Magnetism in Low-Dimensional Systems

From Frustration to Complex Order

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Outline

1. Cool-down
2. Full-Potential ASW Method
3. A Short Walk Through Dimensions
   - Where are the Moments?
   - How to Build a Spin-Ladder
   - Greetings from High-T_c
   - A Recipe Against Frustration

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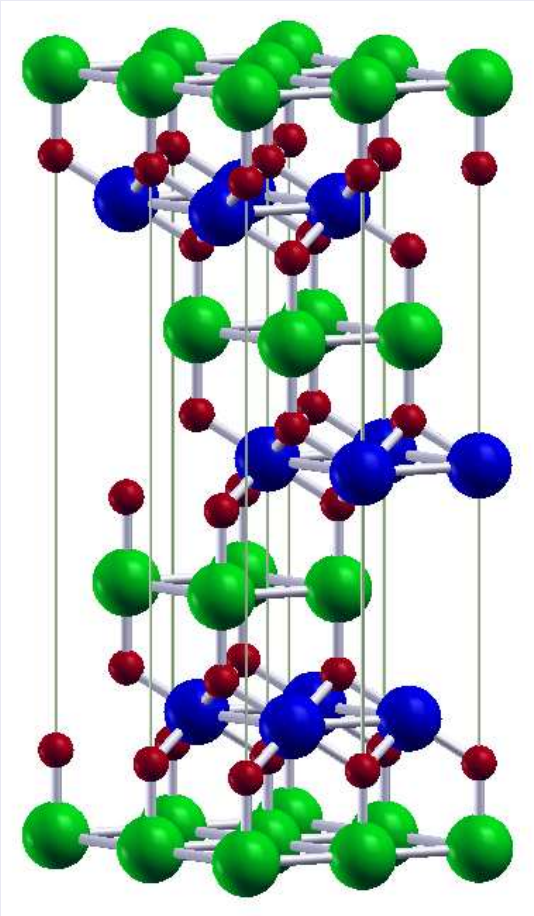
Delafossites ABO_2

Delafossite Structure



Building Blocks

- rhombohedral lattice
- triangular A-atom layers
- BO_2 sandwich layers
- B-atoms octahedrally coordinated
- linear O–A–O bonds

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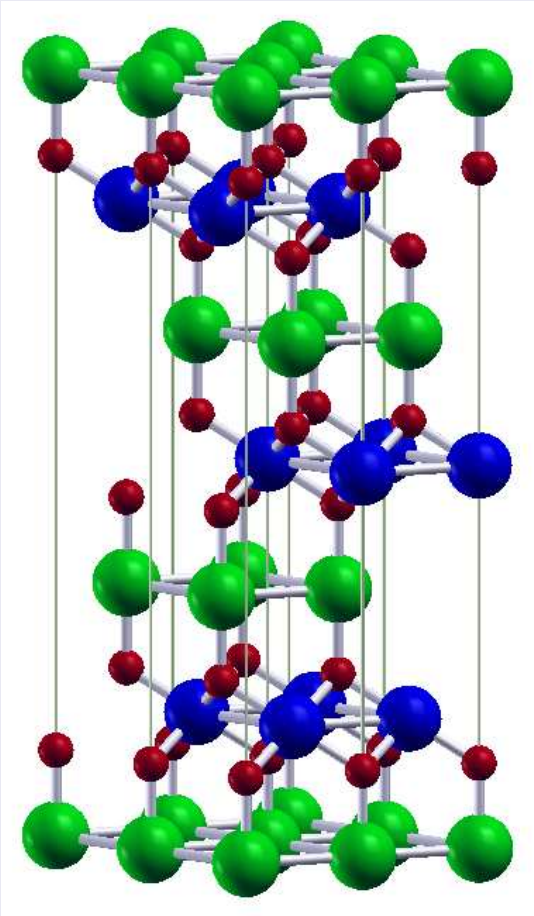

Building Blocks

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Issues

- dimensionality
- frustration effects
- play chemistry

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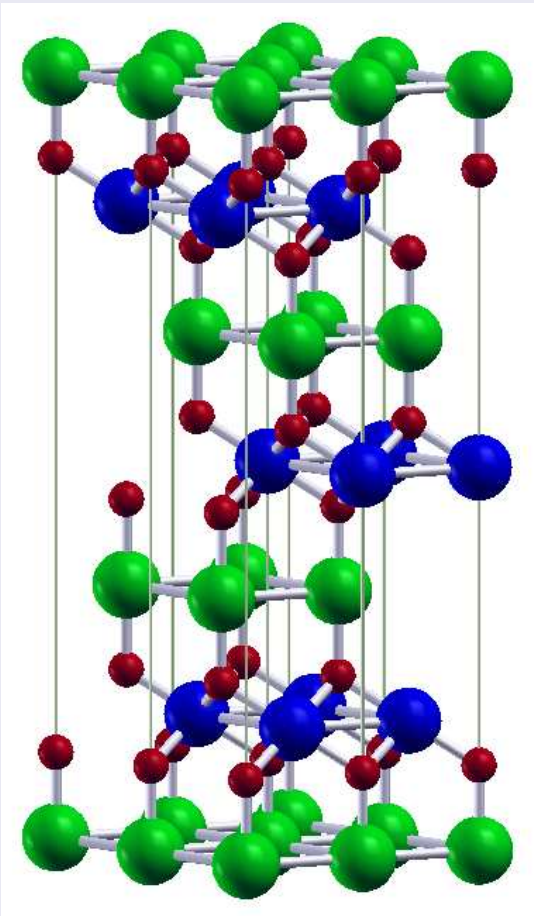

Prototype Materials

- $CuFeO_2$, $CuCrO_2$
- $CuCoO_2$, $CuRhO_2$
- $CuAlO_2$, $CuGaO_2$, $CuInO_2$, ...
- $PdCrO_2$, $PdCoO_2$, $PdRhO_2$, $PtCoO_2$

Properties

- semiconductors, AF interactions, (distorted) triangular
- non-mag. semicond., high TEP
- wide-gap semicond., p-type TCO
- very good metals, highly anisotropic

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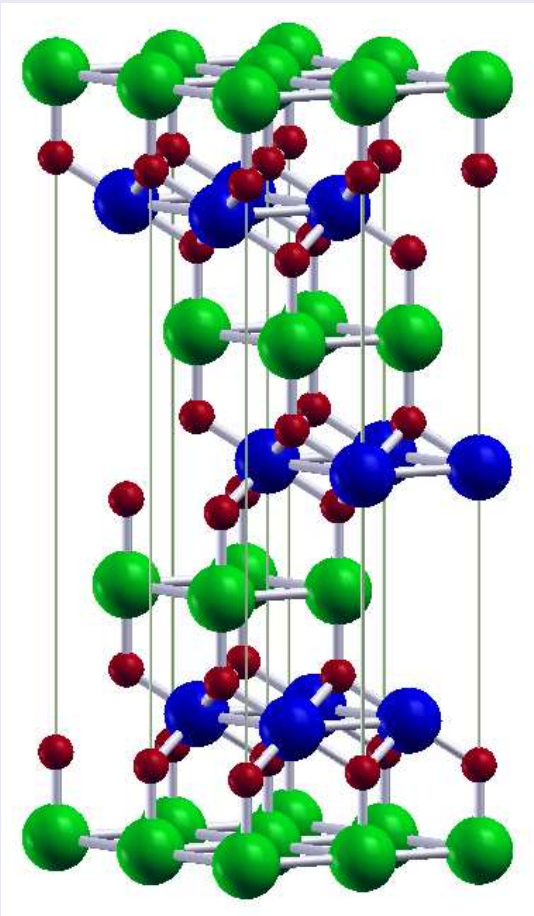

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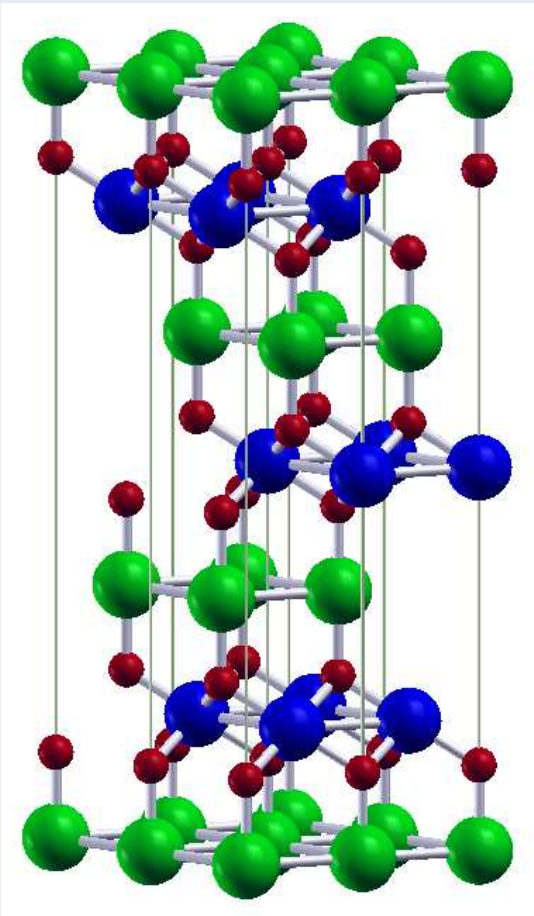

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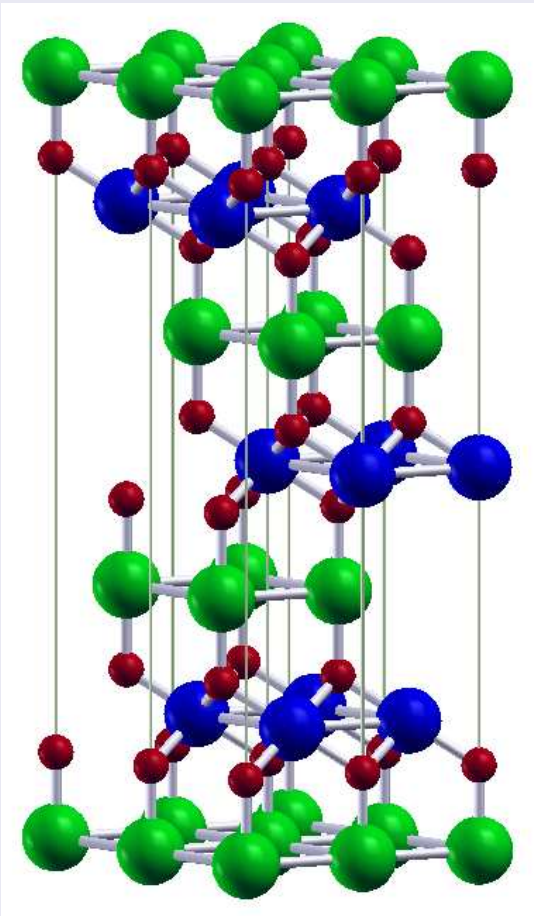

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$PdCoO_2$ and $PtCoO_2$

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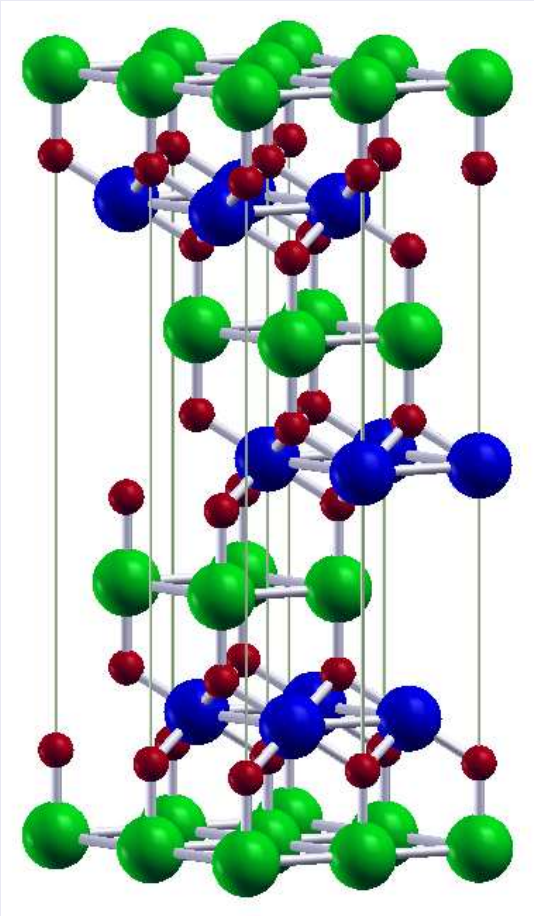

Facts

- very low resistivity
- anisotropy factor ≈ 200
- PES: only Pd $4d$ states at E_F
- PES/IPES: E_F in shallow DOS minimum

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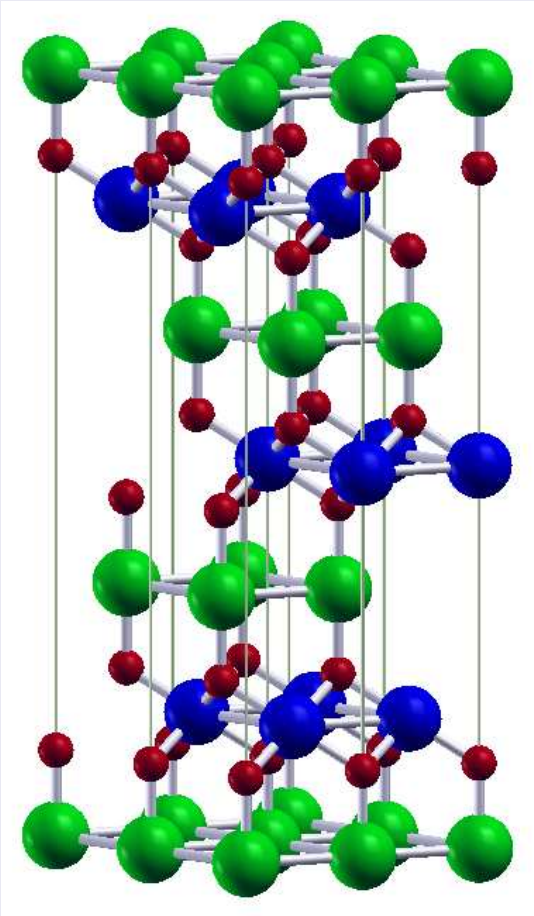

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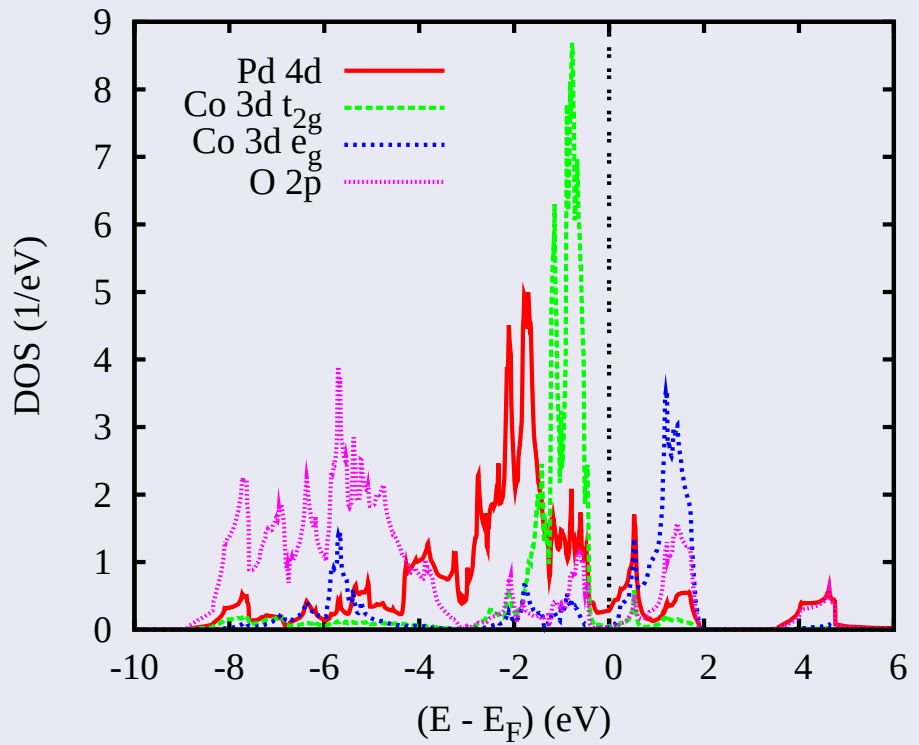
Open Issues

- role of Pd $4d$ orbitals?
- role of Co $3d$ and O $2p$ orbitals?

