1] K. M. Shen,[1,*] D. H. Lu,[1] R. S. Perry,[2] A. P. Mackenzie,[2] Z. Hussain,[3] D. J. Singh,[4] and Z.-X. Shen[1]
[1]*Departments of Applied Physics, Physics, and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305, USA*
[2]*School of Physics and Astronomy, University of St. Andrews, St. Andrews, Fife KY16 9SS, United Kingdom*
[3]*Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[4]*Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032, USA*
(Received 30 December 2005; published 20 June 2006)

- “Stealing” Data:

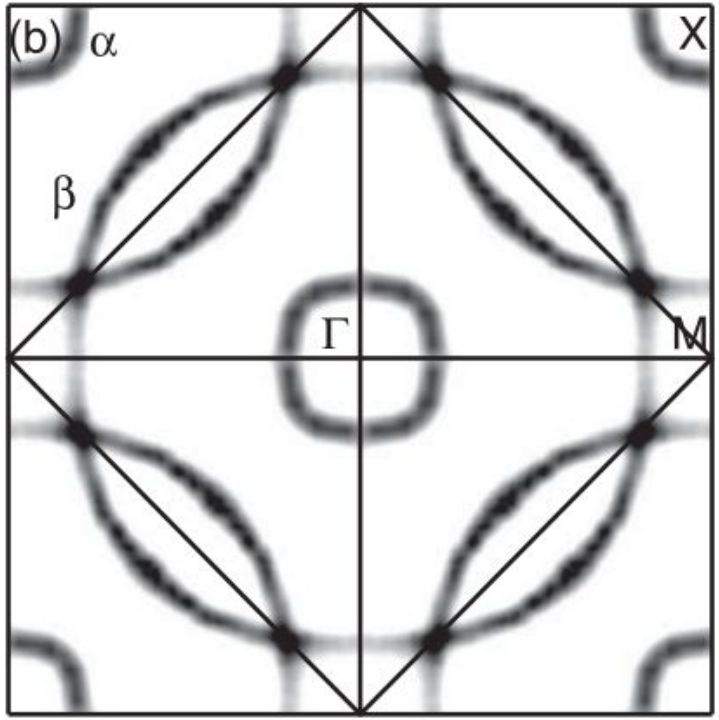


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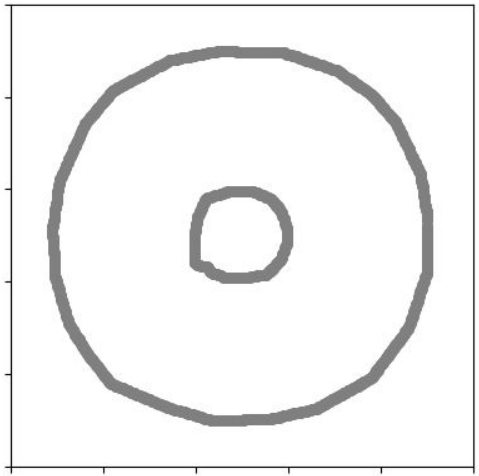




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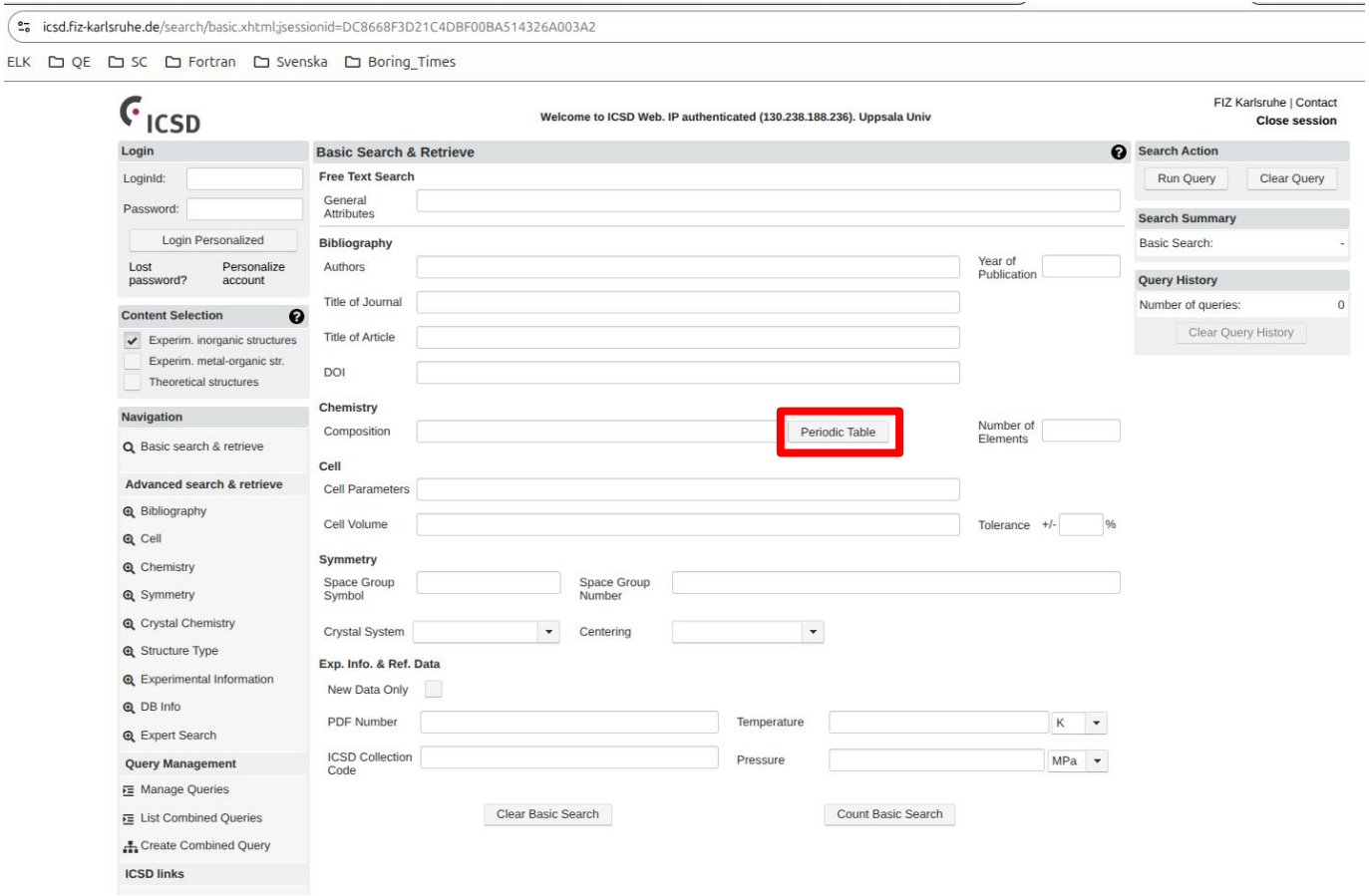




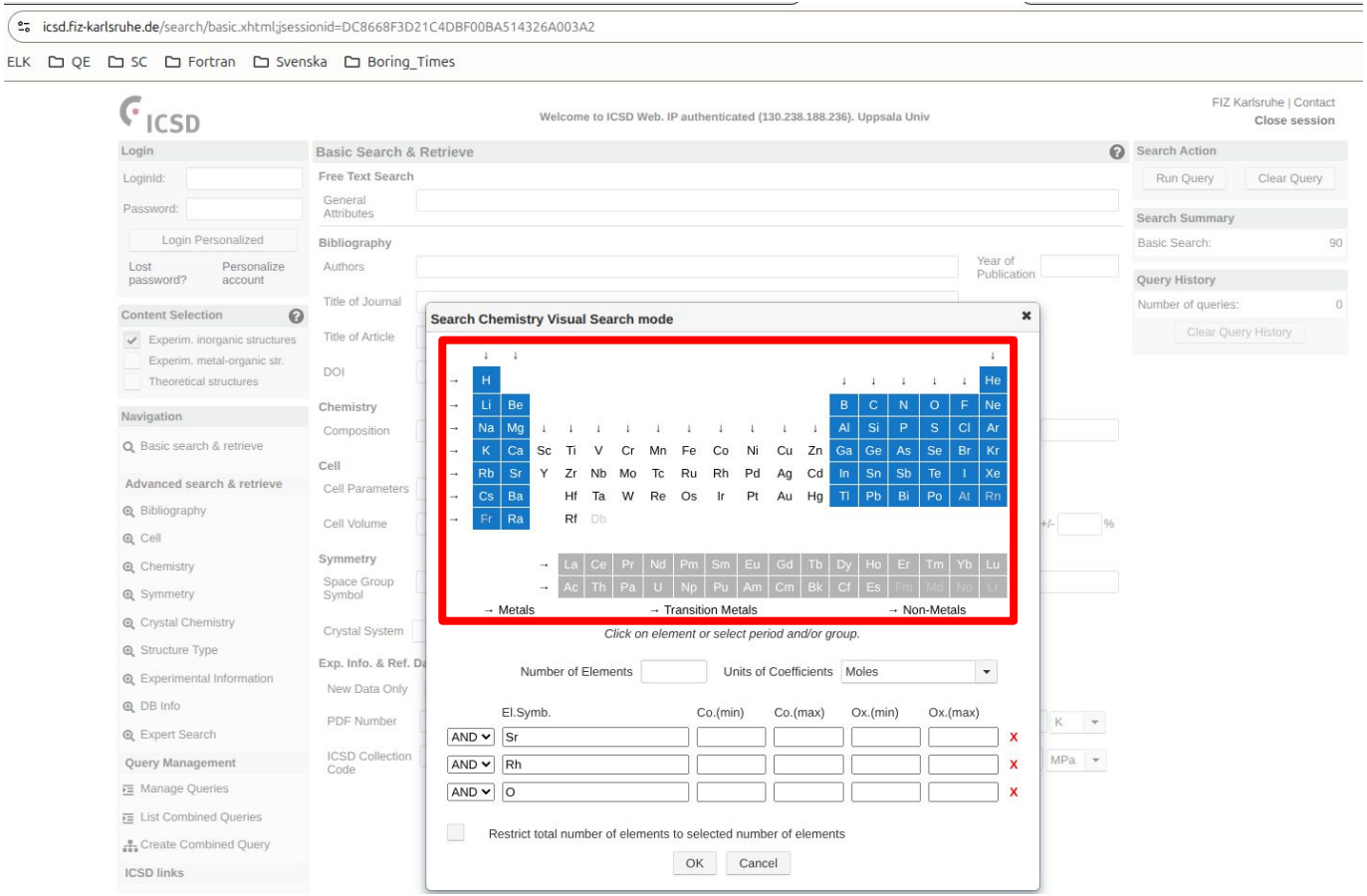


- Finding the structure

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97775	I 4/m m m	(Sr1.2 Nd0.8) (M	K2NiF4	Journal of Mater	3.85783(1) 3.85	184.63	2.00	0.101325	2003	01-072-7856
240257	P b a m	Sr4 (Rh3 O10)		Chemistry of Ma	5.4747(2) 5.474	863.61	3.50	0.101325	2004	01-073-4163
82133	I 41/a c d S	Sr2 (Rh O4)	Ca2MnO4	Journal of Solid	5.43562(9) 5.43	761.54	3.80	0.101325	1996	01-089-0595
82132	I 41/a c d S	Sr2 (Rh O4)	Ca2MnO4	Journal of Solid	5.43593(9) 5.43	761.74	10.00	0.101325	1996	01-089-0594
154943	I 4/m m m	Sr2 ((Ru0.95 Rh	K2NiF4	Journal of Physi	3.86383(5) 3.86	189.94	10.00	0.101325	2002	01-075-2879
154945	I 4/m m m	Sr2 ((Ru0.9 Rh0	K2NiF4	Journal of Physi	3.8651(1) 3.865	190.03	10.00	0.101325	2002	01-075-2881
154952	I 41/a c d S	Sr2 ((Ru0.5 Rh0	Ca2MnO4	Journal of Physi	5.4600(3) 5.460	761.81	10.00	0.101325	2002	
154954	I 41/a c d S	Sr2 ((Ru0.25 Rh	Ca2MnO4	Journal of Physi	5.4392(2) 5.439	762.32	10.00	0.101325	2002	01-075-2887
154956	I 41/a c d S	Sr2 ((Ru0.1 Rh0	Ca2MnO4	Journal of Physi	5.4416(2) 5.441	762.33	10.00	0.101325	2002	01-075-2889
154958	I 41/a c d S	Sr2 ((Ru0.05 Rh	Ca2MnO4	Journal of Physi	5.4490(3) 5.449	763.62	10.00	0.101325	2002	01-075-2891