Electronic Properties of $PdCoO_2$

Partial Densities of States



Results

- Co 3*d*-O 2*p* hybridization
- CoO_6 octahedra: Co 3*d* $\Rightarrow$ t_{2g} and e_g
- Co $3d^6$ (Co^{3+}) LS
- Co 3*d*, O 2*p*: very small DOS at E_F
- Pd $4d^9$ (Pd^{1+})

VE, R. Frésard, A. Maignan, Chem. Mat. **20**, 2370 (2008)

Electronic Properties of $PdCoO_2$

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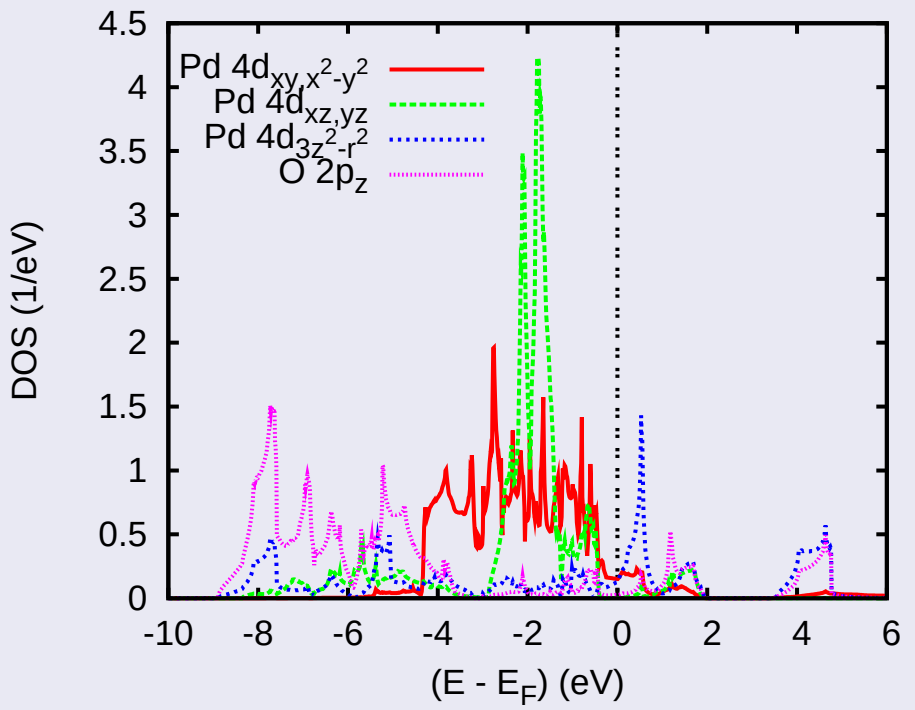

Results

- Pd $4d$-O $2p$ hybridization
- broad Pd d_{xy,x^2-y^2} bands
- states at E_F: Pd d_{xy,x^2-y^2}, $d_{3z^2-r^2}$

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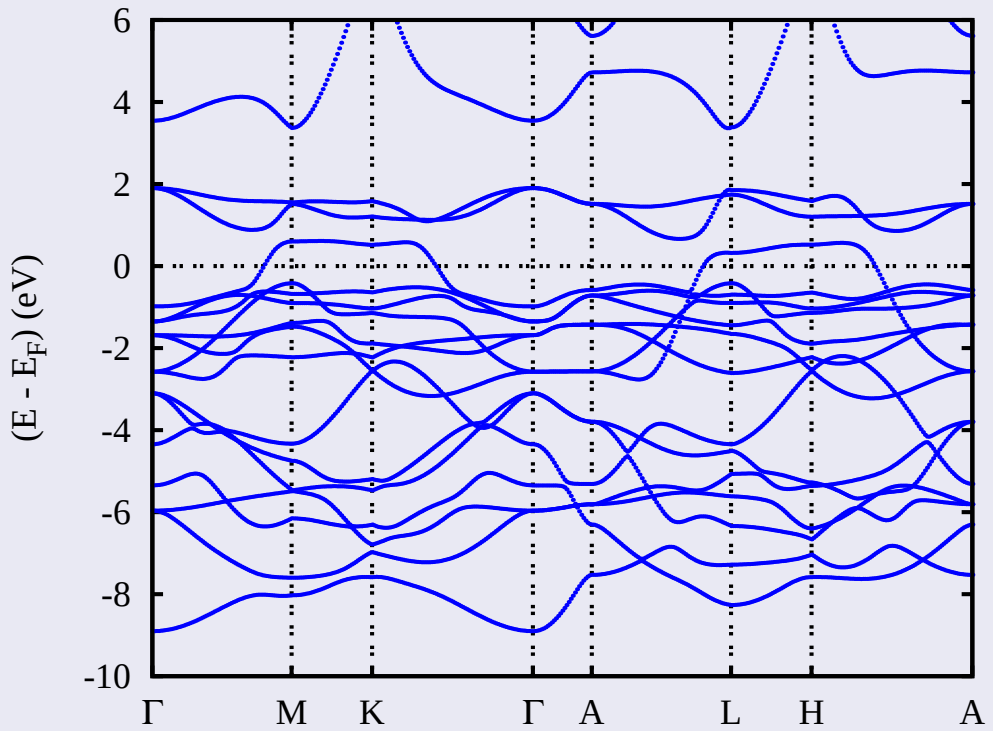
Electronic Properties of $PdCoO_2$

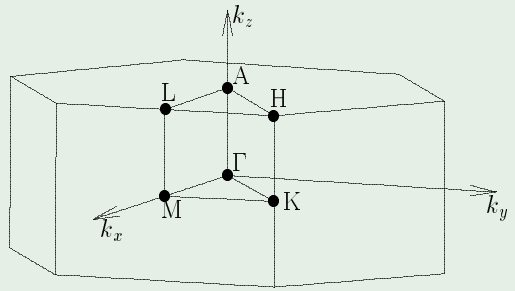
Band Structure



Results

- quasi-2D
- single band crossing E_F

Brillouin Zone



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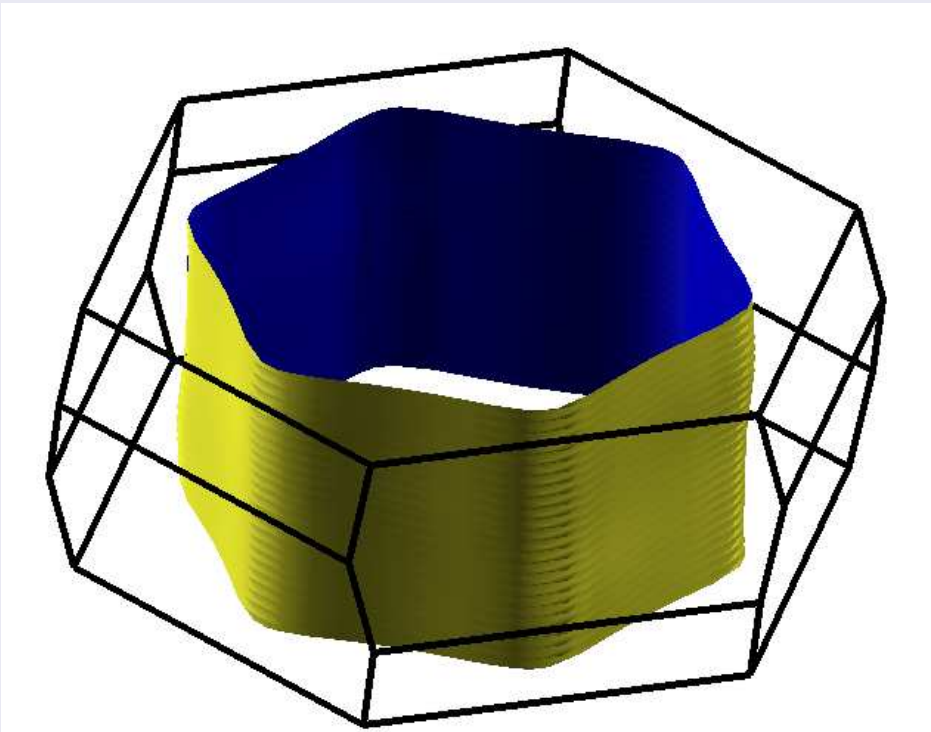
Fermi Surface



Results

- strong anisotropy
- but: bands below E_F disperse along Γ-A

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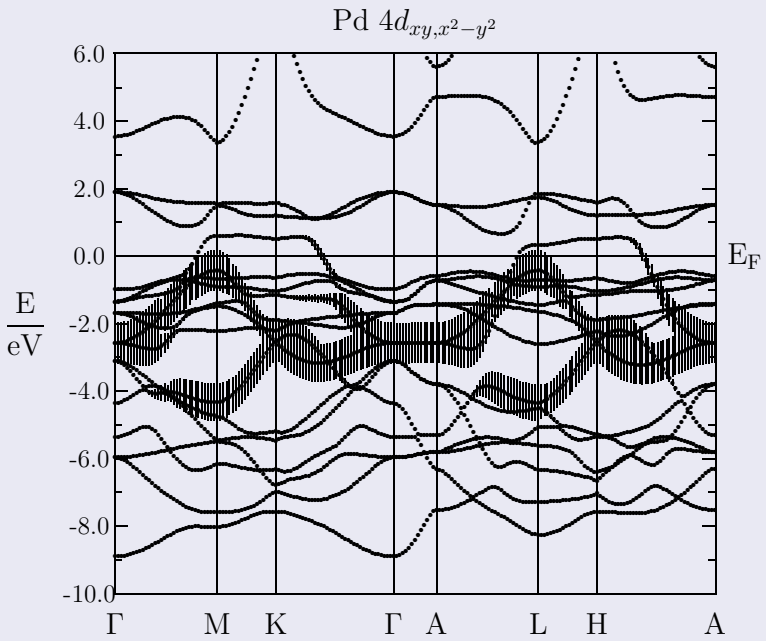
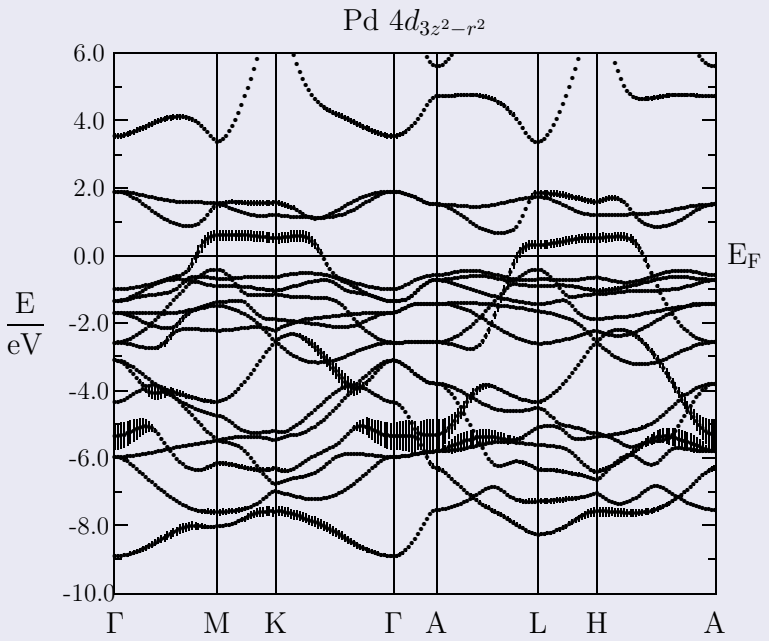
The Fingerprint of Dimensionality

Band Dispersions





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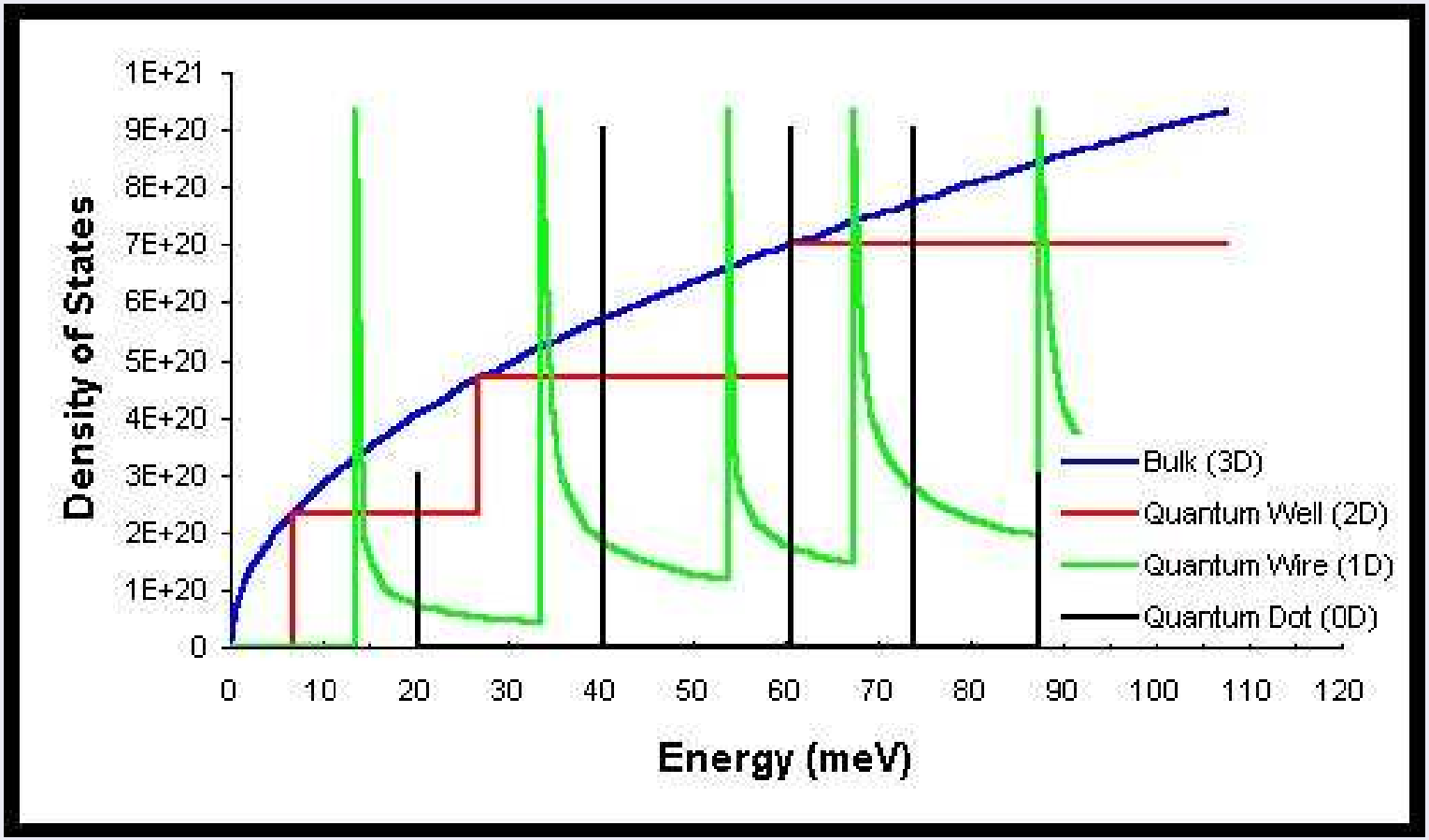
The Fingerprint of Dimensionality