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Detailed View Entry 1 of 1

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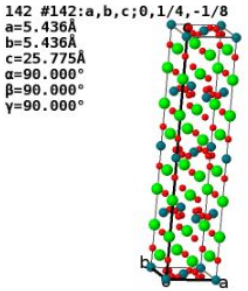
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Struct. formula	Sr2 (Rh O4)	Structure type	Ca2MnO4
Cell parameter	5.43562(9) 5.43562(9) 25.77489(60) 90. 90. 90.	Space group	I 41/a c d S (142)
Cell volume	761.54 [Å³]	Z	8
Temperature	3.8 [K]	Pressure	atmospheric
Data quality	High quality	R-value	0.052
Author	Vogt, T.; Buttrey, D.J.;	Title	Temperature dependent structural behavior of Sr2 Rh O4
Reference	Journal of Solid State Chemistry (1996) 123, p. 186-189 (11 structures)	Fulltext	Get full text by DOI Search full text by Google Scholar
See also	CCDC structures depot		

Details Expand all | Collapse all

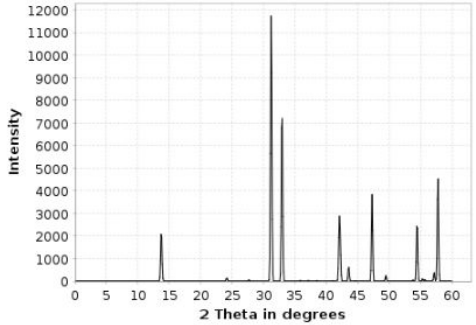
Visualization

Published Crystal Structure



Interactive Visualization

Powder Pattern



Interactive Visualization

Chemistry

Published Crystal Structure Data

Standardized Crystal Structure Data

Distances and Angles

Bibliography

Experimental information

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atoms
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  0.250000000000000   0.750000000000000   0.500000000000000    0.00000000  0.00000000  0.00000000
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scale
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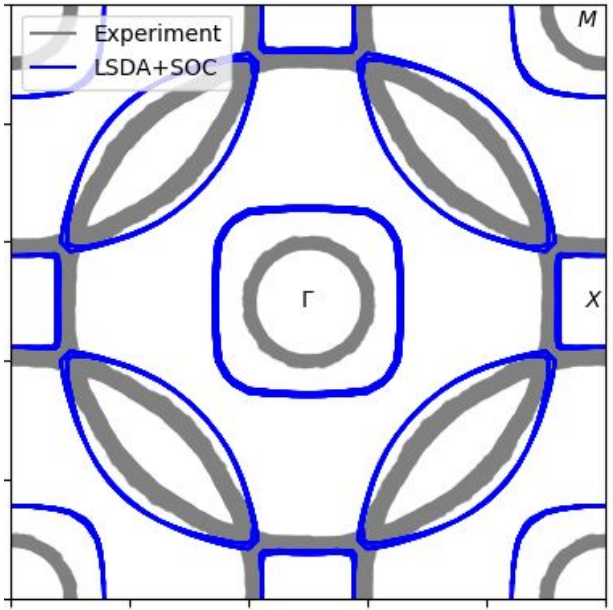
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Crystal = Lattice + Basis.

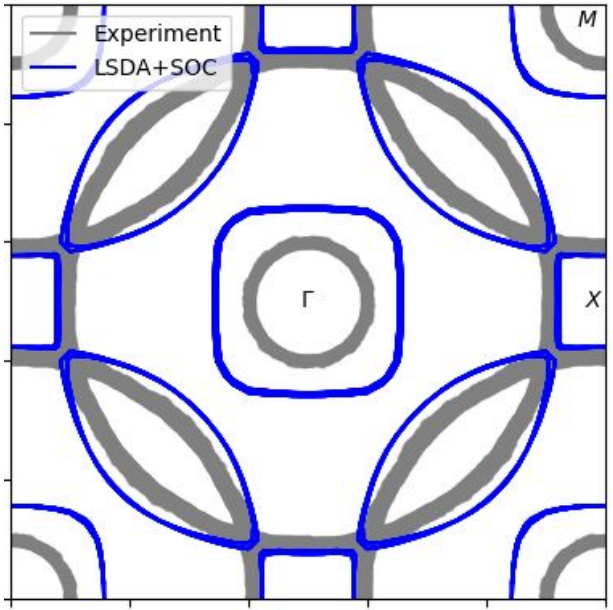
LDA (ELK-9.5.14 Calculation)

LDA (ELK-9.5.14 Calculation)



LDA (ELK-9.5.14 Calculation)

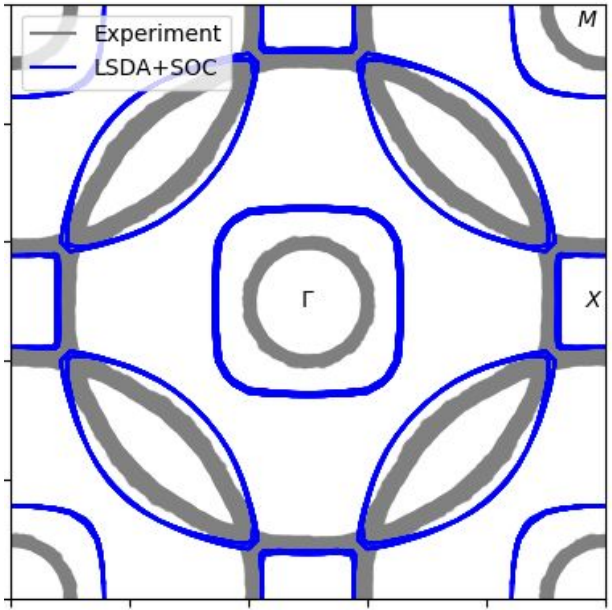
… “behind the scenes”:



LDA (ELK-9.5.14 Calculation)

… “behind the scenes”:

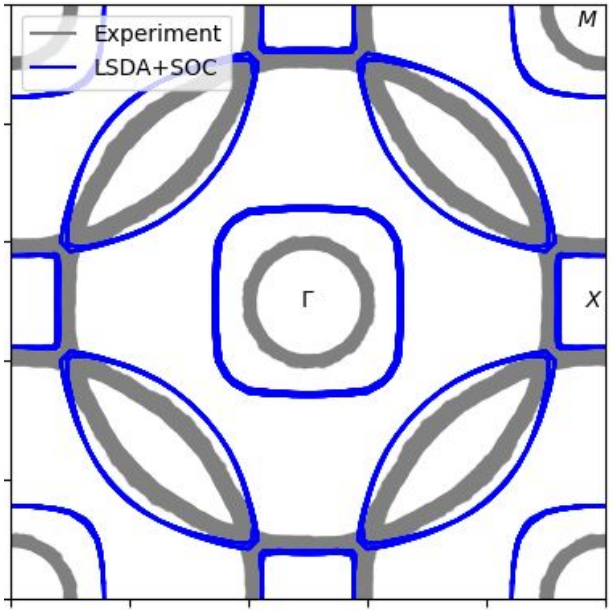
- implementing a new subroutine in ELK to compute / print the relative energies



LDA (ELK-9.5.14 Calculation)

… “behind the scenes”:

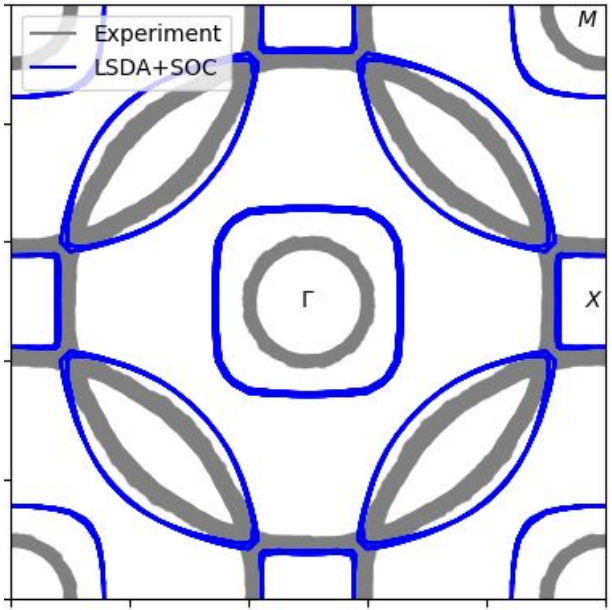
- implementing a new subroutine in ELK to compute / print the relative energies
- reading the data into a python-script



LDA (ELK-9.5.14 Calculation)

… “behind the scenes”:

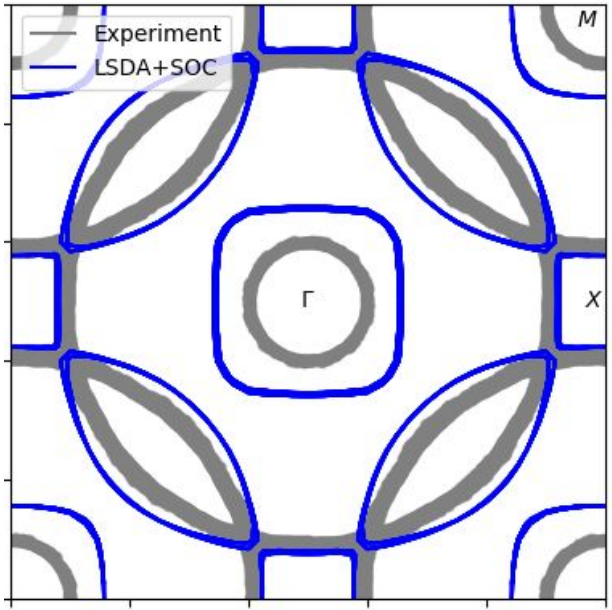
- implementing a new subroutine in ELK to compute / print the relative energies
- reading the data into a python-script
- interpolating energies on the k-sheet



LDA (ELK-9.5.14 Calculation)

… “behind the scenes”:

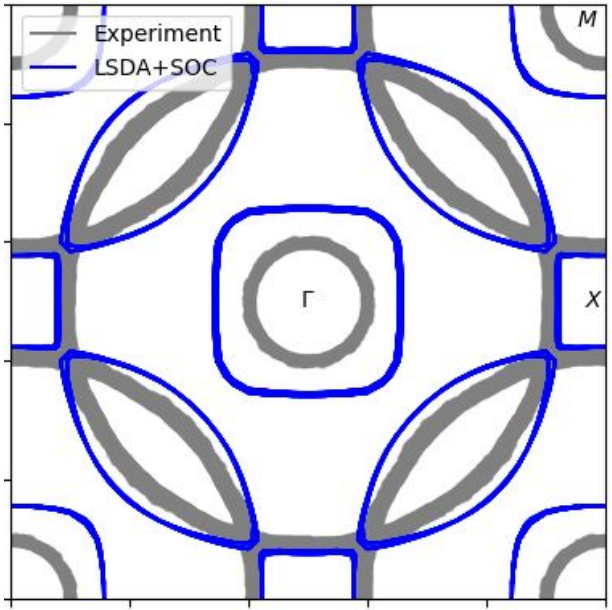
- implementing a new subroutine in ELK to compute / print the relative energies
- reading the data into a python-script
- interpolating energies on the k-sheet
- (finding the “correct” basis)



LDA (ELK-9.5.14 Calculation)

… “behind the scenes”:

- implementing a new subroutine in ELK to compute / print the relative energies
- reading the data into a python-script
- interpolating energies on the k-sheet
- (finding the “correct” basis)
- (further debugging)

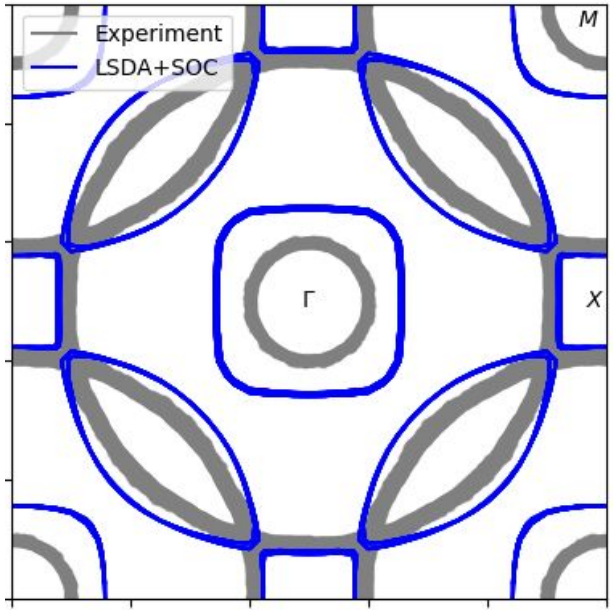


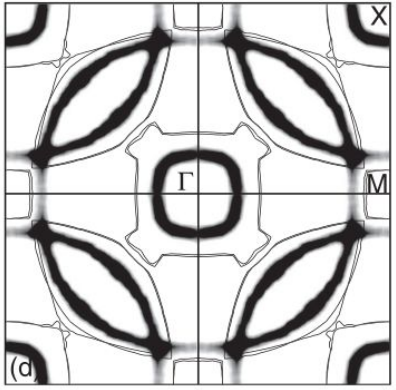
Missing xy-Band Fermi Surface in 4d Transition-Metal Oxide Sr_2RhO_4: Effect of the Octahedra Rotation on the Electronic Structure

B. J. Kim,[1] Jaejun Yu,[1] H. Koh,[2] I. Nagai,[3] S. I. Ikeda,[3] S.-J. Oh,[1] and C. Kim[4]

[1]*School of Physics and Center for Strongly Correlated Materials Research, Seoul National University, Seoul, Korea*
[2]*Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[3]*National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan*
[4]*Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea*

(Received 6 September 2005; published 7 September 2006)



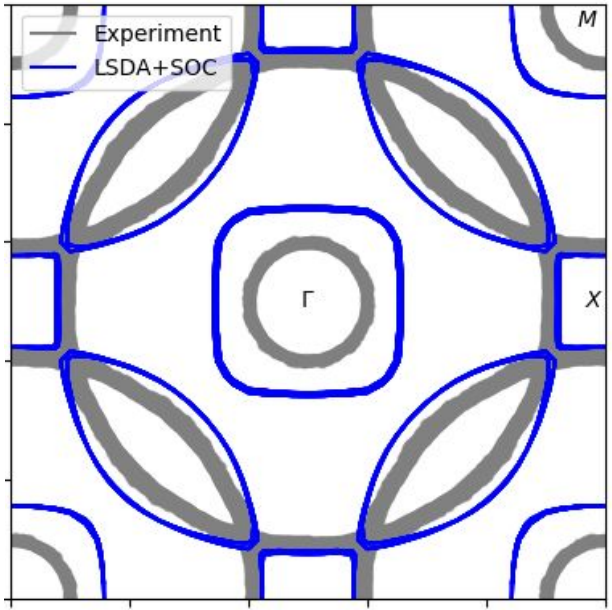


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[1]*School of Physics and Center for Strongly Correlated Materials Research, Seoul National University, Seoul, Korea*
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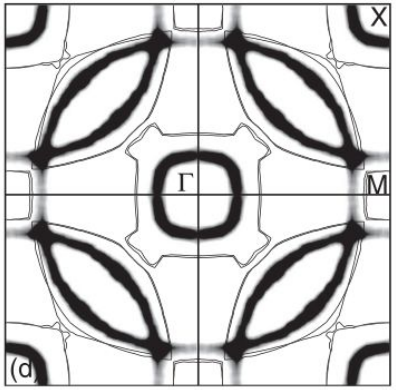


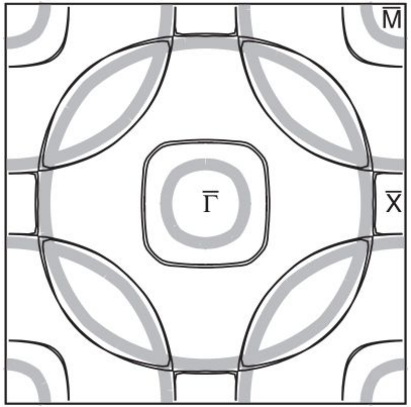
Coulomb-Enhanced Spin-Orbit Splitting: The Missing Piece in the Sr_2RhO_4 Puzzle

Guo-Qiang Liu, V. N. Antonov, O. Jepsen, and O. K. Andersen.

Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany

(Received 2 April 2008; published 11 July 2008)





Fact:

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Sometimes the
“independent electrons”-
approximation fails to reproduce
experimental results

Fact:

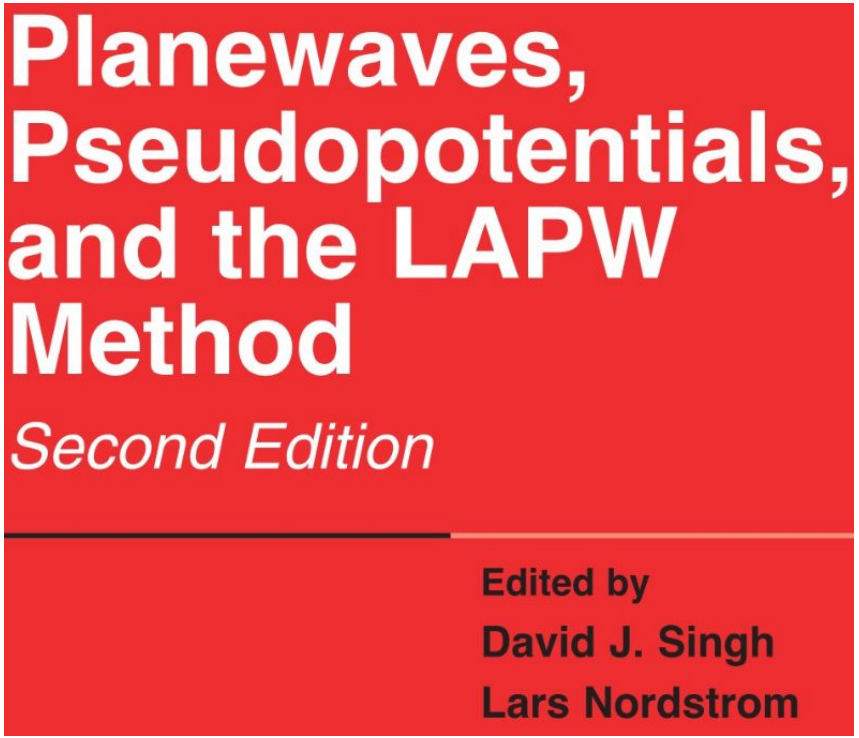
Sometimes the
“independent electrons”-
approximation fails to reproduce
experimental results

→ DFT+U

Fact:

Sometimes the "independent electrons"-approximation fails to reproduce experimental results

→ DFT+U

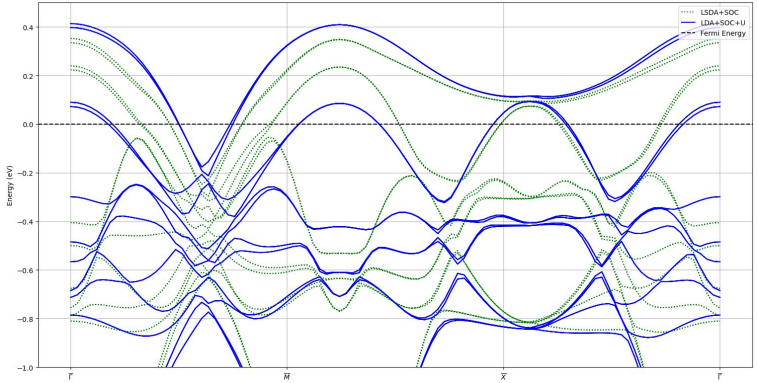


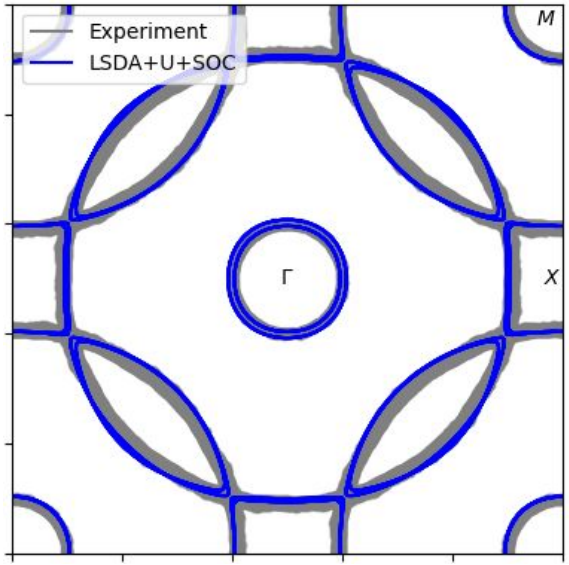
ℓ. This method, known as LDA+U, was first developed to be able to cope with so-called Mott insulators, *i.e.* systems where LDA and GGA incorrectly predict a metallic state. By construction, the resulting potential is orbital dependent.

[Introduction to DFT+U]

DFT+U (ELK-9.5.14 Calculation):

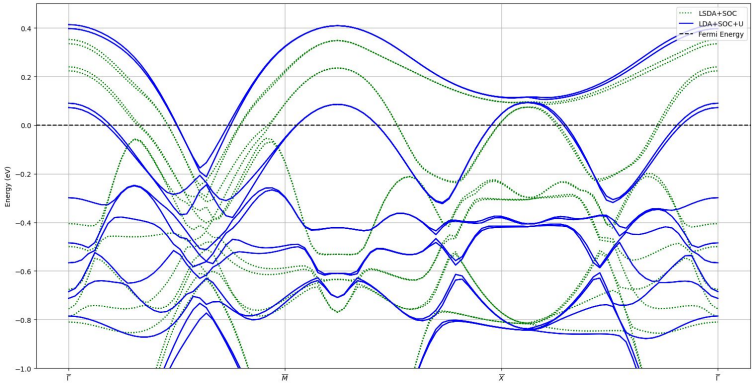
- Yukawa-type of screening with U = 3.6 eV
- Around Mean Field Approximation

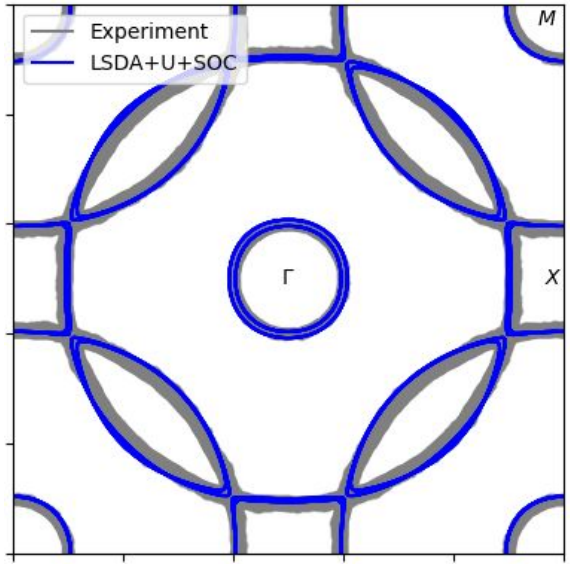


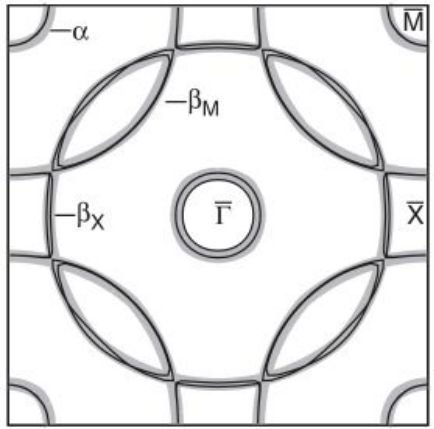


DFT+U (ELK-9.5.14 Calculation):

- Yukawa-type of screening with U = 3.6 eV
- Around Mean Field Approximation







PRL **101,** 026408 (2008) PHYSICAL REVIEW LETTERS week ending 11 JULY 2008

Coulomb-Enhanced Spin-Orbit Splitting: The Missing Piece in the Sr_2RhO_4 Puzzle

Guo-Qiang Liu, V. N. Antonov, O. Jepsen, and O. K. Andersen.
Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany
(Received 2 April 2008; published 11 July 2008)

Not done in the literature so far:

A quantitative interpretation of what is happening to the system, without referring to a TB-Model!