Free Electron Density of States

$$\begin{aligned}
\rho(E) &\sim \int_{\Omega_{BZ}} d^d\mathbf{k}\, \delta\left(E - \frac{\hbar^2|\mathbf{k}|^2}{2m}\right) \\
&\sim \int_{\Omega_{BZ}} d|\mathbf{k}||\mathbf{k}|^{d-1}\, \delta\left(|\mathbf{k}| - \sqrt{\frac{2mE}{\hbar^2}}\right) \\
&\sim \frac{m}{\hbar^2}\sqrt{\frac{2mE}{\hbar^2}}^{d-2}
\end{aligned}$$

The Fingerprint of Dimensionality

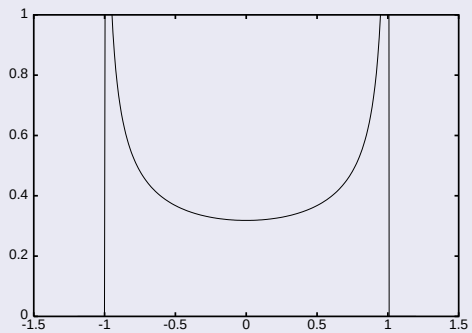
Free Electron Density of States

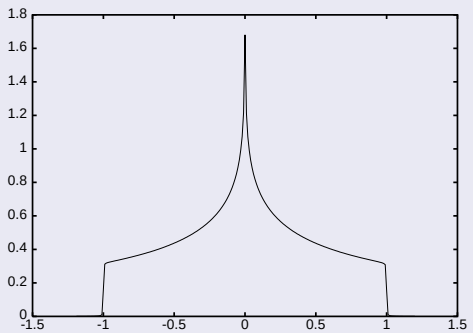


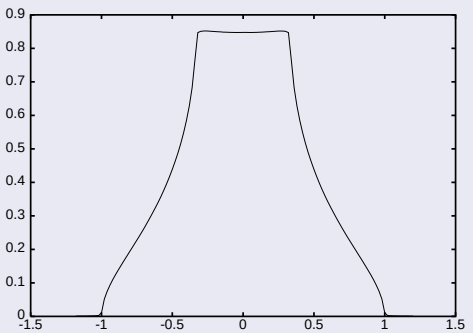
The Fingerprint of Dimensionality

Tight-Binding Bands

$$\varepsilon_{\mathbf{k}} = E_0 + E_1 \sum_{\{\Delta\}} e^{i\mathbf{k}\Delta}$$





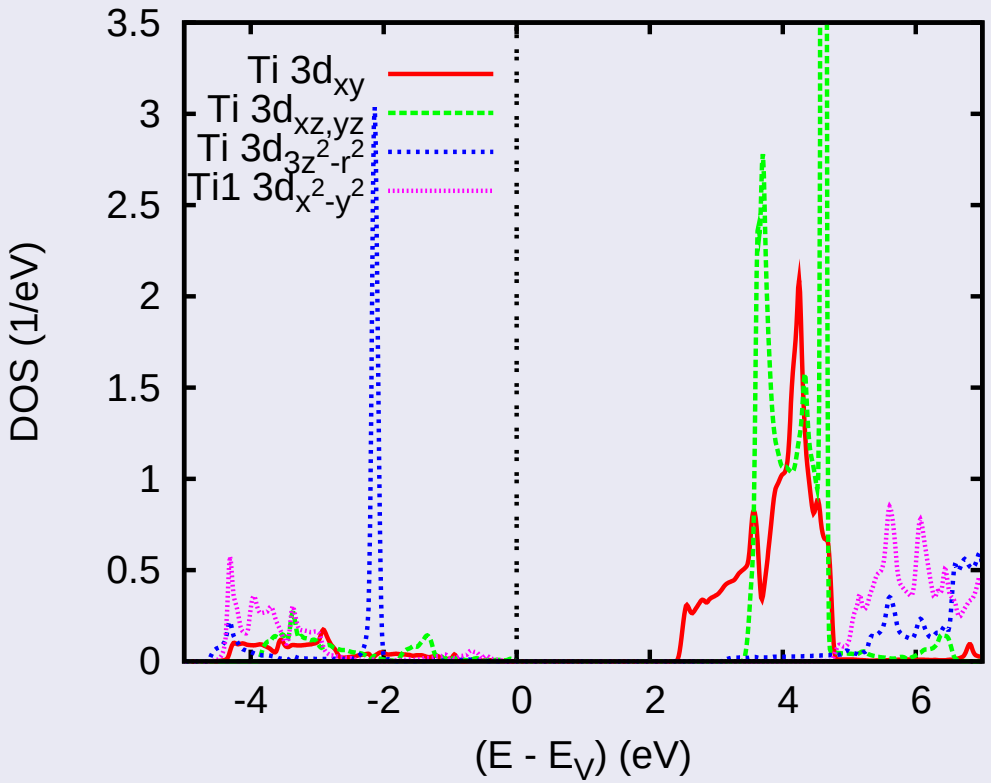


$d = 1$ $d = 2$ $d = 3$

(from: G. Czycholl, Theoretische Festkörperphysik, Springer)

The Fingerprint of Dimensionality

Single-layer $SrTiO_3$



$$d_{3z^2-r^2} : d = 0$$
$$d_{xz,yz} : d = 1$$
$$d_{xy} : d = 2$$

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Augmented Spherical Wave (ASW) Method

Characteristics

- a “dialect” of Andersen’s LMTO method
  - different linearization schemes
  - different interstitial energies
  - different implementations

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  - different linearization schemes
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0th Generation (Williams, Kübler, Gelatt, 1970s)

PRB **19**, 6094 (1979)

Augmented Spherical Wave (ASW) Method

1st Generation (VE, 1990s) — IJQC **77**, 1007 (2000)

- monolithic implementation from scratch
- new algorithms $\longrightarrow$ improved accuracy, numerical stability
- much improved functionality, usability, and portability
- xAnderson convergence acceleration scheme
- all LDA-parametrizations, most GGA-schemes
- still based on atomic-sphere approximation

ASW Method: Basic Formalism

Wave Function Expanded in Basis Functions

$$\psi_\sigma(\mathbf{r}) = \sum_{L\kappa i} c_{L\kappa i\sigma} H^{\infty}_{L\kappa\sigma}(\mathbf{r}_i)$$

$\longrightarrow$ $c_{L\kappa i\sigma}$ determined variationally

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Basis Functions: Augmented Spherical Waves

$$H^\infty_{L\kappa\sigma}(\mathbf{r}_i) = \begin{cases} H^I_{L\kappa}(\mathbf{r}_i) & \text{interstitial region} \\ \tilde{H}_{L\kappa\sigma}(\mathbf{r}_i) & \text{on-centre sphere } i \\ \sum'_{L'j} \tilde{J}_{L'\kappa\sigma}(\mathbf{r}_j) B_{L'L\kappa} & \text{off-centre spheres } j \end{cases}$$

$B_{L'L\kappa}(\mathbf{R}_j - \mathbf{R}_i)$: structure constants
ASW classified by atomic site $\mathbf{R}_i$, $L = (l, m)$, decay κ, spin σ

ASW Method: Basic Formalism

Envelope Functions

$$H^l_{L\kappa}(\mathbf{r}_i) := i\kappa^{l+1} h^{(1)}_l(\kappa r_i) Y_L(\hat{\mathbf{r}}_i)$$

$h^{(1)}_l(\kappa r_i)$: spherical Hankel function

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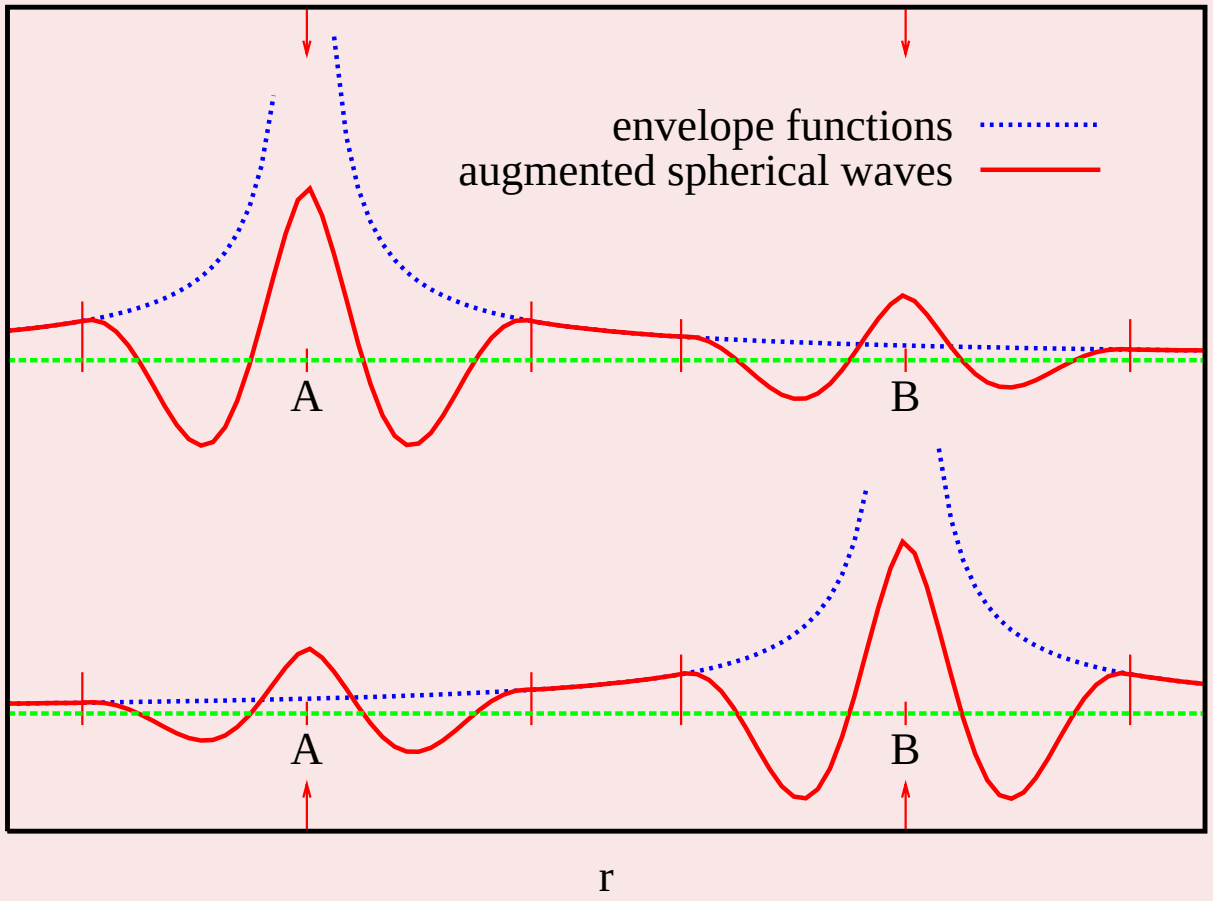
Augmented Functions

$$\begin{aligned} \tilde{H}_{L\kappa\sigma}(\mathbf{r}_i) &:= \tilde{h}_{l\kappa\sigma}(r_i) Y_L(\hat{\mathbf{r}}_i) \\ \tilde{J}_{L'\kappa\sigma}(\mathbf{r}_j) &:= \tilde{j}_{l'\kappa\sigma}(r_j) Y_{L'}(\hat{\mathbf{r}}_j) \end{aligned}$$

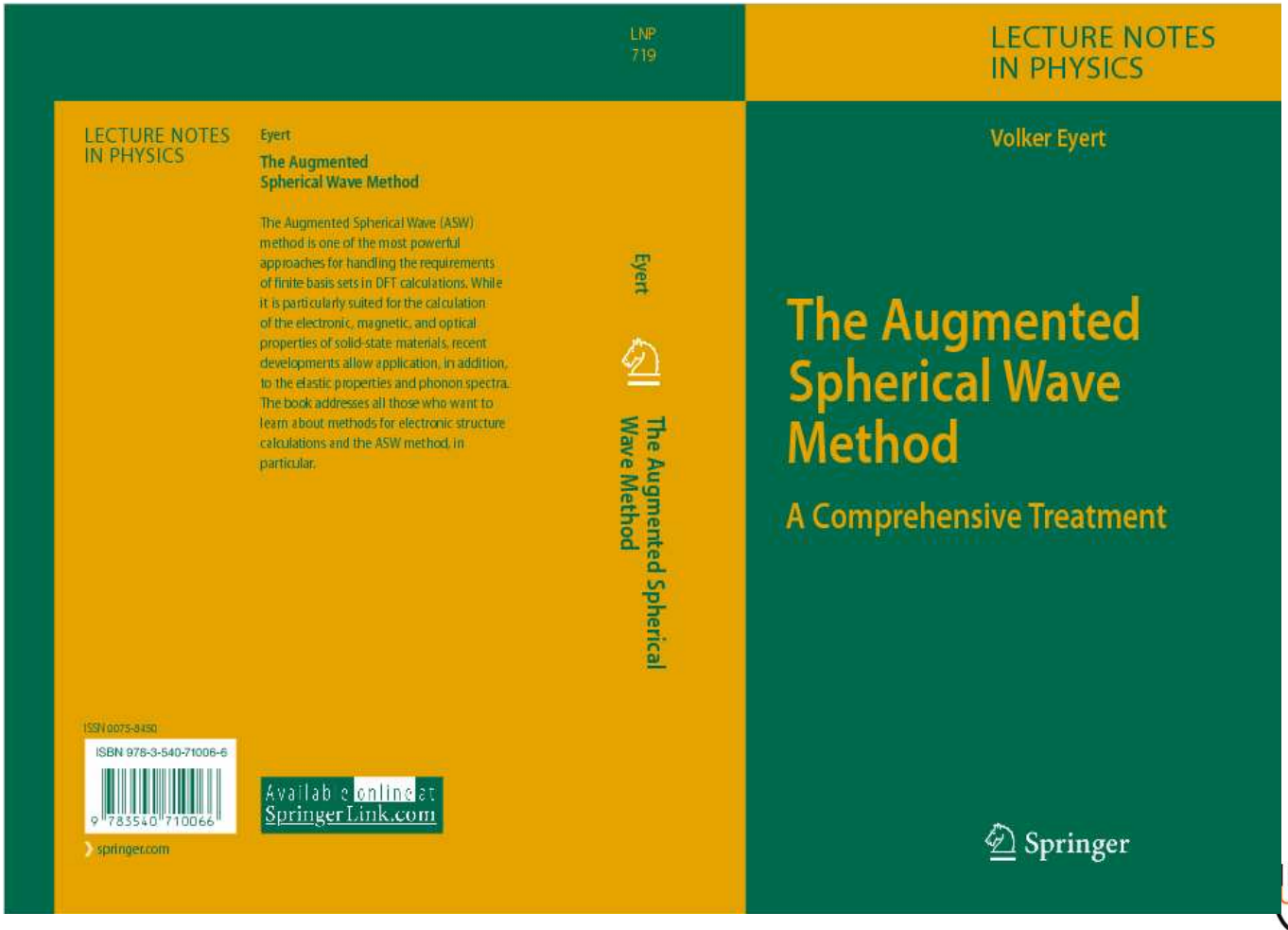
$\tilde{h}$, $\tilde{j}$: numerical solutions of radial Kohn-Sham equation
boundary conditions from envelope functions
correspond to φ and $\dot{\varphi}$ of LMTO

ASW Method: Basic Formalism

Augmented Spherical Waves



ASW Method: Further Reading



Towards a Full-Potential Spherical-Wave Method

Status

- ASA (space-filling atomic spheres)
  - $\mathcal{O}$(ASA) speed
  - systematic error in total energy
- non-overlapping muffin-tin spheres
  - prerequisite for accurate total energies
  - larger basis set $\rightarrow$ inefficient