Recap:

Notation 6.1 We consider the following sequence of Hilbert-spaces and densities

$$\rho_{\mathscr{F}} = \frac{1}{Z} e^{-\beta(H^{2Q} - \mu N^{2Q})} \qquad \in \mathscr{D}\Big[\quad \mathscr{H} = \mathscr{F}(\mathcal{H}) \quad \Big]$$

Theorem 6.2 For any one-body operator X on $\mathcal{H}$ one finds for the expectation-values

$$\begin{aligned} \text{"Observable Quantity"} &= \langle X^{2Q} \rangle \\ &= \mathrm{Tr}_{\mathscr{F}} \left(\rho_{\mathscr{F}} X^{2Q} \right) \end{aligned}$$

Notation 6.1 We consider the following sequence of Hilbert-spaces and densities

$$\rho_{\mathscr{F}} = \frac{1}{Z} \mathrm{e}^{-\beta\left(H^{2\mathrm{Q}} - \mu N^{2\mathrm{Q}}\right)} \qquad \in \mathscr{D}\Big[\quad \mathscr{H} = \mathscr{F}(\mathcal{H}) \quad \Big]$$

$$\bigcup$$

$$\rho_{\mathcal{H}} = \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_{\beta}(\epsilon_{N\mathbf{k}} - \mu) |\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}\rangle\langle\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}| \qquad \in \mathscr{D}\Big[\quad \mathcal{H} \equiv L^2(\mathrm{Crystal}) \otimes \mathbb{C}^2 \simeq \bigoplus_{\mathbf{k}\in\mathrm{Q}} \mathcal{H}_{\mathbf{k}} \quad \Big]$$

Theorem 6.2 For any one-body operator X on $\mathcal{H}$ one finds for the expectation-values

$$\begin{aligned} \text{"Observable Quantity"} &= \langle X^{2\mathrm{Q}} \rangle \\ &= \mathrm{Tr}_{\mathscr{F}} \left(\rho_{\mathscr{F}} X^{2\mathrm{Q}} \right) \\ &= \mathrm{Tr}_{\mathcal{H}} \left(\rho_{\mathcal{H}} X \right) \end{aligned} \qquad = \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_{\beta}(\epsilon_{N\mathbf{k}} - \mu) \left\langle \Psi^{\ \mathrm{sv}}_{N\mathbf{k}} | X | \Psi^{\ \mathrm{sv}}_{N\mathbf{k}} \right\rangle$$

Notation 6.1 We consider the following sequence of Hilbert-spaces and densities

$$\begin{aligned}
\rho_{\mathscr{F}} = \frac{1}{Z}\mathrm{e}^{-\beta\left(H^{2\mathrm{Q}}-\mu N^{2\mathrm{Q}}\right)} \qquad & \in \mathscr{D}\Big[\quad \mathscr{H} = \mathscr{F}(\mathcal{H}) \quad \Big] \\
& \qquad \bigcup \\
\rho_{\mathcal{H}} = \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}}-\mu) |\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}\rangle\langle\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}| \qquad & \in \mathscr{D}\Big[\quad \mathcal{H} \equiv L^2(\mathrm{Crystal}) \otimes \mathbb{C}^2 \simeq \bigoplus_{\mathbf{k}\in\mathrm{Q}} \mathcal{H}_{\mathbf{k}} \quad \Big] \\
& \qquad \bigcup \\
\rho_{N\mathbf{k}} = |u^{\ \mathrm{sv}}_{N\mathbf{k}}\rangle\langle u^{\ \mathrm{sv}}_{N\mathbf{k}}| \qquad & \in \mathscr{D}\Big[\quad \mathcal{H}_{\mathbf{k}} = L^2(\mathrm{UC}) \otimes \mathbb{C}^2 \quad \Big]
\end{aligned}$$

Theorem 6.2 For any one-body operator X on $\mathcal{H}$ one finds for the expectation-values

$$\begin{aligned}
\text{"Observable Quantity"} = \langle X^{2\mathrm{Q}} \rangle & \\
= \mathrm{Tr}_{\mathscr{F}} \left(\rho_{\mathscr{F}} X^{2\mathrm{Q}} \right) & \\
= \mathrm{Tr}_{\mathcal{H}} \left(\rho_{\mathcal{H}} X \right) & \qquad = \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}}-\mu) \left\langle \Psi^{\ \mathrm{sv}}_{N\mathbf{k}} | X | \Psi^{\ \mathrm{sv}}_{N\mathbf{k}} \right\rangle \\
= N_p \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}}-\mu) \, \mathrm{Tr}_{\mathcal{H}_{\mathbf{k}}} \left(\rho_{N\mathbf{k}} X \right) & \qquad = N_p \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}}-\mu) \left\langle u^{\ \mathrm{sv}}_{N\mathbf{k}} | X | u^{\ \mathrm{sv}}_{N\mathbf{k}} \right\rangle_{\mathrm{UC}}
\end{aligned}$$

Fact:

For *some* observables, there is an *extended* decomposition, that allows us extract even more information!

Theorem 2.7 Let U, V, W be vector spaces over the same field $\mathbb{F}$. Then there is an isomorphism

$$(U \oplus V) \otimes W \simeq (U \otimes W) \oplus (V \otimes W).$$

Proof 2.7 See Appendix, Proofs, page 71.

Remark 2.7.1 This property is called *the distributivity-law of the tensor product over direct sums*.

Fact 2.15 Note that the Hilbert-space of a single-electron in a bulk crystalline environment is given as[3]

$$\mathcal{H} = L^2(\text{Crystal}) \otimes \mathbb{C}^2 = \left\{ \Psi : \text{Crystal} \times \{\uparrow, \downarrow\} \to \mathbb{C} \;\middle|\; \oint\!\!\!\!\!\!\sum_{\substack{\text{Crystal} \\ \sigma \in \{\uparrow,\downarrow\}}} |\Psi(\mathbf{r}, \sigma)|^2 = 1 \right\} \tag{2.14}$$

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Fact 2.16 Recall that using the Bloch-theorem, we know that we can expand any wavefunction $\Psi \in L^2(\text{Crystal}) \otimes \mathbb{C}^2$ as

$$\Psi(\mathbf{r}, \sigma) = \sum_{\mathbf{k} \in Q} \sum_{N=1}^{\infty} c_{N\mathbf{k}} \Psi_{N\mathbf{k}}(\mathbf{r}, \sigma) = \sum_{\mathbf{k} \in Q} \sum_{N=1}^{\infty} c_{N\mathbf{k}} u_{N\mathbf{k}}(\mathbf{r}, \sigma) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{2.15}$$

with a lattice-periodic spinors $u_{N\mathbf{k}}(\mathbf{r}, \sigma) = u_{N\mathbf{k}}(\mathbf{r} + \mathbf{R}_\mathbf{n}, \sigma)$ that obey certain differential equations[4].

Notation 2.17 We denote the space of lattice-periodic functions as

$$L^2(\mathrm{UC}) = \mathcal{H}_{\mathbf{k}} = \left\{ u_{\mathbf{k}} : \mathrm{UC} \to \mathbb{C} \;\middle|\; u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G} \in \mathrm{RL}} c_{\mathbf{k}}^{\mathbf{G}} e^{\mathrm{i}\mathbf{G}\cdot\mathbf{r}}, \int_{\mathrm{UC}} |u_{\mathbf{k}}(\mathbf{r})|^2 \mathrm{d}^{\mathrm{d}}\mathbf{r} < \infty \right\} \tag{2.17}$$

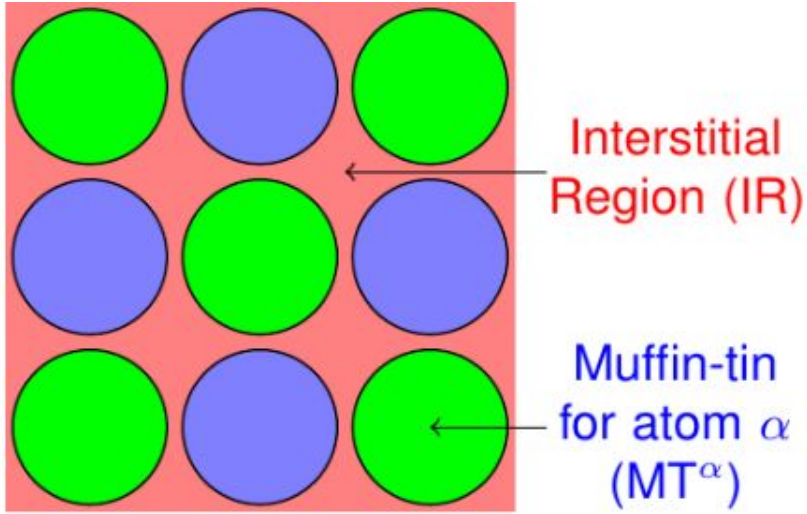
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Theorem 2.18 Using Equation (2.7) this gives us an isomorphism

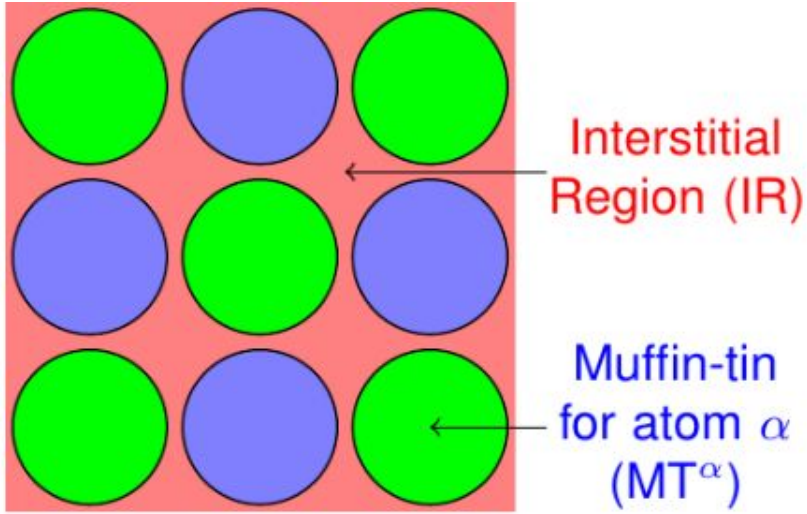
$$\mathcal{H} = L^2(\mathrm{Crystal}) \otimes \mathbb{C}^2 \simeq \left(\bigoplus_{\mathbf{k}\in\mathrm{Q}} \mathcal{H}_{\mathbf{k}} \right) \otimes \mathbb{C}^2 \simeq \bigoplus_{\mathbf{k}\in\mathrm{Q}} \left(\mathcal{H}_{\mathbf{k}} \otimes \mathbb{C}^2 \right) \tag{2.18}$$

Proof 2.18 Analogous to the proof of Theorem 2.12, in combination with Theorem 2.7.


Interstitial
Region (IR)
Muffin-tin
for atom α
(MT$^{\alpha}$)

Fact 2.19 Using the decomposition of the unit cell into muffin-tins and interstitial regions, we obtain a corresponding decomposition of the electronic Hilbert-space

$$\mathcal{H}_{\mathbf{k}} \simeq \left(\bigoplus_{\alpha=1}^{r} L^2([0, R_\alpha], r^2 \mathrm{d}r) \otimes L^2(S^2, \mathrm{d}\Omega) \otimes \mathbb{C}^2 \right) \oplus \left(L^2(\mathrm{IR}) \otimes \mathbb{C}^2 \right) \tag{2.19}$$

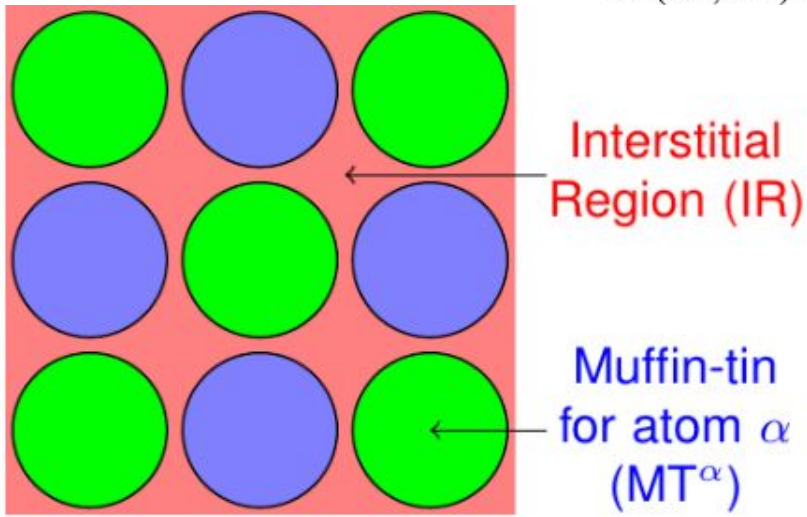


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with

$$L^2(S^2, \mathrm{d}\Omega) = \bigoplus_{l=0}^{\infty} \mathrm{span}_{\mathbb{C}} \bigcup_{m=-l}^{l} \{ Y_{lm} \equiv |lm\rangle \} \tag{2.20}$$



Remark 2.20.1 Summarizing, we have in the spin-independent case the following hierarchy of Hilbert-(sub)spaces:

$$\mathcal{H} \equiv L^2(\text{Crystal}) \otimes \mathbb{C}^2$$

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$$\rho_{\mathscr{F}} = \frac{1}{Z} e^{-\beta\left(H^{2Q} - \mu N^{2Q}\right)} \qquad \in \mathscr{D}\Big[\quad \mathscr{H} = \mathscr{F}(\mathcal{H}) \quad \Big]$$

"Observable Quantity" $= \langle X^{2Q} \rangle = \mathrm{Tr}_{\mathscr{F}} \left(\rho_{\mathscr{F}} X^{2Q} \right) = \mathrm{Tr}_{\mathcal{H}} \left(\rho_{\mathcal{H}} X \right) = \ldots$

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$$\rho_{\mathcal{H}} = \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) |\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}\rangle\langle\Psi^{\ \mathrm{sv}}_{N\mathbf{k}}| \quad \in \mathscr{D}\Big[\quad \mathcal{H} \equiv L^2(\mathrm{Crystal}) \otimes \mathbb{C}^2 \simeq \bigoplus_{\mathbf{k}\in\mathrm{Q}} \mathcal{H}_{\mathbf{k}} \quad \Big]$$

$$\bigcup$$

$$\rho_{N\mathbf{k}} = |u^{\ \mathrm{sv}}_{N\mathbf{k}}\rangle\langle u^{\ \mathrm{sv}}_{N\mathbf{k}}| \quad \in \mathscr{D}\Bigg[\quad \mathcal{H}_{\mathbf{k}} = L^2(\mathrm{UC}) \otimes \mathbb{C}^2 = \Bigg[\left(\bigoplus_{\alpha=1}^{r} L^2([0, R_\alpha], r^2 \mathrm{d}r) \otimes L^2(S^2, \mathrm{d}\Omega) \otimes \mathbb{C}^2 \right) \oplus \left(L^2(\mathrm{IR}) \otimes \mathbb{C}^2 \right) \Bigg] \Bigg]$$