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  - go to non-overlapping muffin-tin spheres
  - go beyond constant-potential approximation
- inside muffin-tin spheres
  - non-spherical contributions

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  - straightforward to implement
  - inefficient
- interstitial quantities expanded in spherical waves
  - elegant, no periodicity required
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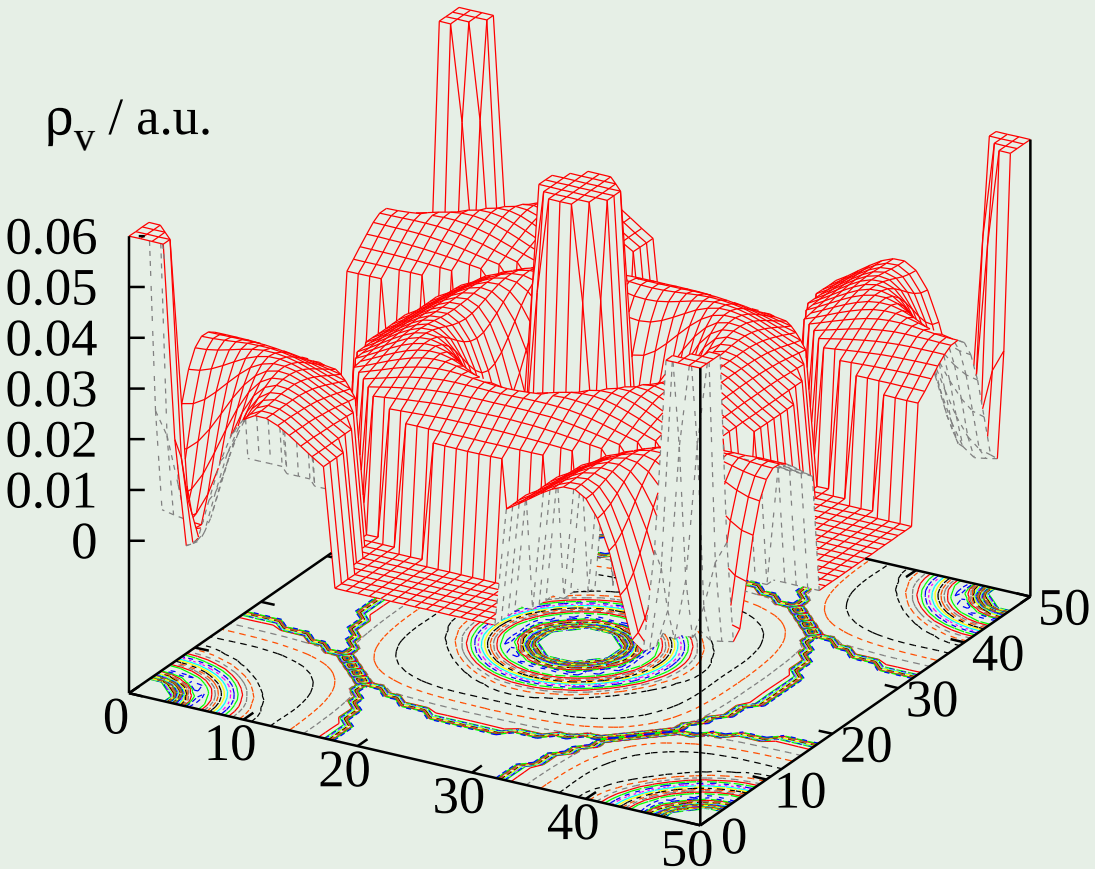
  - inside muffin-tin spheres
    - use spherical-harmonics expansions
  - in the interstitial region
    - no exact spherical-wave representation available!

From Wave Functions to Electron Density

Density inside MT-Spheres (Al)



From Wave Functions to Electron Density

Products of Basis Functions in Interstitial Region

$$p^I(\mathbf{r}) = \sum_n d_n F_n(\mathbf{r})$$

$$\int d^3\mathbf{r}\, F^*_{n'}(\mathbf{r}) p^I(\mathbf{r}) = \sum_n d_n \int d^3\mathbf{r}\, F^*_{n'}(\mathbf{r}) F_n(\mathbf{r})$$

From Wave Functions to Electron Density

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- $F_n(\mathbf{r})$: plane waves
  - integrals exact
  - inefficient
  - Weyrich 1988, Blöchl 1989, VE 1991, Savrasov 1992, Methfessel 2000

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  - would be efficient
  - integrals not known analytically
  - Springborg/Andersen 1987, Methfessel 1988, VE 2002, VE 2006

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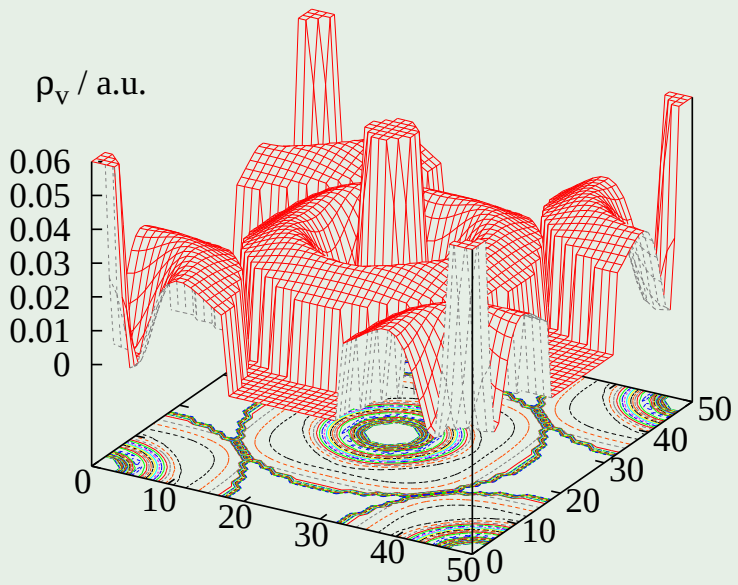
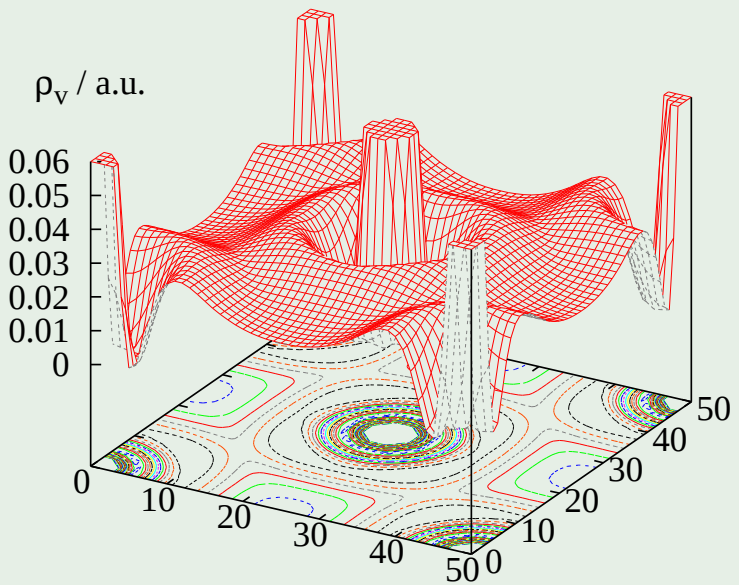
  - Springborg/Andersen 1987, Methfessel 1988, VE 2002, VE 2006
  - Methfessel 1988:
    match values and slopes at MT-sphere surfaces

From Wave Functions to Electron Density

Density from Value/Slope Matching at MT-Radii (Al)





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From Electron Density to Full Potential

Inside Muffin-Tin Spheres

- density, Hartree-potential and xc-potential numerically

Interstitial Region

- density from value/slope matching
- Hartree-potential analytically
- xc-potential from value/slope matching

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From Full Potential to Basis Functions

Previous Approaches

- project full potential to muffin-tin potential
- construct basis functions from muffin-tin potential
- no minimal basis set! (large basis set!)

Present Approach

- project full potential to ASA potential
- construct basis functions from ASA potential
- minimal basis set!

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Comparison of Approaches

Ole K. Andersen

- ASA geometry used for basis functions
  → minimal basis set — good!
- ASA geometry used for density and potential
  → error in total energy — bad!

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- MT geometry used for density and potential
  → accurate total energy — good!
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Comparison of Approaches

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present approach

- ASA geometry used for basis functions
  $\rightarrow$ minimal basis set $\rightarrow \mathcal{O}$(ASA) speed — great!
- MT geometry used for density and potential
  $\rightarrow$ accurate total energy — great!

Full-Potential ASW Method

2nd Generation ASW (VE, 2000s)

- based on 1st generation code
- full-potential ASW method — at $\mathcal{O}$(ASA) speed!
  - electron densities, spin densities
  - electric field gradients
  - elastic properties, phonon spectra
- optical properties
  - based on linear-response theory
  - direct calculation of $\Re\sigma$ and $\Im\sigma$
  - no Kramers-Kronig relations needed
- transport properties, thermoelectrics
- LDA+U method
  - all „flavours“ for double-counting terms (AMF, FLL, DFT)

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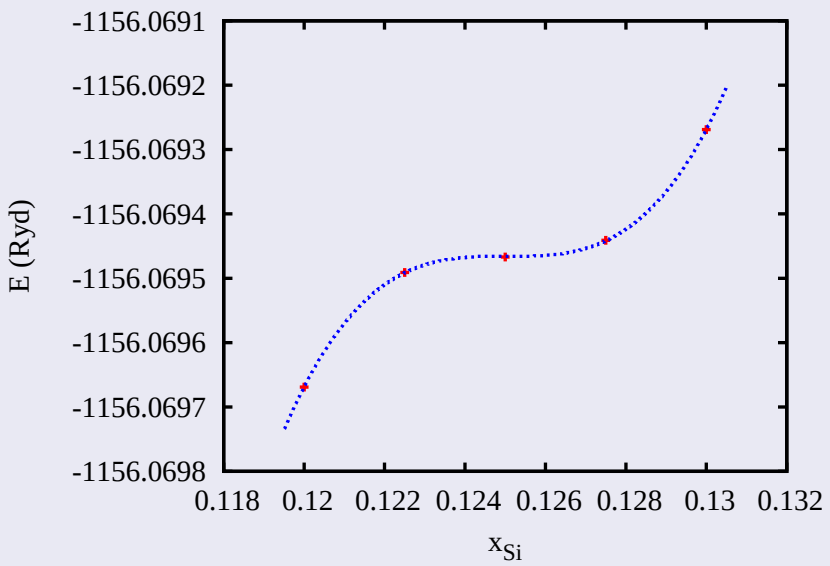
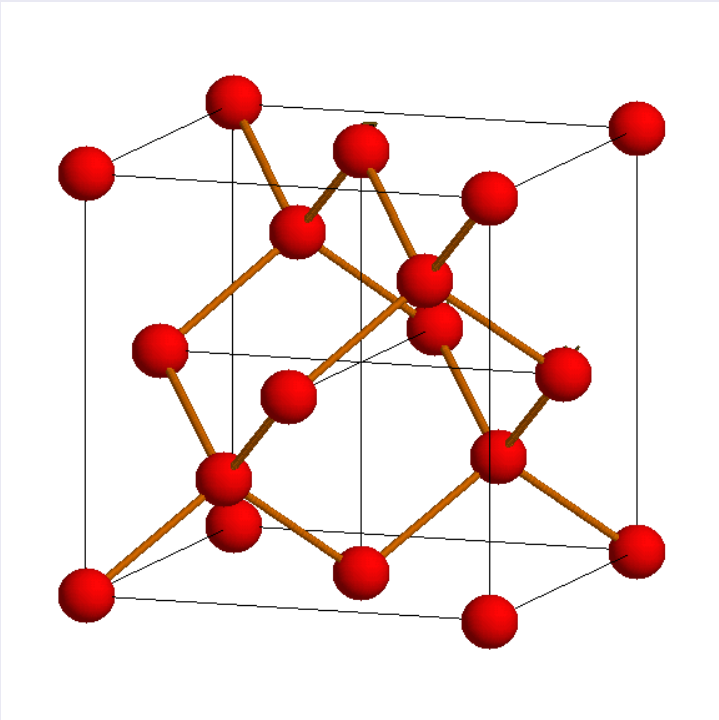
LTO(Γ)-Phonon in Silicon

ASA$^+$ Code





Bad

- no stable Si position # nature

LTO(Γ)-Phonon in Silicon

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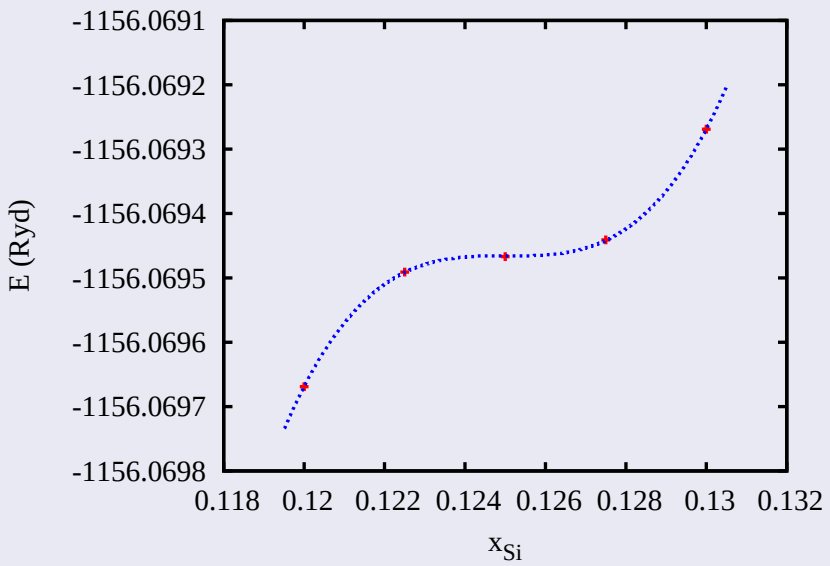
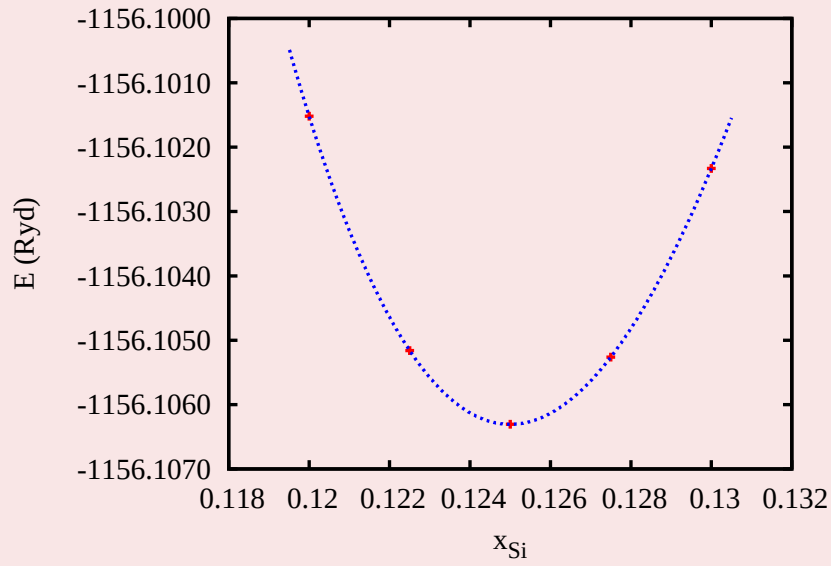


Full-Potential Code



New!

- phonon frequency: $f_{calc} = 15.34\,\mathrm{THz}$ ($f_{exp} = 15.53\,\mathrm{THz}$)

Outline

1. Cool-down
2. Full-Potential ASW Method
3. A Short Walk Through Dimensions
   - Where are the Moments?
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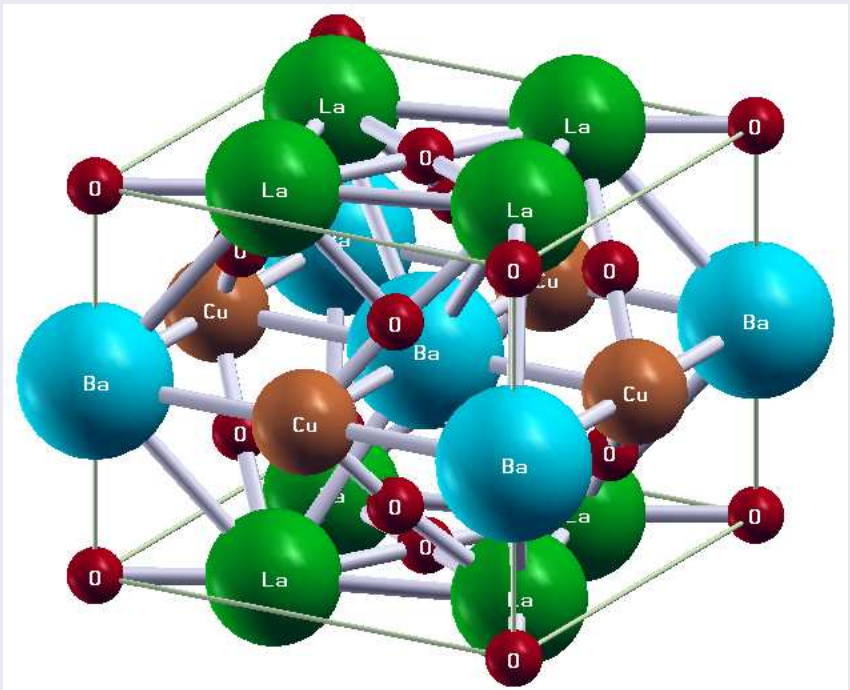
La_2BaCuO_5: A 0D(?) Ferromagnetic Semiconductor

Crystal Structure

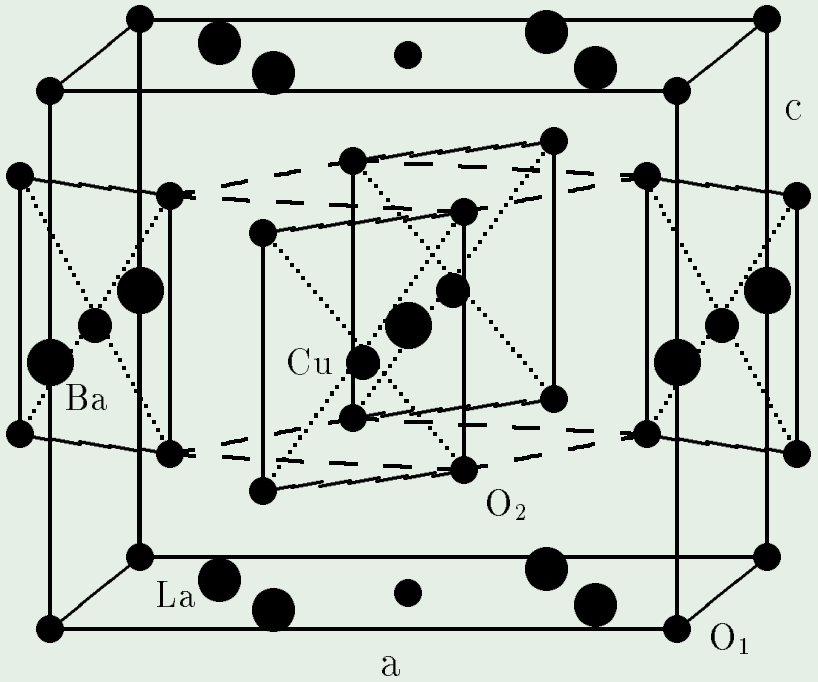


Building Blocks

- *P4/mbm* (D^5_{4h})
- a = 6.8447 Å, c = 5.8637 Å
- Ba-Cu and La-O1 layers
- O2 interlayers
- LaO_8 and BaO_{10} polyhedra
- CuO_4 plaquettes
  - Cu-Cu distance 4.84 Å
  - chains $\parallel$ c
  - $\perp$ in (a,b) planes
  - coupled by La atoms

La_2BaCuO_5: A 0D(?) Ferromagnetic Semiconductor

Plaquettes



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  - $\perp$ in (a,b) planes
  - coupled by La atoms

La_2BaCuO_5: A 0D(?) Ferromagnetic Semiconductor

Magnetic Properties

- $T_C = 5.2\,K$
- $m = 0.95\,\mu_B/Cu \parallel c$
- $T > 80\,K$: Curie-Weiss
  - $\mu_{eff} = 1.54\,\mu_B$
  - $\Theta < 0\,K$
- $T < 80\,K$: Curie-Weiss
  - $\Theta = 5\,K$
- 3D Spin-$\frac{1}{2}$ Heisenberg Model
- + Ising-like anisotropy

Electronic Properties

- $Cu^{2+} \longrightarrow d^9$
- Cu d hole $\hat{=}$ $d_{x^2-y^2}$ plaquette orbital

Cluster Model

- ferromagnetic order
  - interference of different exchange paths

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La_2BaCuO_5: A 0D(?) Ferromagnetic Semiconductor

Open Issues

- Role of Cu 3*d*, O 2*p*, La 5*d* Orbitals?
- Dimensionality?
- Effective Magnetic Sites?
- Exchange Paths?
- Heisenberg model?

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TODOs

- Spin-Degenerate Calculations
  - Role of Orbitals
  - Chemical Bonding
- Spin-Polarized Calculations
  - Magnetic Instability
  - Exchange Paths

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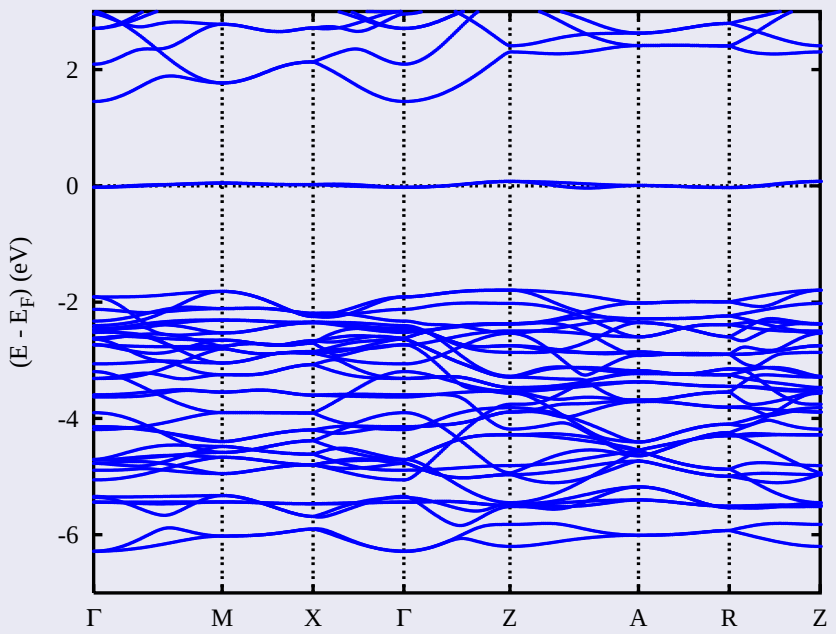
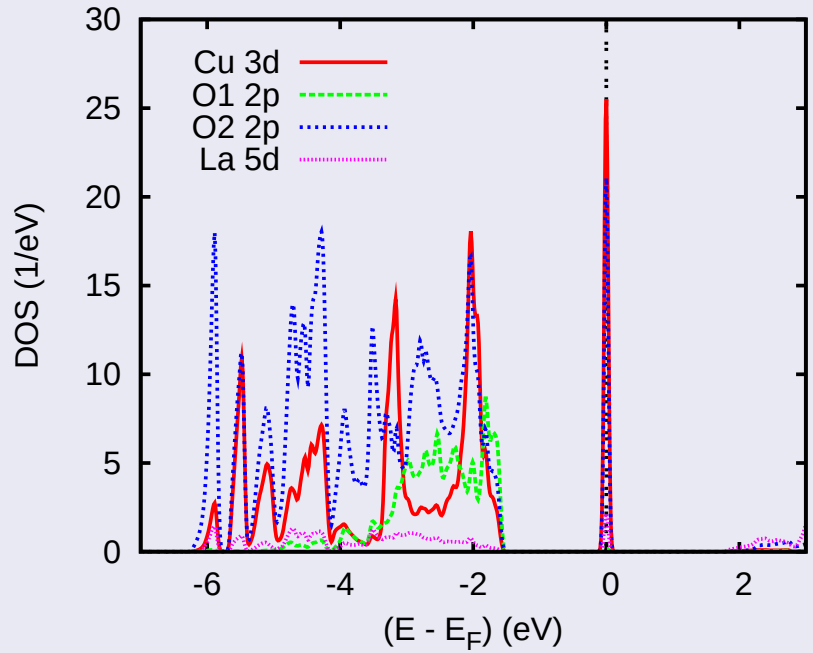
Spin-Degenerate Calculations for La_2BaCuO_5

Band Structure



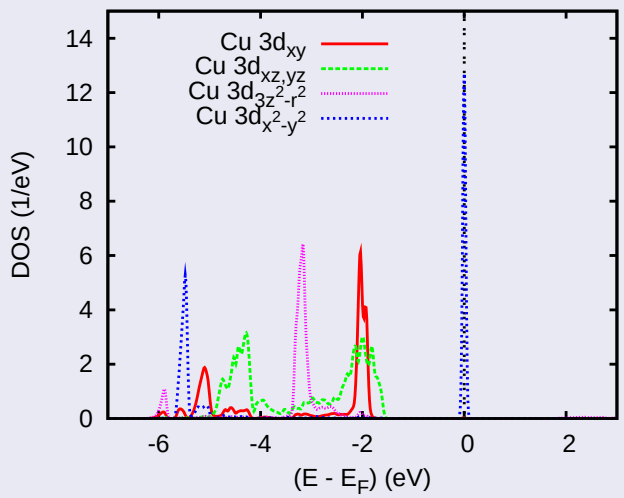
Partial DOS



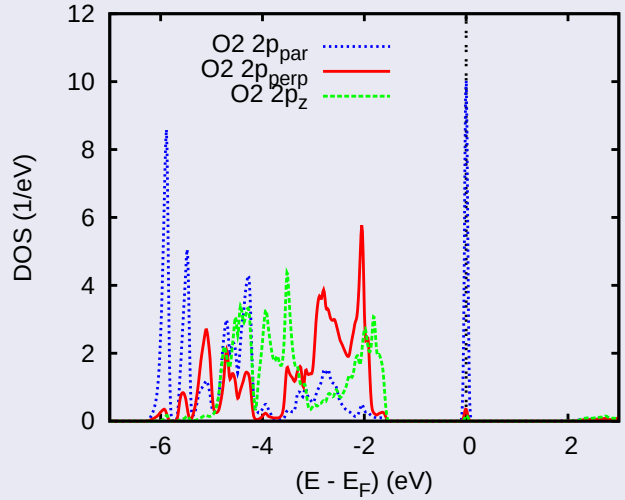
VE, K.-H. Höck, P. S. Riseborough, EPL **31**, 385 (1995)

Spin-Degenerate Calculations for La_2BaCuO_5

Cu 3*d* Partial DOS



O 2*p* Partial DOS



Bonding/Antibonding Splitting from *p*-*d* Overlap

$\approx 2.5 - 3.0$ eV for t_{2g}-like states (π-type)
≈ 5.5 eV for $d_{x^2-y^2}/p_{\|}$ states (σ-type)
$= 0$ eV for $d_{3z^2-r^2}$ states (apex $\rightarrow \infty$)

Spin-Polarized Calculations for La_2BaCuO_5

Magnetic Moments (μ_B)

	(↑↑)	(↑↓)
Cu	0.51	0.53
O2	0.12	0.07
La	0.02	0.03
Ba	-0.01	0.00
O1	0.00	0.00
f.u.	1.00	0.87

Total Energies (mRyd/f.u.)

spin-deg.	(↑↑)	(↑↓)
0.0	-9.35	-3.30

Band Gap (eV)

spin-deg.	(↑↑)	(↑↓)
0.0	0.66	0.38

VE, K.-H. Höck, P. S. Riseborough, EPL **31**, 385 (1995)

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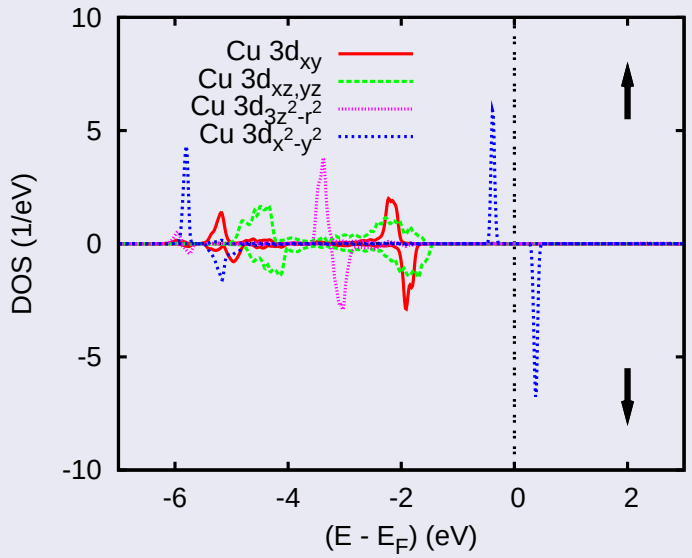

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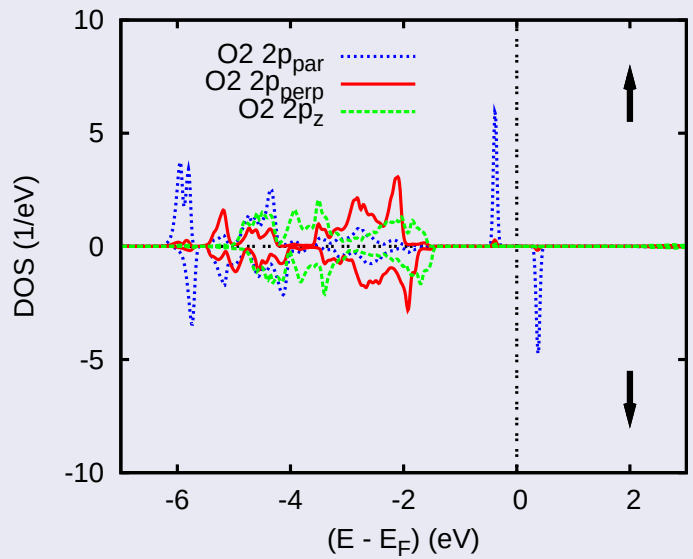
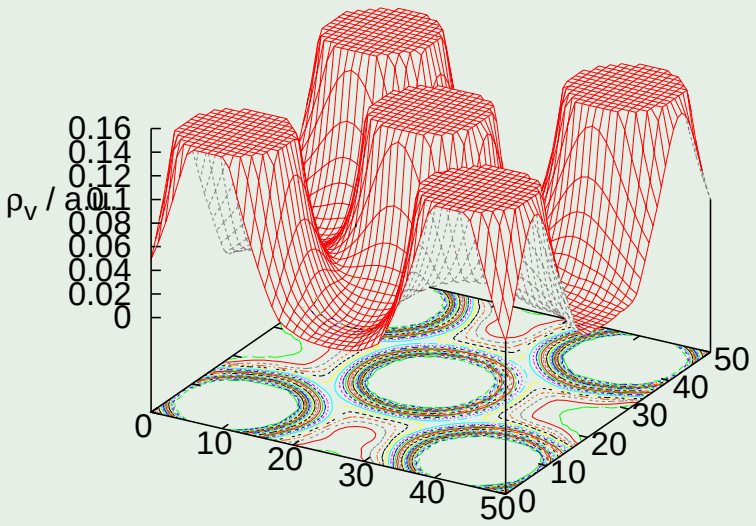