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$$\rho^{\ \alpha}_{N\mathbf{k}} \quad \in \mathscr{D}\Bigg[\quad \mathcal{H}_\alpha = L^2([0, R_\alpha], r^2 \mathrm{d}r) \otimes L^2(S^2, \mathrm{d}\Omega) \otimes \mathbb{C}^2 \Bigg]$$

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$$\approx N_p \sum_{\mathbf{k}\in\mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \mathrm{Tr}_{\mathcal{H}_{\alpha LS}} \left(\rho^{\ N\mathbf{k}}_{\alpha LS} X \right)$$

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for example …

- the spin-operator $X \equiv S_i$ with $i \in \{x, y, z\}$,
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$$\rho_{\mathscr{F}} = \frac{1}{Z} e^{-\beta(H^{2Q} - \mu N^{2Q})} \quad \in \mathscr{D}\Big[\quad \mathscr{H} = \mathscr{F}(\mathcal{H}) \quad \Big]$$

$$\bigcup$$

$$\rho_{\mathcal{H}} = \sum_{\mathbf{k}\in Q} \sum_{N=1}^{\text{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) |\Psi^{\text{sv}}_{N\mathbf{k}}\rangle\langle\Psi^{\text{sv}}_{N\mathbf{k}}| \quad \in \mathscr{D}\Big[\quad \mathcal{H} \equiv L^2(\text{Crystal}) \otimes \mathbb{C}^2 \simeq \bigoplus_{\mathbf{k}\in Q} \mathcal{H}_{\mathbf{k}} \quad \Big]$$

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"Observable Quantity" $= \langle X^{2Q} \rangle = \text{Tr}_{\mathscr{F}} \left(\rho_{\mathscr{F}} X^{2Q} \right) = \text{Tr}_{\mathcal{H}} \left(\rho_{\mathcal{H}} X \right) = \dots$

$$\begin{aligned}
\dots &= N_p \sum_{\mathbf{k}\in Q} \sum_{N=1}^{\text{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \, \text{Tr}_{\mathcal{H}_{\mathbf{k}}} \left(\rho_{N\mathbf{k}} X \right) \\
&= N_p \sum_{\mathbf{k}\in Q} \sum_{N=1}^{\text{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \text{Tr}_{\mathcal{H}_\alpha} \left(\rho^{\ N\mathbf{k}}_{\ \alpha} X \right) \\
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&= N_p \sum_{\mathbf{k}\in Q} \sum_{N=1}^{\text{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \sum_{l=0}^{\infty} \text{Tr}_{\mathcal{H}_{\alpha L(l)S}} \left(\rho^{\ N\mathbf{k}}_{\ \alpha L(l)S} X \right)
\end{aligned}$$

dim H_{ alpha L(l) S}
=
2 * [l] = 2 * (2 * l + 1)

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Notation 7.1 For the discussion of tensor-moments, we consider a density-matrix ρ that has the dimensions $2[l] \times 2[l]$ with matrix elements denoted as

$$\rho \equiv \rho_{ms,m's'} \quad \in \quad \mathrm{Herm}_{2[l]\times 2[l]}(\mathbb{C}) \tag{7.1}$$

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We will now introduce

triple upper-index tensor-moments $w_t^{kpr} \in \mathbb{C}$ with $k \in \{0, 1, 2, \ldots, 2l\}$, $p \in \{0, 1\}$, $r \in \{|k-p|, \ldots, |k+p|\}$ and $t \in \{-r, \ldots, +r\}$

$$w_t^{kpr} = \mathrm{Tr}\left(\Gamma_t^{kpr}\rho\right)$$

with *tensor-matrices*[5]

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$$\Gamma_{t,ab}^{kpr} = N_{kprls}^{-1}(-1)^{l-m_a+s-s_a} \sum_{\substack{x\in\{-k,\ldots,+k\}\\ y\in\{-p,\ldots,+p\}}} (-1)^{+k-x+p-y} \begin{pmatrix} l & k & l \\ -m_a & x & m_b \end{pmatrix} \begin{pmatrix} s & p & s \\ -s_a & y & s_b \end{pmatrix} \begin{pmatrix} k & r & p \\ -x & t & -y \end{pmatrix},$$

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$$w_t^{kpr} = \mathrm{Tr}\left(\Gamma_t^{kpr}\rho\right) \qquad \Longleftrightarrow \qquad \rho_{ab} = \sum_{kprt} \left(\Lambda_t^{kpr}\right)_{ab} \cdot w_t^{kpr}$$

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$$\Lambda_{t,ab}^{kpr} = N_{kprls}[kpr](-1)^{m_b-l+s_b-s} \sum_{\substack{x\in\{-k,\ldots,+k\}\\ y\in\{-p,\ldots,+p\}}} (-1)^{x-k+y-p} \begin{pmatrix} l & k & l \\ -m_b & x & m_a \end{pmatrix} \begin{pmatrix} s & p & s \\ -s_b & y & s_a \end{pmatrix} \begin{pmatrix} k & r & p \\ -x & t & -y \end{pmatrix}$$

Definition 7.16 Let $\mathbf{J} \in \{\mathbf{L}, \mathbf{S}\}$ denote either the orbital angular momentum operator or the spin operator. For $q \in \{-1, 0, +1\}$, we introduce[7] the associated *rank 1 spherical tensor-operator* $\mathbf{J}_q^{(1)}$ as

$$
\begin{aligned}
J_{-1}^{(1)} &= -\frac{J_x - \mathrm{i}J_y}{\sqrt{2}}, \\
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Theorem 7.19 The *Wigner-Eckart-Theorem* states (in our particular case) that

$$\begin{aligned} \langle lm' | L_q^{(1)} | lm \rangle &= (-1)^{l-m'} \sqrt{l(l+1)(2l+1)} \begin{pmatrix} l & 1 & l \\ -m' & q & m \end{pmatrix} \\ \langle ss_a | S_q^{(1)} | ss_b \rangle &= (-1)^{s-s_a} \sqrt{s(s+1)(2s+1)} \begin{pmatrix} s & 1 & s \\ -s_a & q & s_b \end{pmatrix} \end{aligned} \tag{7.33}$$

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Proof 7.19 See Code-Folder, ELK-related, Topic 12, Python-script.

Summary of Lemmata and Theorems

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$$\text{"Observable Quantity"} = \langle X^{2Q} \rangle = \ldots \approx N_p \sum_{\mathbf{k} \in Q} \sum_{N=1}^{\text{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \sum_{l=0}^{\infty} \mathrm{Tr}_{\mathcal{H}_{\alpha L(l) S}} \left(\rho_{\substack{N\mathbf{k} \\ \alpha L(l) S}} X \right)$$

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$$= \ldots$$

Theorem 8.2 We obtain

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$$\mathrm{Tr}\,(\rho\mathbb{1}) \equiv \mathrm{Tr}\,\rho = N_{000ls} n_{l0}^{-1} n_{s0}^{-1} w_0^{000} \tag{8.4}$$

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$$\mathrm{Tr}\left[\rho S_q^{(1)}\right] = \sqrt{s(s+1)(2s+1)} N_{011ls}[r=1](-1)^{q-1} \begin{pmatrix} 0 & 1 & 1 \\ 0 & q & -q \end{pmatrix} n_{l0}^{-1} w_q^{011} \tag{8.6}$$

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$$\langle N\rangle = \langle \mathbb{1}^{2\mathrm{Q}}\rangle \approx N_p \sum_{\mathbf{k}\in \mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \sum_{l=0}^{\infty} N_{000ls} n_{l0}^{-1} n_{s0}^{-1} w^{000}_{0\ N\mathbf{k}\alpha l} \tag{8.5}$$

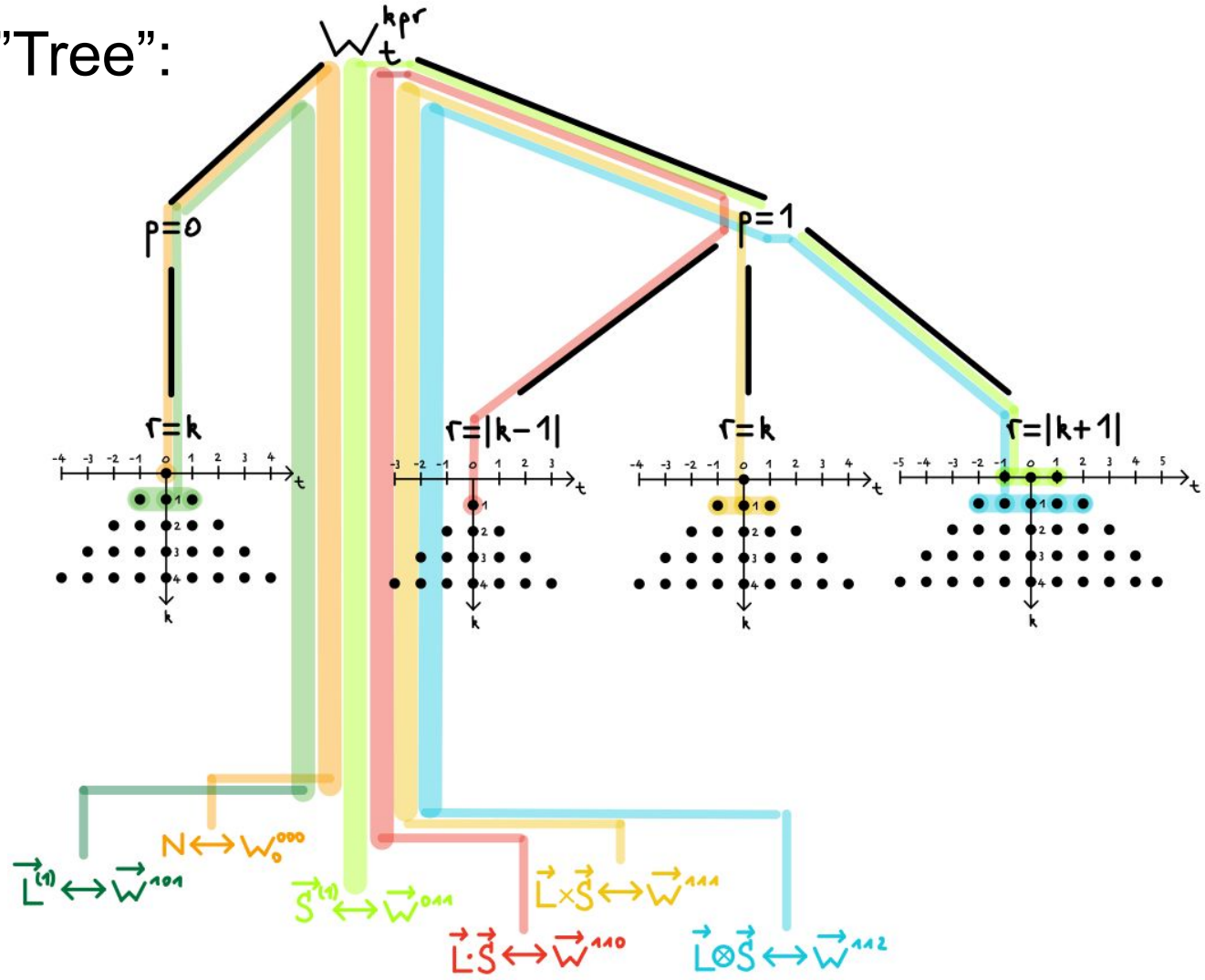
$$\left\langle \left(S_q^{(1)}\right)^{2\mathrm{Q}} \right\rangle \approx N_p \sum_{\mathbf{k}\in \mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \sum_{l=0}^{\infty} \sqrt{s(s+1)(2s+1)} N_{011ls}[r=1](-1)^{q-1} \begin{pmatrix} 0 & 1 & 1 \\ 0 & q & -q \end{pmatrix} n_{l0}^{-1} w^{011}_{q\ N\mathbf{k}\alpha l}$$

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$$\left\langle (\mathbf{L}\cdot\mathbf{S})^{2\mathrm{Q}} \right\rangle \approx N_p \sum_{\mathbf{k}\in \mathrm{Q}} \sum_{N=1}^{\mathrm{nstsv}} \mathrm{F}_\beta(\epsilon_{N\mathbf{k}} - \mu) \sum_{\alpha=1}^{r} \sum_{l=0}^{\infty} \sqrt{l(l+1)(2l+1)} \sqrt{s(s+1)(2s+1)} N_{110ls}[r=0] \sum_{q=-1}^{+1} \begin{pmatrix} 1 & 0 & 1 \\ q & 0 & -q \end{pmatrix} (-1)^q w^{110}_{0\ N\mathbf{k}\alpha l}$$