Results

- extended localized moments on plaquettes
  - carried by Cu $3d_{x^2-y^2}$ and O2 $2p_{||}$ states

Spin-Polarized Calculations for La_2BaCuO_5

Electron Density



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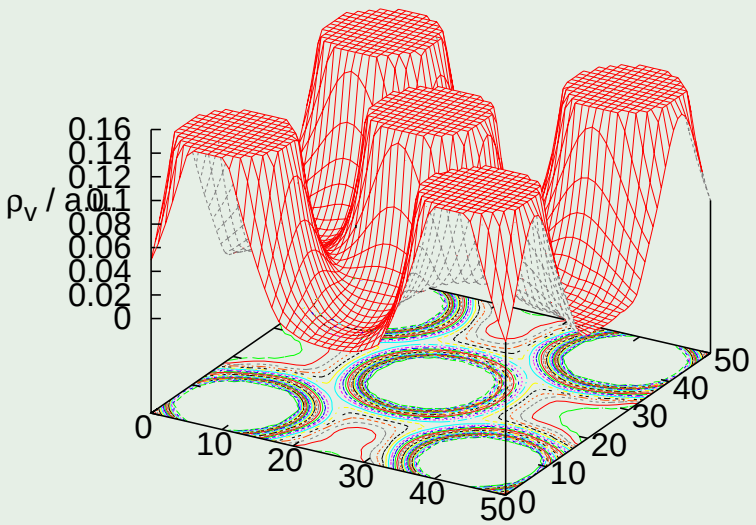
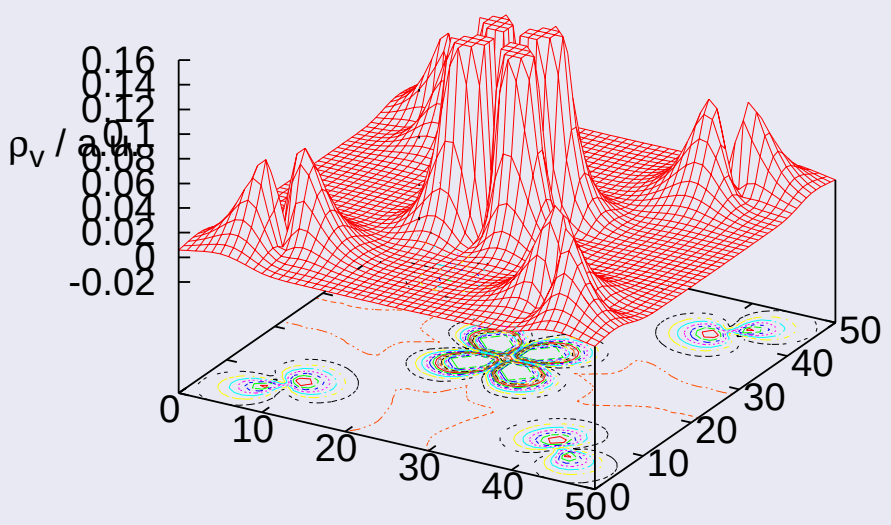


Electron Spin Density



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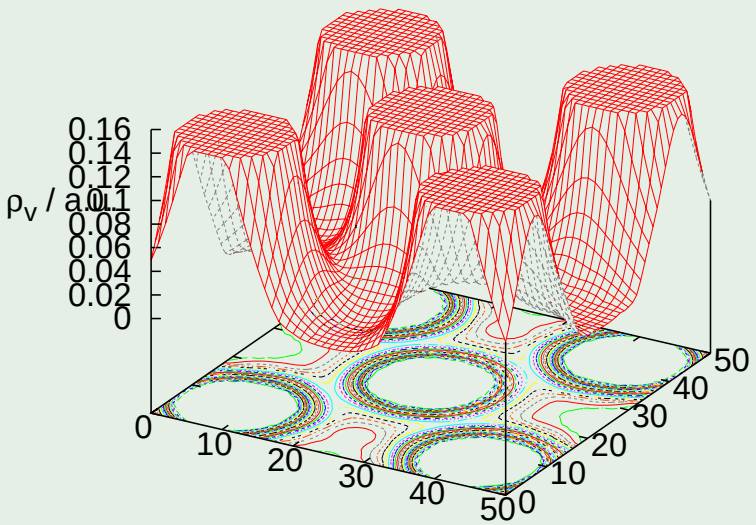
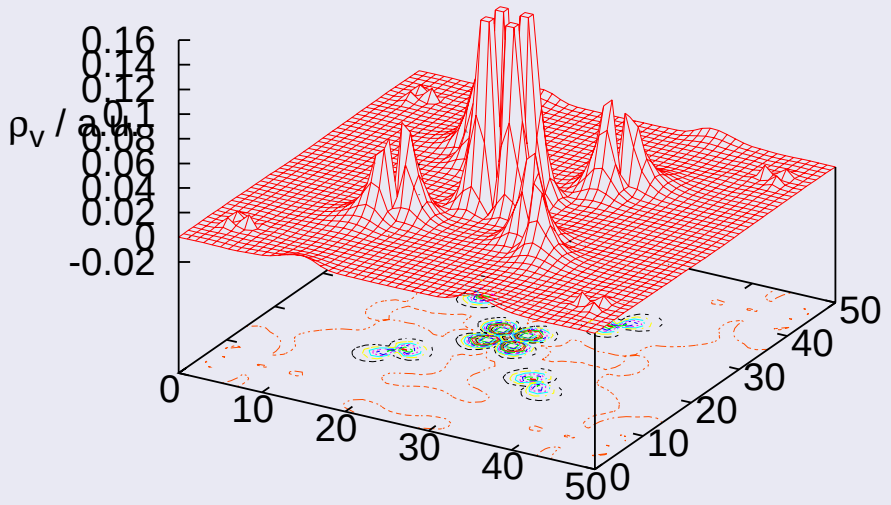


Electron Spin Density



Results

- extended localized moments on plaquettes
  - carried by Cu $3d_{x^2-y^2}$ and O2 $2p_{\|}$ states
  - coupled via La $5d_{x^2-y^2}$ states

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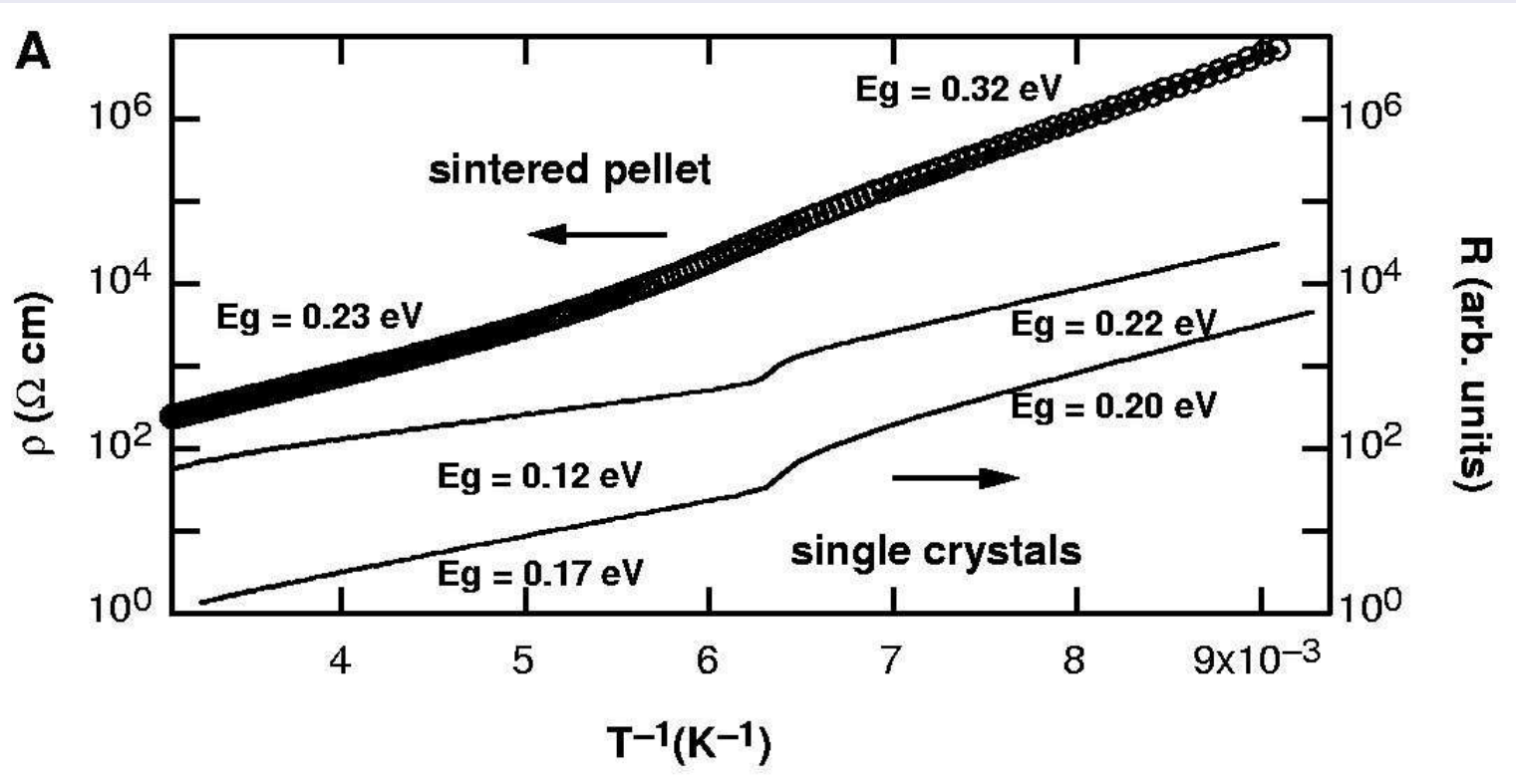
Orbital Ordering Transition in La_2RuO_5

Semiconductor-Semiconductor Transition at 160 K



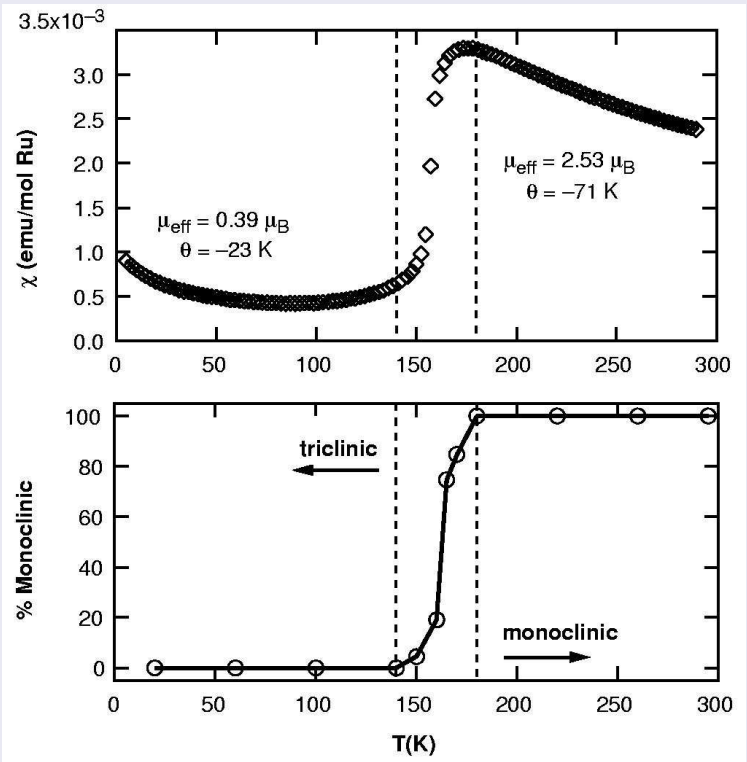
P. Khalifah et al., Science **297**, 2237 (2002)

Orbital Ordering Transition in La_2RuO_5

Basics

- $Ru^{4+} \rightarrow 4d^4$
- low-spin ($S = 1$)
- above 160 K: CW
- below 160 K:
  - $\chi \neq \chi(H), H < 9\,\mathrm{T}$
  - no supercell reflects. no AF order (?)
  - local moments?
  - $S = 1$, $S = 0$?

Magnetism, Crystal Structure



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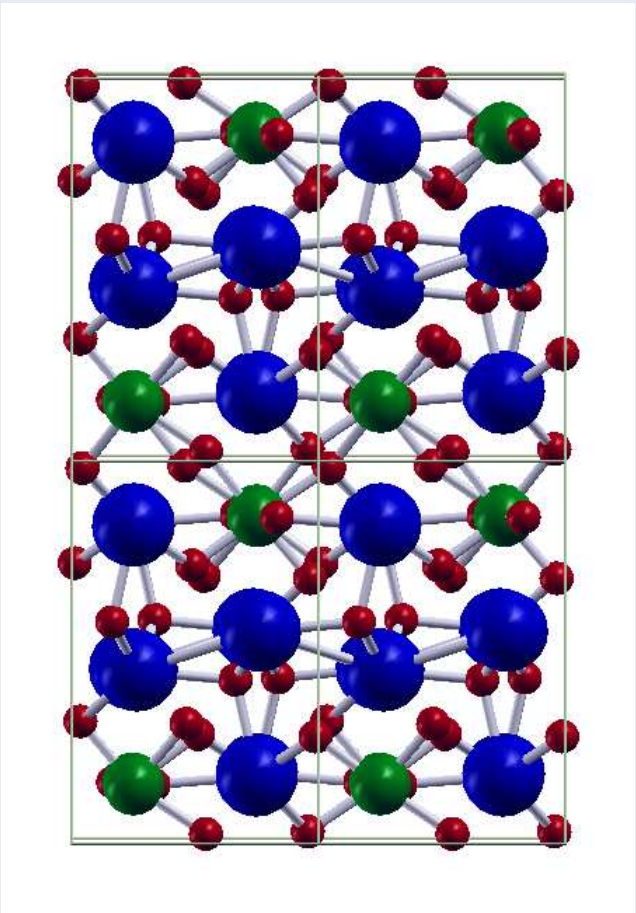
HT-Structure



Building Blocks

- RuO_6 octahedra
  - corner-sharing
  - chains $\|c$
  - zigzag pattern $\|b$
  - double layers $\|b, c$
- LaO_9 tricapped trigonal prisms
- La_4O tetrahedra

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Orbital Ordering Transition in La_2RuO_5

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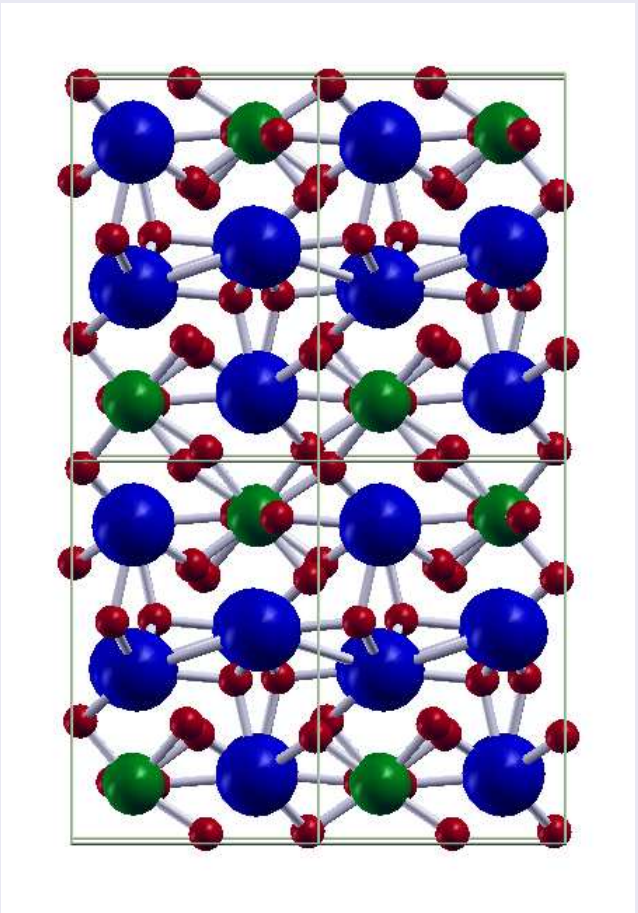
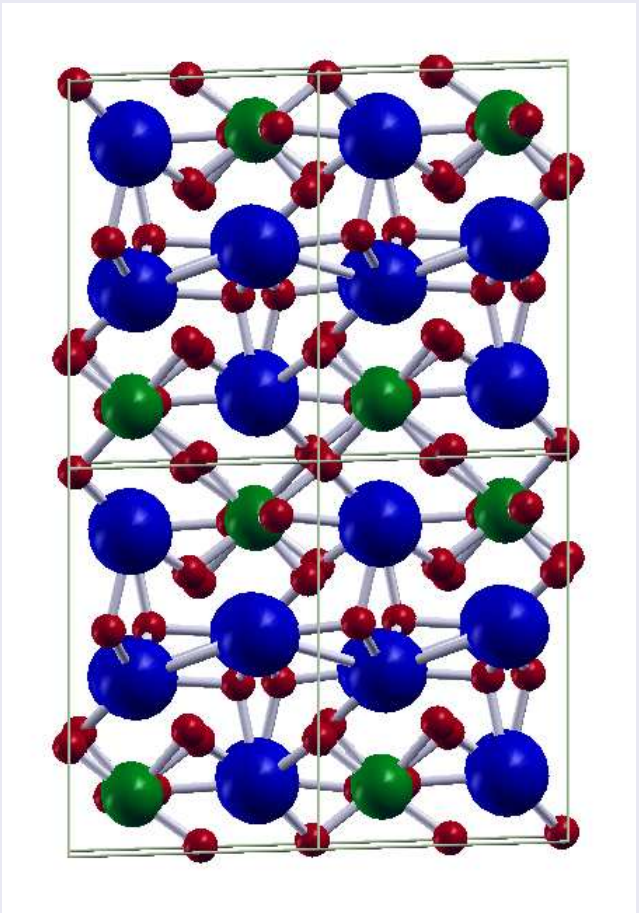


LT-Structure



Orbital Ordering Transition in La_2RuO_5

HT-Structure

- monoclinic, $P2_1/c$
- $d_{Ru-Ru} = 3.975\,\text{Å}$
- $d_{O-Ru-O-Ru-O} = 7.772\,\text{Å}$

LT-Structure

- triclinic, $P\bar{1}$
- $d_{Ru(1)-Ru(2)} = 3.868, 4.045\,\text{Å}$
- $d_{O-Ru(1)-O-Ru(2)-O} = 7.579, 7.977\,\text{Å}$

P. Khalifah et al., Science **297**, 2237 (2002)

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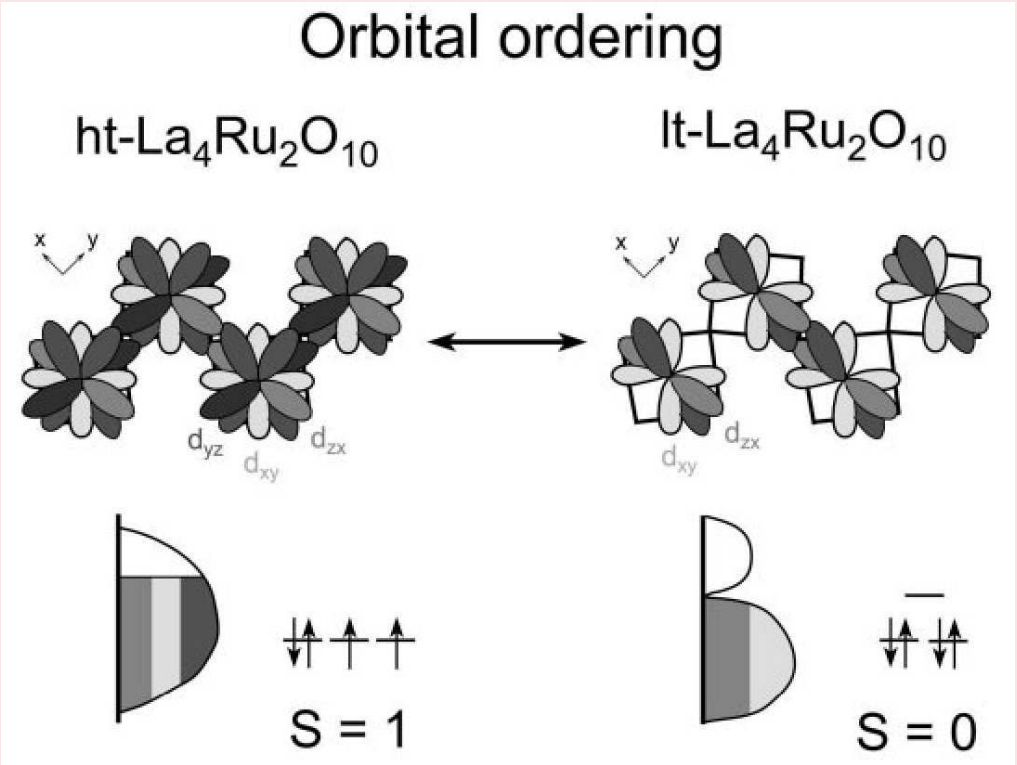
Orbital Ordering Transition in La_2RuO_5

Where are the Electrons?



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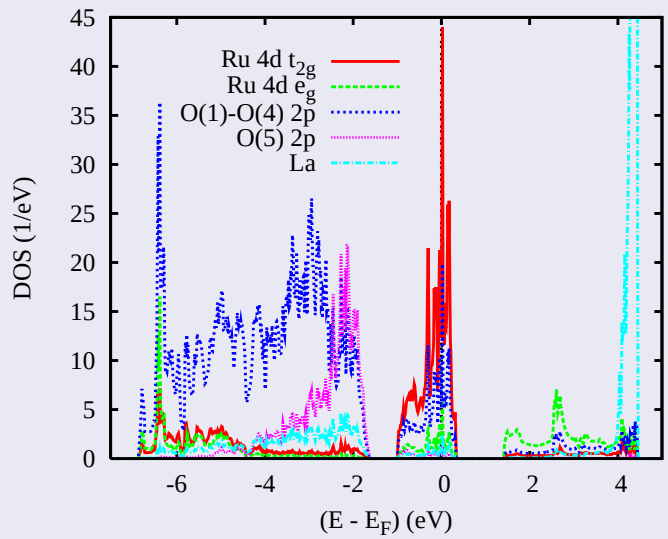
Spin-Degenerate Calculations for La_2RuO_5

HT-Structure



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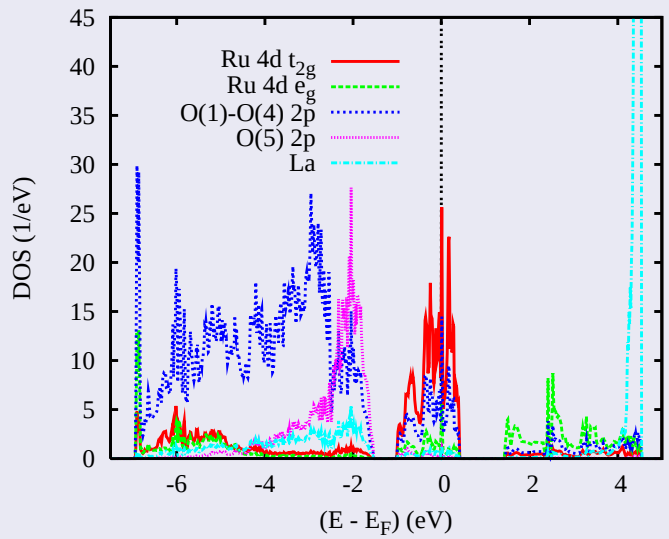

Results

- quasi-1D dispersion $\|c$
- CEF $\rightarrow$ Ru 4*d* t_{2g}/e_g
- strong Ru 4*d*-O 2*p* overlap

Spin-Degenerate Calculations for La_2RuO_5

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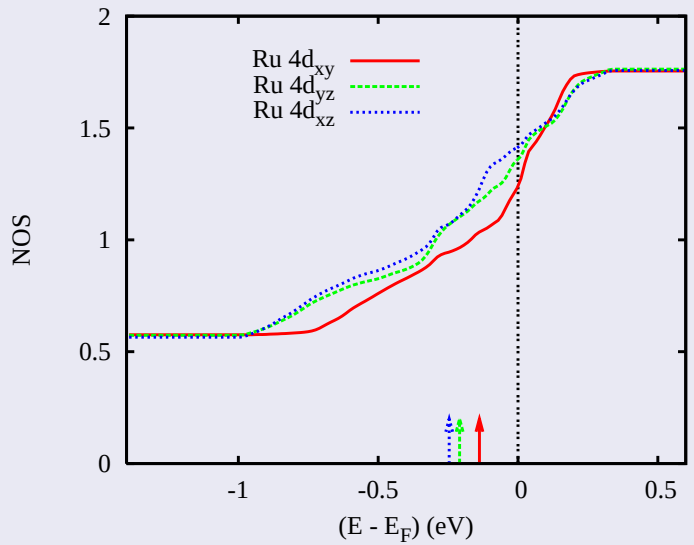

Results

- $d_{xy} \approx d_{xz} \approx d_{yz}$
- Hund's rule: $S = 1$

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Spin-Degenerate Calculations for La_2RuO_5

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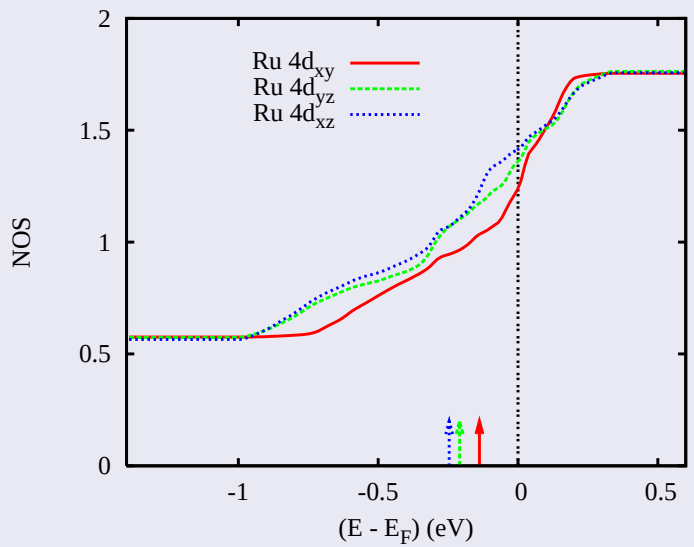

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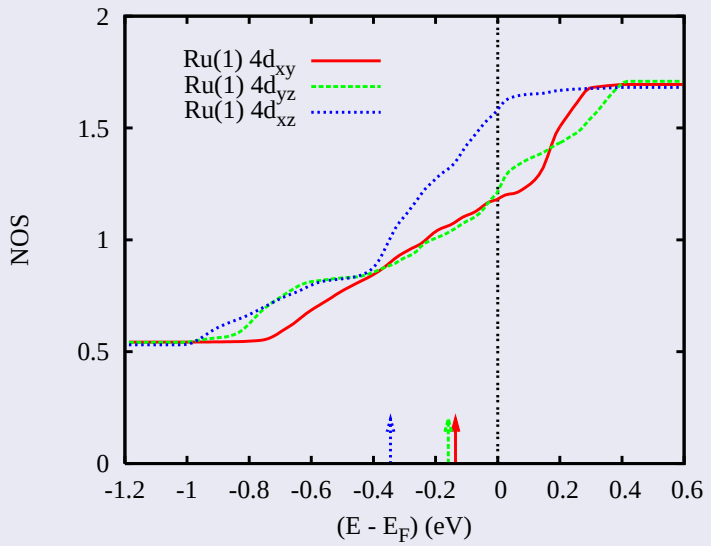

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Results

- $d_{xy} \approx d_{yz}$
- $d^1_{xy} d^2_{xz} d^1_{yz}$: $S = 1$

Spin-Polarized Calculations for La_2RuO_5

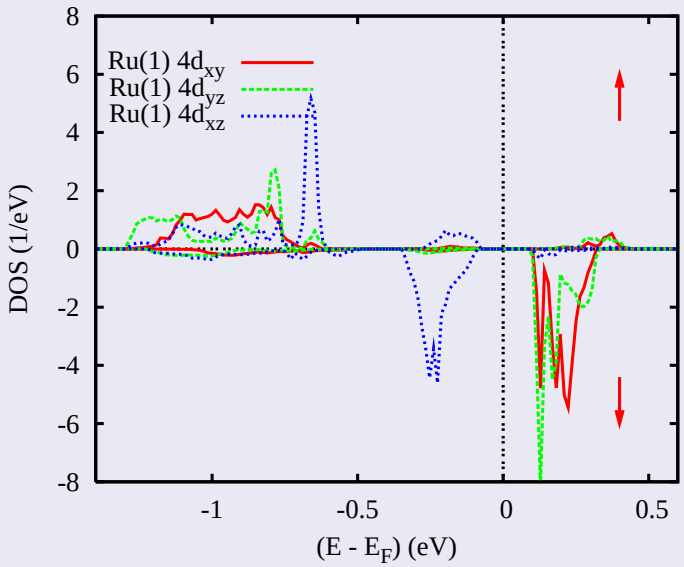
Total Energies (mRyd/f.u.), Moments (μ_B), Band Gaps (eV)

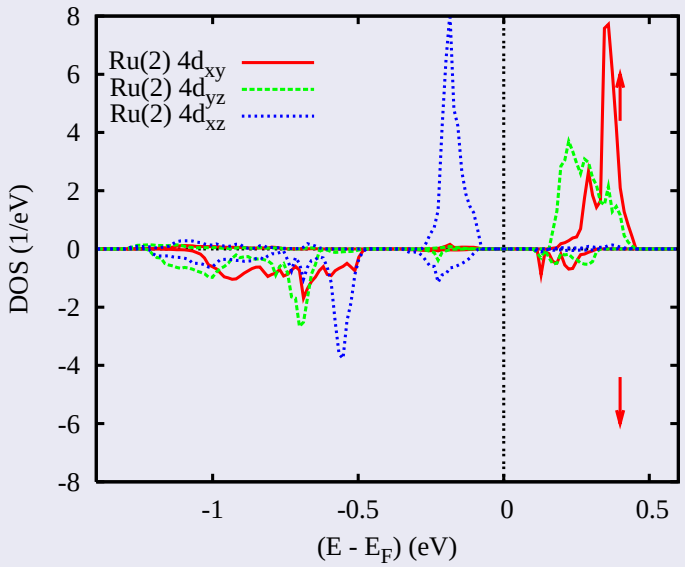
structure	funct.	order	ΔE	m_{RuO_6}	E_g
monoclinic	GGA	-	0.0		-
monoclinic	GGA	ferri	−6.6	1.24	-
monoclinic	GGA+U	ferri	−49.3	1.41	0.54
triclinic	GGA	-	−20.9		-
triclinic	GGA	ferri	−28.5	1.29	0.02
triclinic	GGA+U	ferri	−70.1	1.44	0.65

VE, S. G. Ebbinghaus, T. Kopp, PRL **96**, 256401 (2006)