Tensor-Moment-”Tree”:

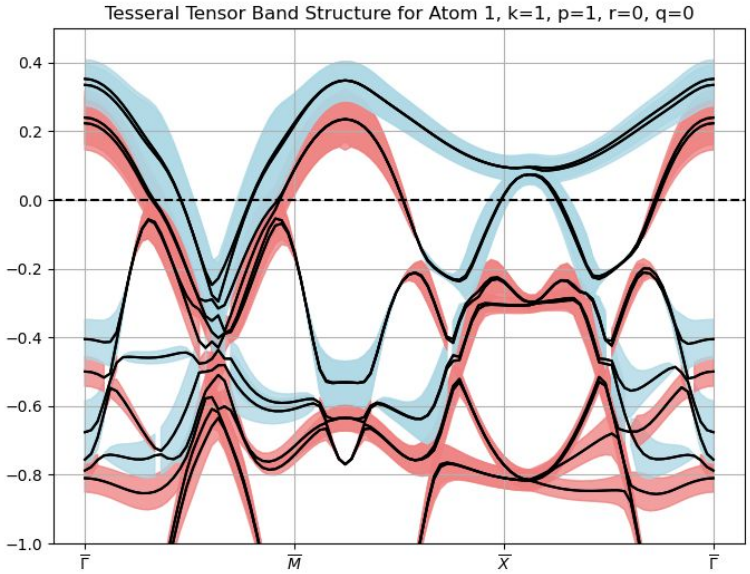
Tensor-Moment-"Tree":



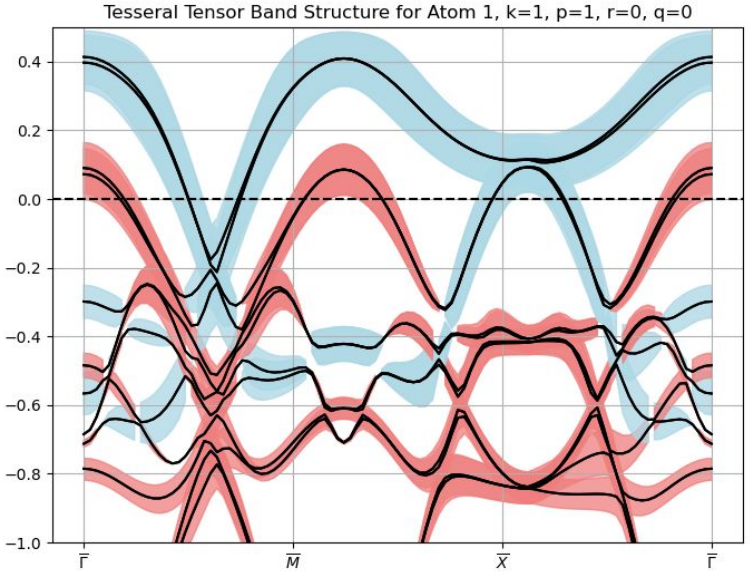
Featuring:

- Bandstructure with Tensor-Moment 110 for Rh-atoms as linewidth
- blue / red LW = positive / negative sign

U = 0.0 eV

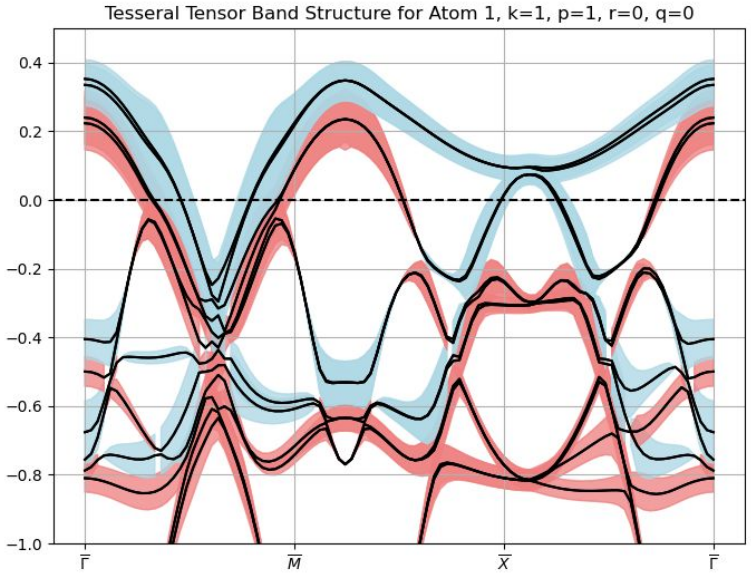


U = 3.6 eV

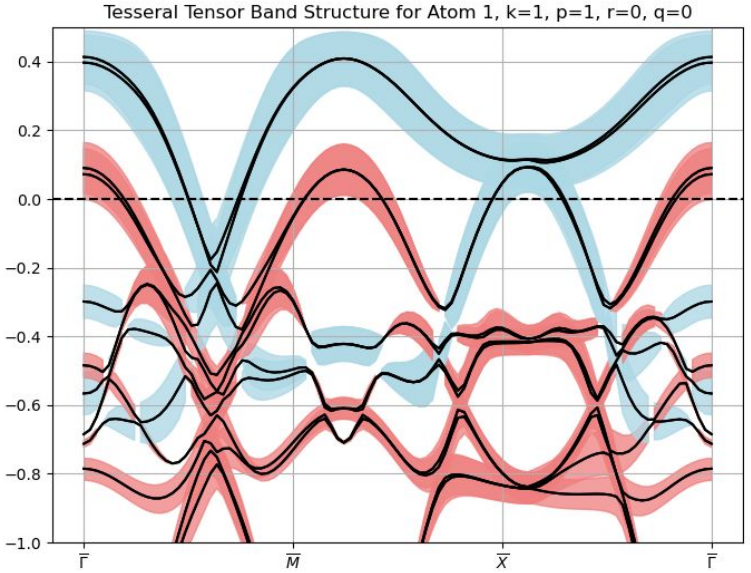


“Behind the Scenes” …

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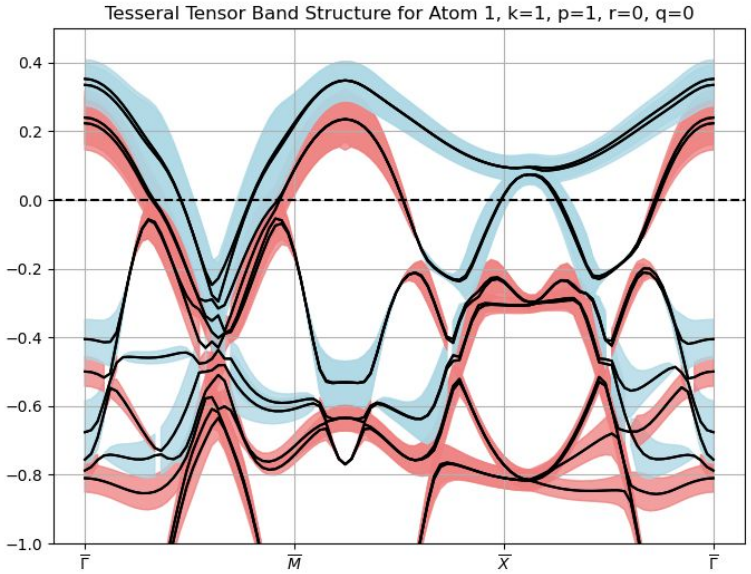
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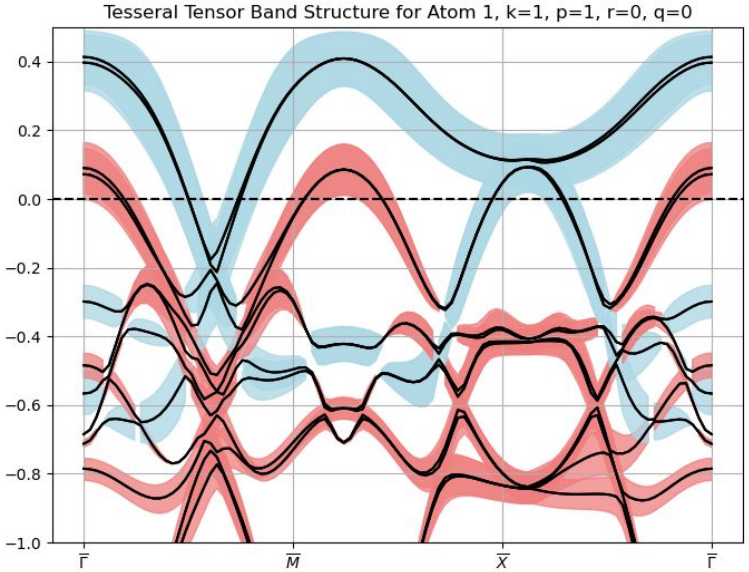
“Behind the Scenes” …

- Implementing a new subroutine into ELK-9.5.14 to compute (and write) the orbital representation of the densities corresponding to Bloch-states along a k-path (to file)

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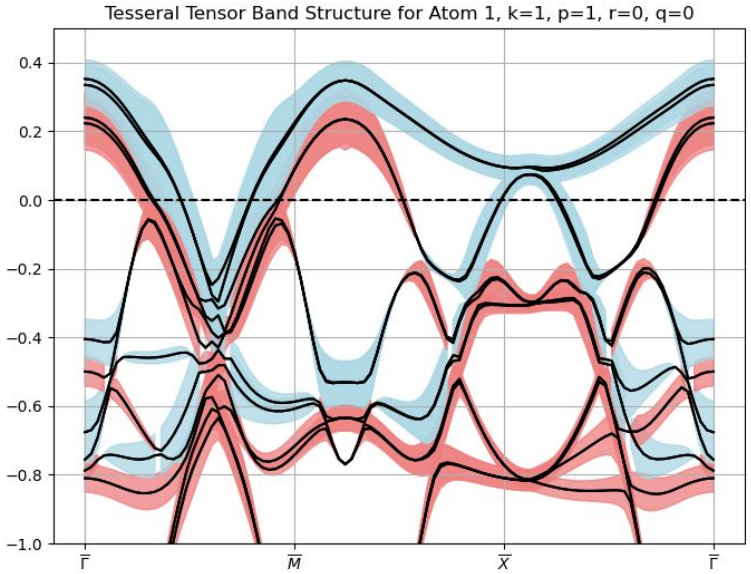
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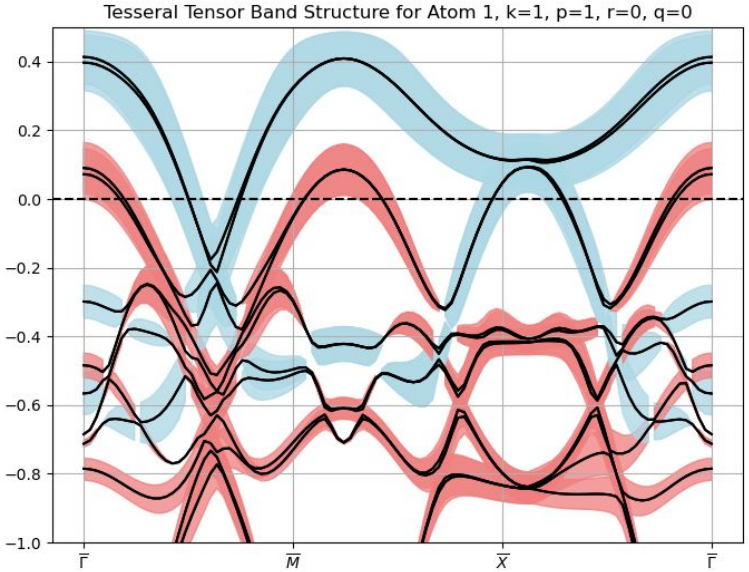
“Behind the Scenes” …

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- Post-processing in Python
- (Debugging)

U = 0.0 eV



U = 3.6 eV

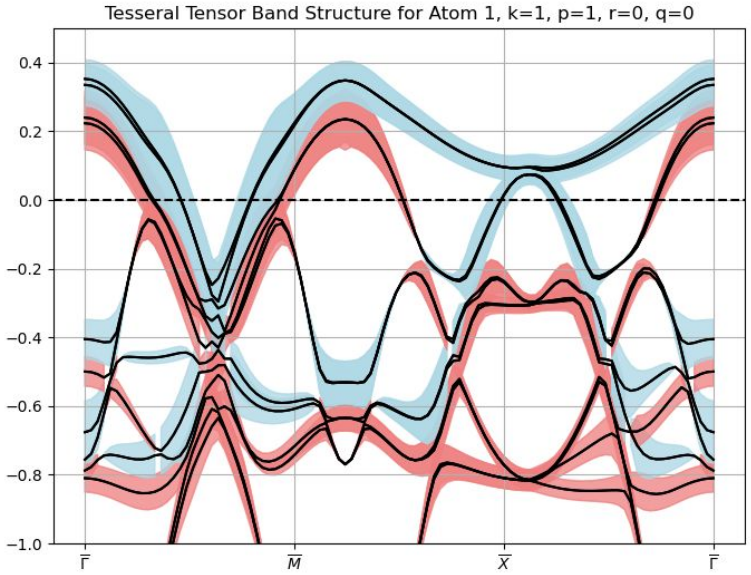


Featuring:

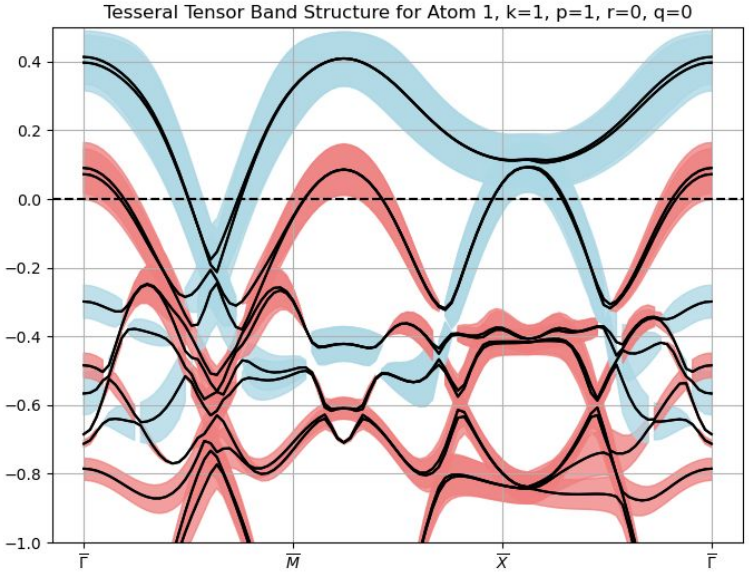
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U = 0.0 eV



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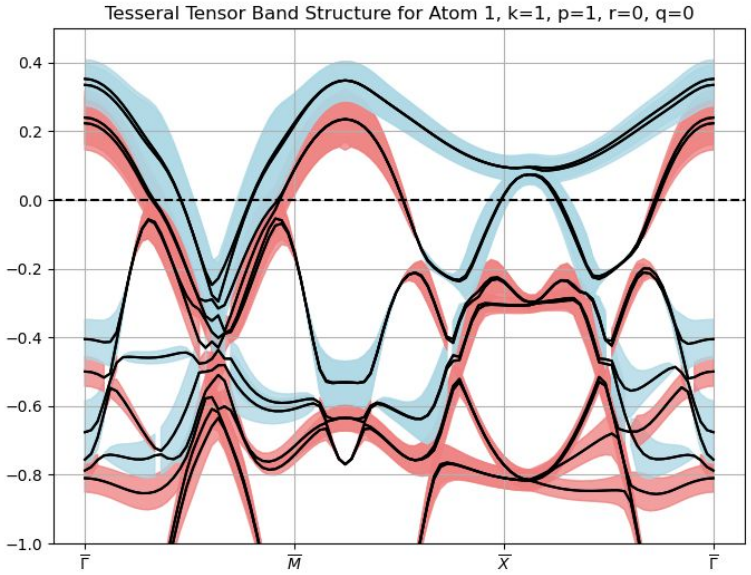


Featuring:

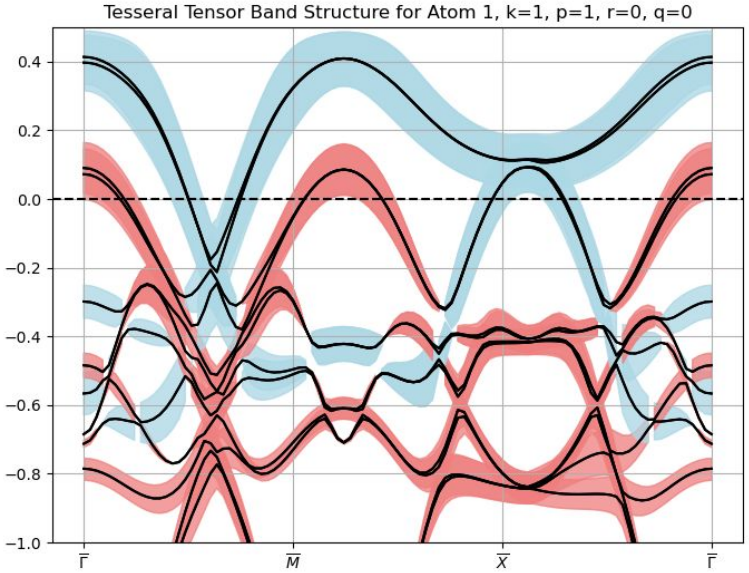
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- blue / red LW = positive / negative sign

Interpretation: The spin-orbit-interaction of the system increases, when U increases!

U = 0.0 eV



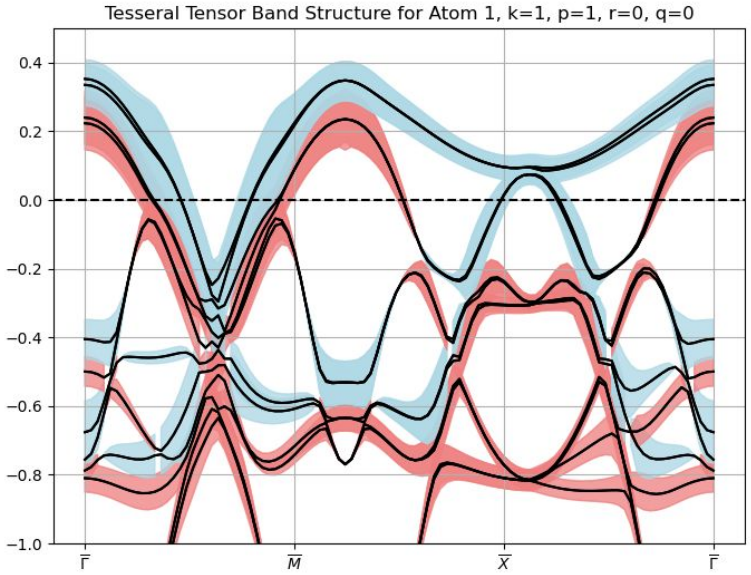
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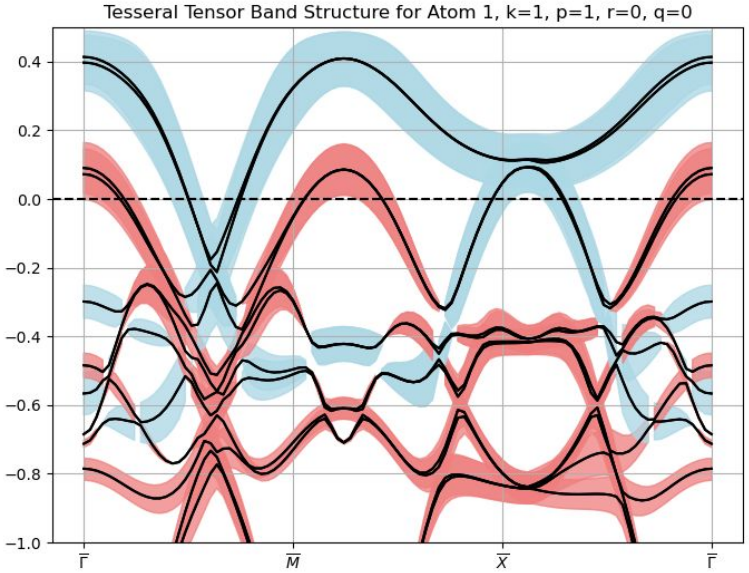
Hypothesis:

- The shift in energy bands corresponds to an increase in spin-orbit-interactions!

U = 0.0 eV



U = 3.6 eV



Recap:

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$$H_{v\ll c}\bullet = \left[mc^2 + \frac{p^2}{2m} + V(\mathbf{r}) - \frac{p^4}{8m^3c^2} + \frac{\hbar^2}{8m^2c^2}(\Delta V)(\mathbf{r}) + \frac{\hbar}{4m^2c^2}\sigma \cdot \left[(\nabla V)(\mathbf{r}) \times [\mathbf{p}\bullet] \right] \right]$$

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Notice that if V is a central potential

$$\mathbb{R} \ni \mathbf{r} \longmapsto V(\mathbf{r}) \equiv V(|r|) \in \mathbb{R} \tag{1.36}$$

then its gradient is given by

$$\left(\vec{\nabla} V\right)(\mathbf{r}) = \left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)(\mathbf{r})\frac{\mathbf{r}}{r} \tag{1.37}$$

and the expression simplifies to the form encountered in atom physics courses

$$H_{\mathrm{soc}} = \frac{\hbar}{4m^2c^2}\frac{1}{r}\left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)(\mathbf{r})\,\vec{\sigma}\cdot[\mathbf{r}\times\mathbf{p}] = \frac{1}{2m^2c^2}\frac{1}{r}\left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)(\mathbf{r})\,\mathbf{S}\cdot\mathbf{L} \tag{1.38}$$

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elk.pdf 133,9%

5.99 socscf

socscf	scaling factor for the spin-orbit coupling term in the Hamiltonian	real	1.0

This can be used to enhance the effect of spin-orbit coupling in order to accurately determine the magnetic anisotropy energy (MAE).

Now: Tuning the effective SOC in our calculation “by hand”:

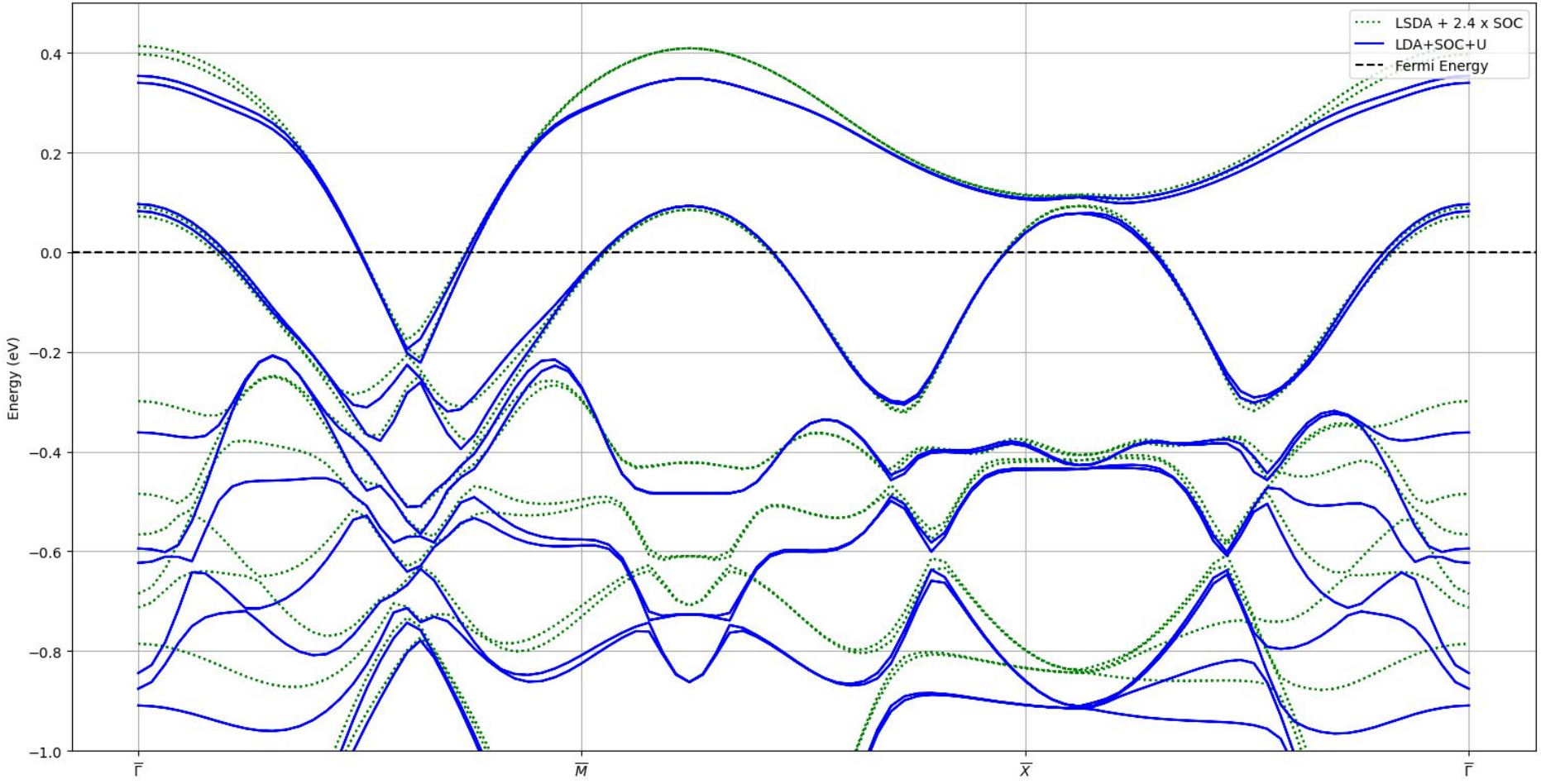
```
/home/sebastian/04_SL_Dropbox/AA_Sebast~e_SOC_Test/SOC_eq_2.40_Files4PP/elk.in


! ============================================================ !
! ============================================================ !
!  Part 3: Input blocks that can be varied to fit exp.-data.
! ============================================================ !
! ============================================================ !

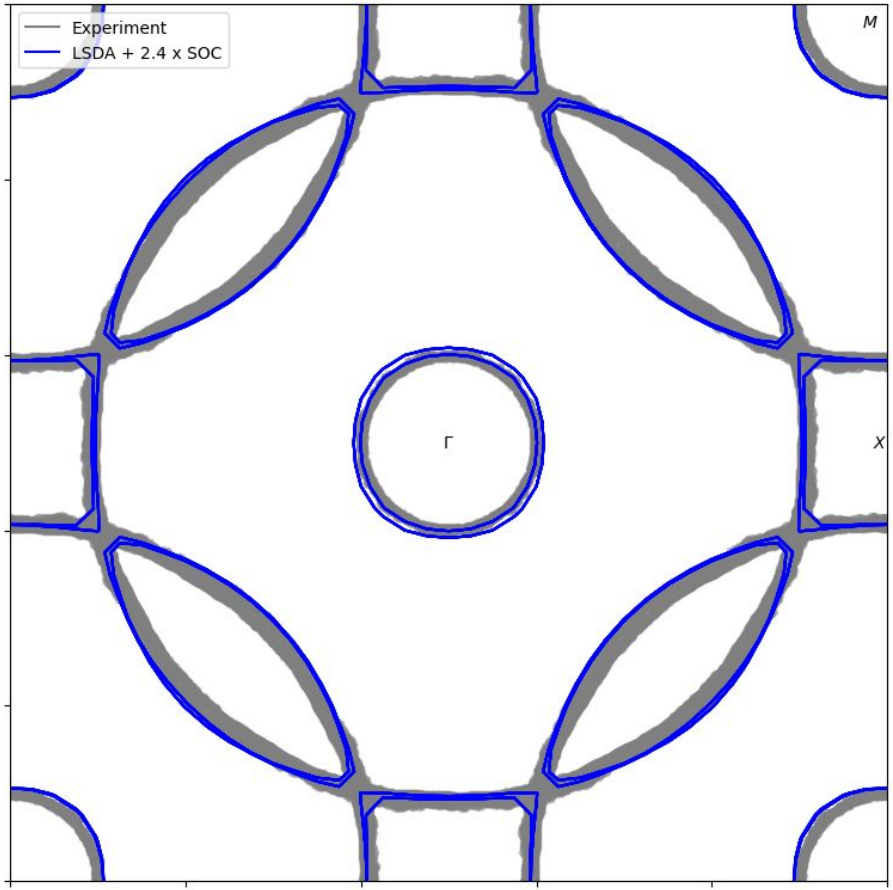
! Note: No SOC :<=> socscf = 0.0.
socscf
  2.40

! dftu=0    corresponds to No DFT+U-Calculation.
! inpdftu=5 corresponds to the Yukawa screening.
dft+u
  0  5          : dftu,inpdftu
  1  2  0.132   : is, l, U fixed
```

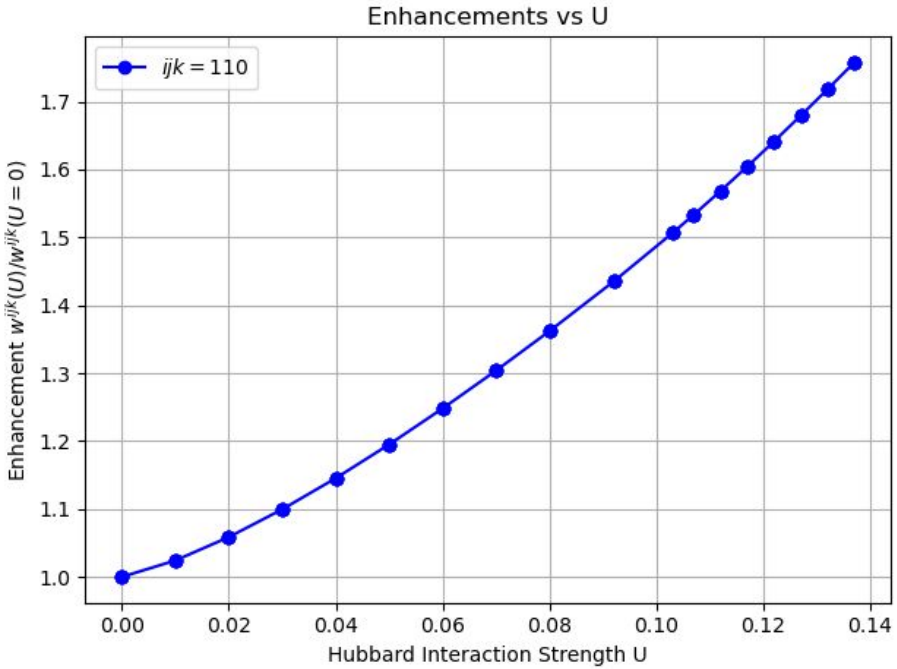
[Band-Structure-Calculation]


LSDA + 2.4 x SOC
LDA+SOC+U
Fermi Energy
Energy (eV)
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
$\overline{\Gamma}$
$\overline{M}$
$\overline{X}$
$\overline{\Gamma}$

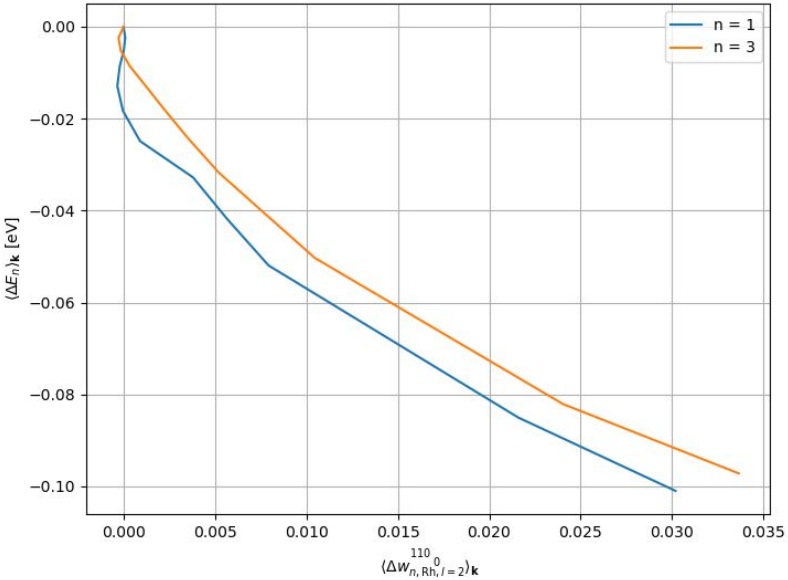
Fermi-Surface LDA+2.4SOC-Calculation



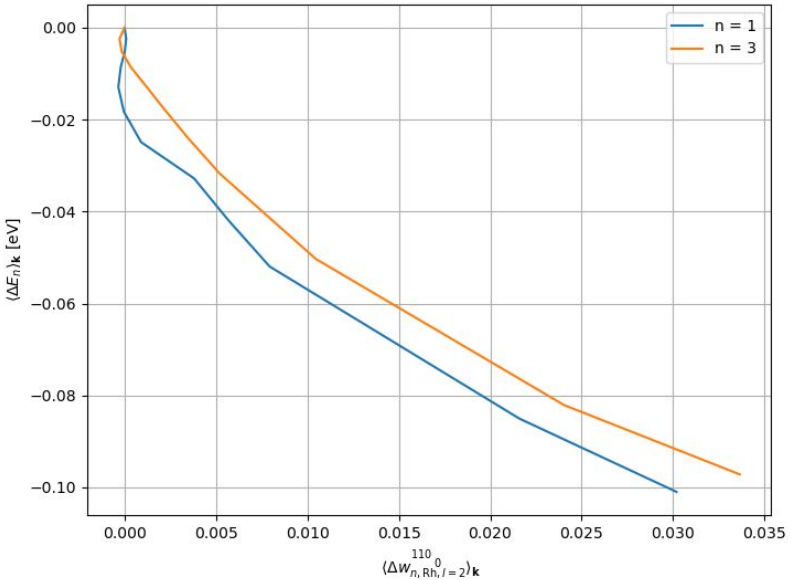
DFT+U Calculations



Heuristically:
The energies depend quadratically on the changes (w.r.t. U) of the 110 Tensor-Moment



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$$H_0 \left| n^{(0)} \right\rangle = E_n^{(0)} \left| n^{(0)} \right\rangle, \qquad n = 1, 2, 3, \cdots$$

$$H = H_0 + \lambda V$$

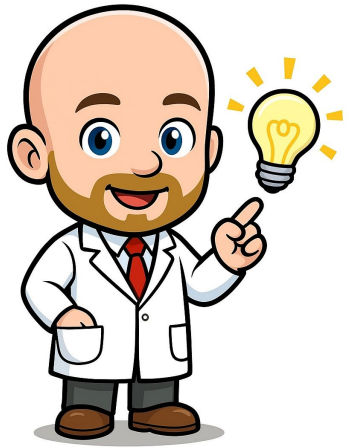
$$(H_0 + \lambda V) \left| n \right\rangle = E_n \left| n \right\rangle.$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

$$E_n(\lambda) = E_n^{(0)} + \lambda \left\langle n^{(0)} \right| V \left| n^{(0)} \right\rangle + \lambda^2 \sum_{k \neq n} \frac{\left| \left\langle k^{(0)} \right| V \left| n^{(0)} \right\rangle \right|^2}{E_n^{(0)} - E_k^{(0)}} + O(\lambda^3)$$

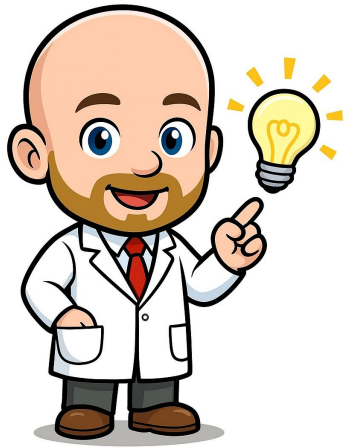
“Approximately Quadratic”! =)

Summary / Lessons Learned:



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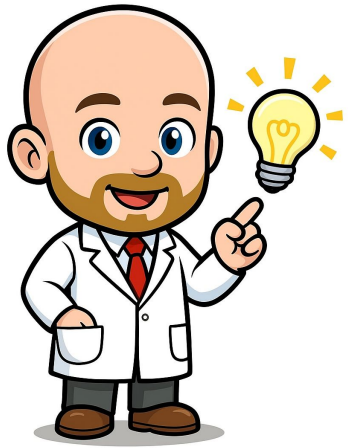
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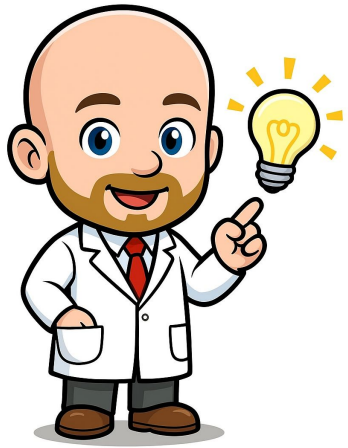


Summary / Lessons Learned:

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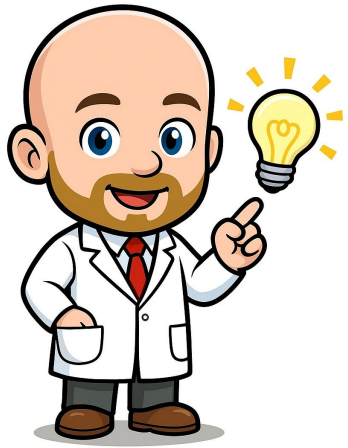
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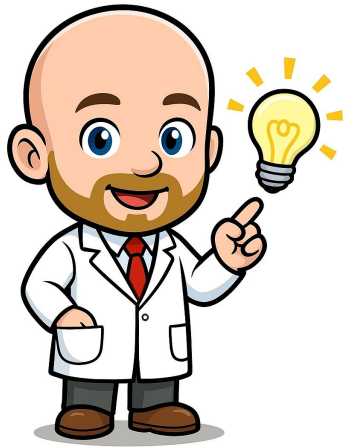
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- Electron-Electron-Interactions can increase the effective Spin-Orbit-Coupling,

- Tensor-Moments provide a technique to conclude this and further, from which atoms the mechanism arise.



Acknowledgements

- Jonas (Quantum Statistical Mechanics)
- Johan (ELK on Dardel (!!!))
- Oscar (ELK)
- Jakub (ELK-scripts)
- Nastaran (Fortran)
- (Lars) (ELK and all the rest…)

Thank you for your Attention!

(Applause…)

Questions / Suggestions / Comments?