Spin-Polarized Calculations for La_2RuO_5

LT-Structure



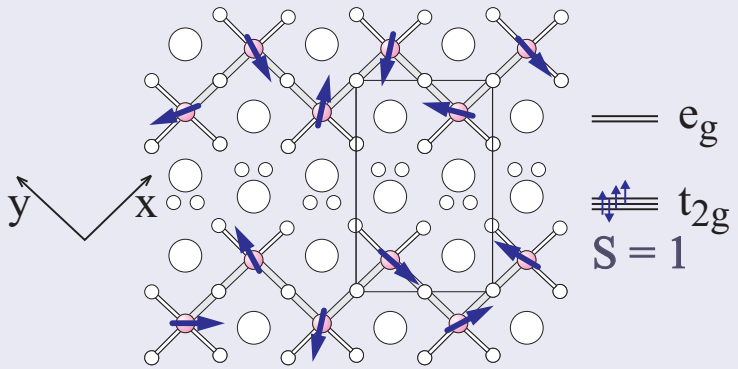


Results

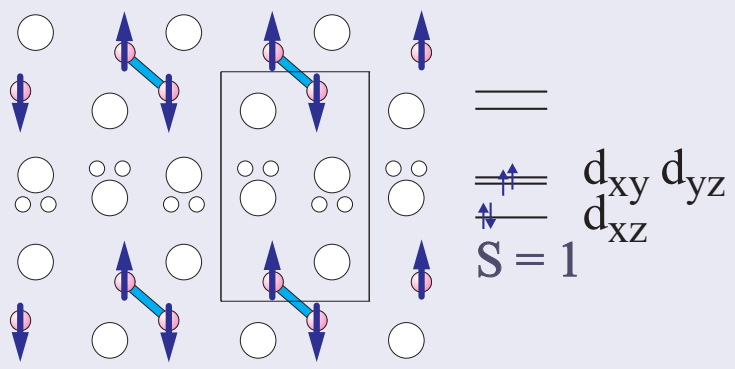
- Ru(1) $\approx$ Ru(2)
- $d_{xy} \approx d_{yz}$
- m(Ru): d_{xy} and d_{yz} $(d^1_{xy} d^2_{xz} d^1_{yz})$
- m(Ru(1)) $\neq -$m(Ru(2))

Scenario for La_2RuO_5

HT-Structure



LT-Structure



Spin-Ladders

- AF couping on rungs
- $m(Ru(1)O_6) = -m(Ru(2)O_6)$

VE, S. G. Ebbinghaus, T. Kopp, PRL **96**, 256401 (2006)

Outline

1 Cool-down

2 Full-Potential ASW Method

3 A Short Walk Through Dimensions
- Where are the Moments?
- How to Build a Spin-Ladder
- Greetings from High-T_c
- A Recipe Against Frustration

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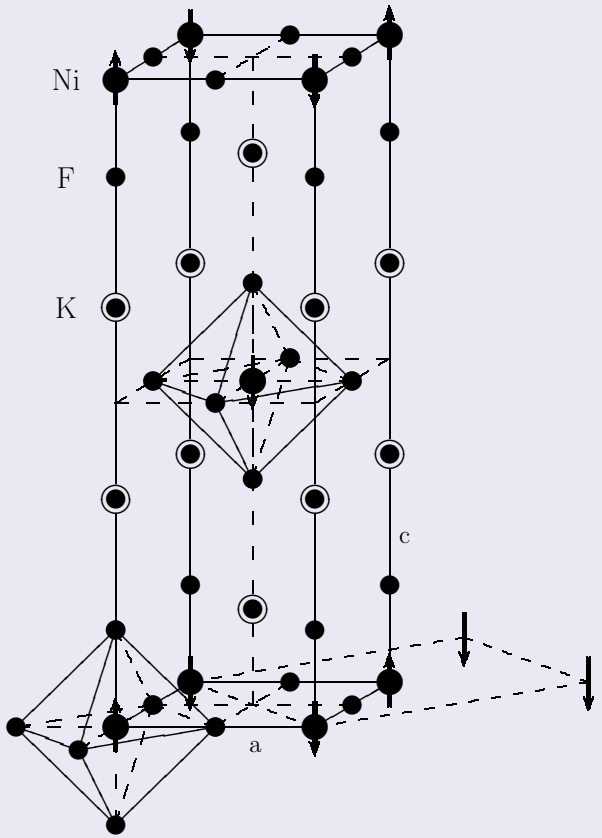
Magnetic Order in K_2NiF_4 and K_2CuF_4

K_2NiF_4 and K_2NiF_4

- “classical” two-dimensional systems
- based on K_2NiF_4 structure
- parent compounds of La_2CuO_4
- magnetic semiconductors
- role of TM 3*d* and F 2*p* orbitals?
- intralayer/interlayer magnetic coupling?
- antiferromagnetism vs. ferromagnetism
- symmetry breaking by magnetic order vs. symmetry breaking by orbital order

Magnetic Order in K_2NiF_4 and K_2CuF_4

K_2NiF_4 Structure



Basics

- I4/mmm (centered tetragonal)
- NiF_2 planes ($\hat{=}CuO_2$ planes)
- K and F interlayers
- corner sharing NiF_6 octahedra
- $d(Ni - F_{apex}) < d(Ni - F_{plane})$
- AF order
  - Cmca (side-centered orthorh.)
  - $a \longrightarrow \sqrt{2}a$

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K_2NiF_4

Magnetic Properties

- $T_N = 97.23$ K
- $m = 2.22\,\mu_B$
- magnetic moments $\parallel$ c
- $J/k_B \approx -100$ K

- 2D spin-wave dispersion
  - $J'/J < 0.0037$
- 2D ($S = 1$) Heisenberg Model
- + Ising-like anisotropy

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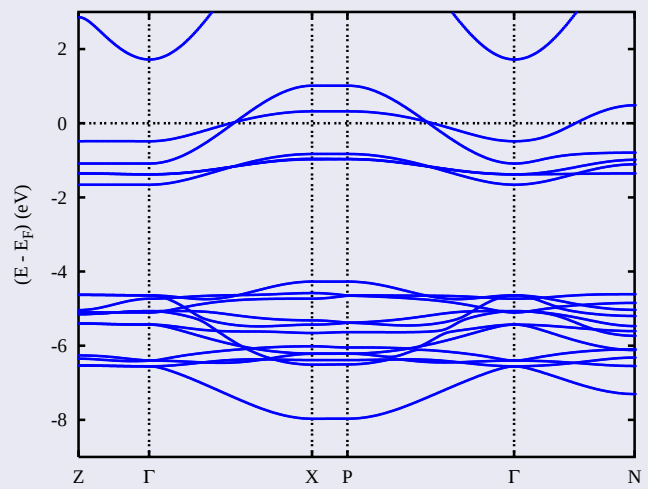
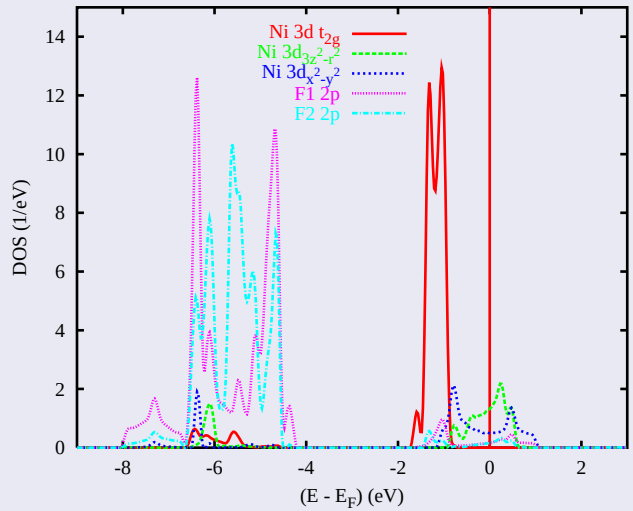
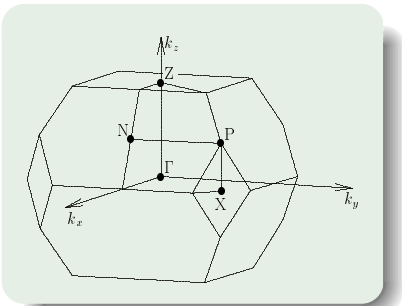
K_2NiF_4: Spin-Degenerate Calculations

Band Structure



Partial DOS



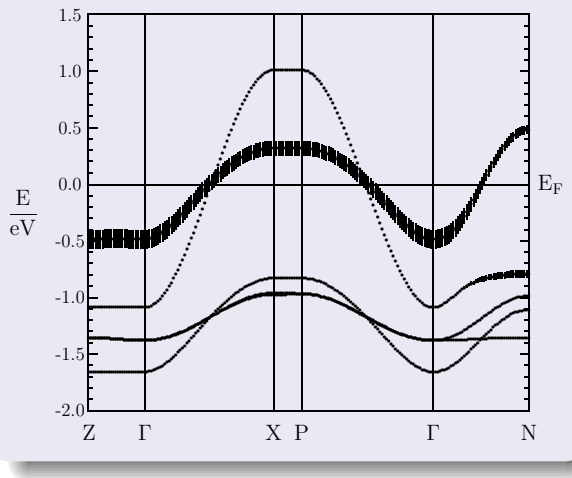


Results

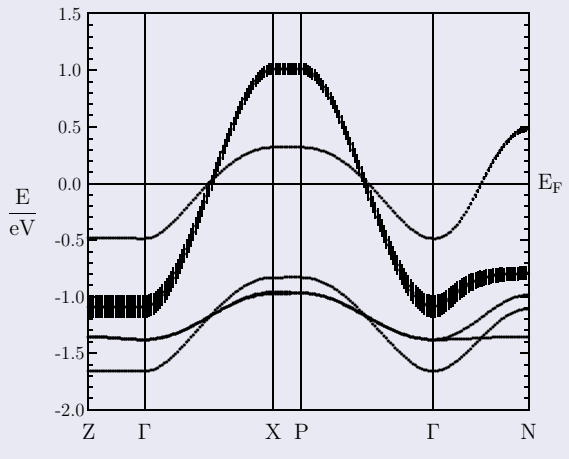
- $E < -4\,\text{eV}$: d-p bonding
- $E > -2\,\text{eV}$: d-p antib.
- 2D dispersion
- at E_F: Ni 3d e_g

K_2NiF_4: Weighted Bands

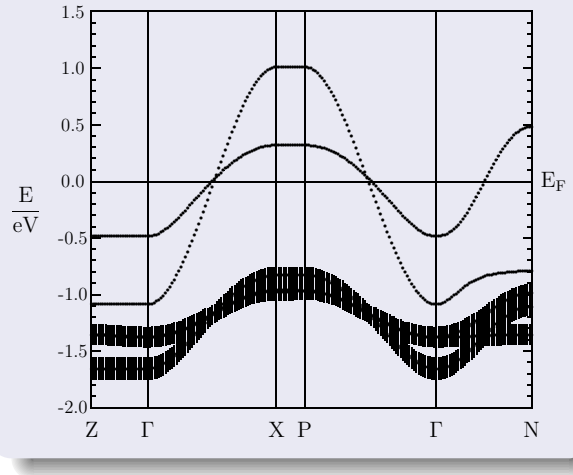
Ni $3d_{3z^2-r^2}$



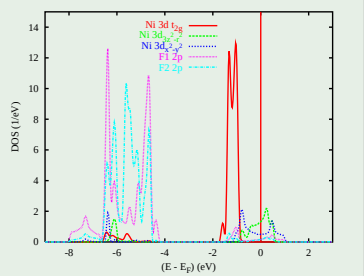
Ni $3d_{x^2-y^2}$



Ni $3dt_{2g}$



Partial DOS

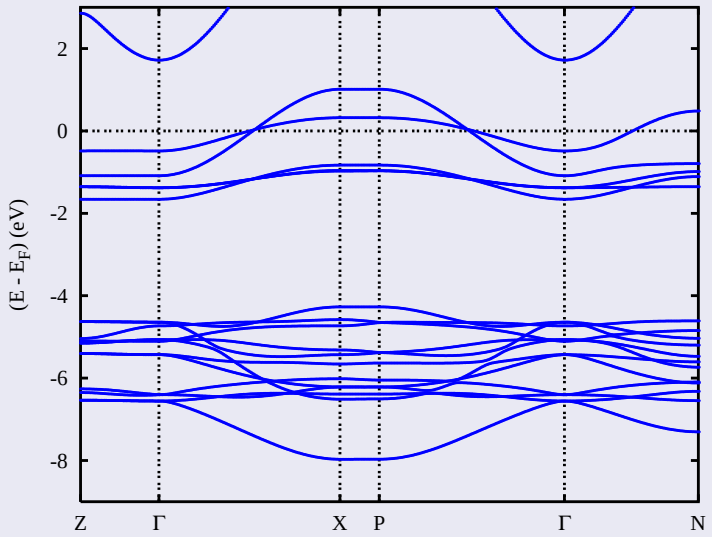


Results

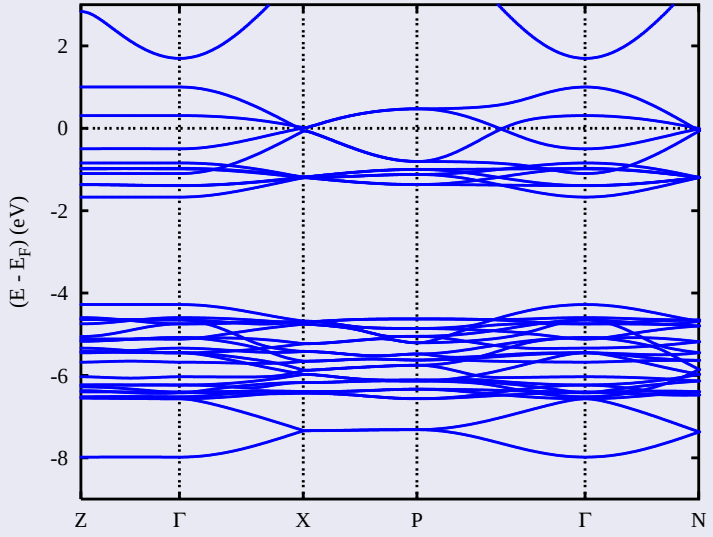
- CEF $(t_{2g}/e_g) \approx 0.9$ eV
- $W(d_{x^2-y^2}) \approx 2\, W(d_{3z^2-r^2})$
- perfect FS nesting

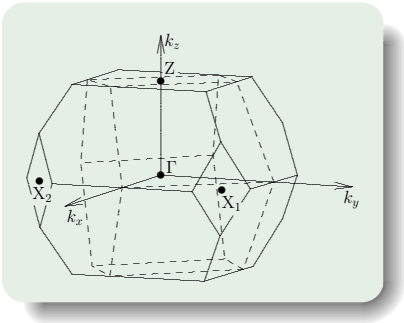
K_2NiF_4: Doubling the Unit Cell

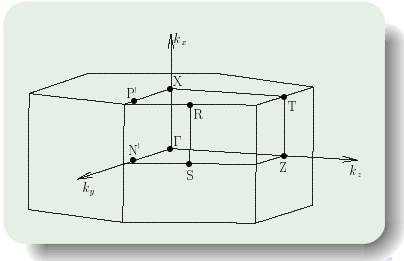
centered tetragonal



side-centered orthorh.







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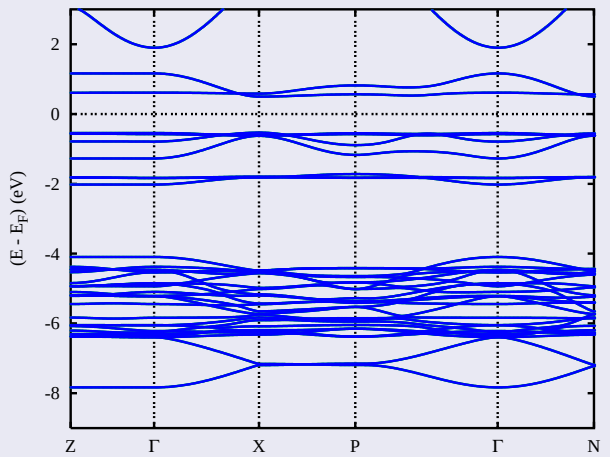
K_2NiF_4: Spin-Polarized Calculations

Band Structure



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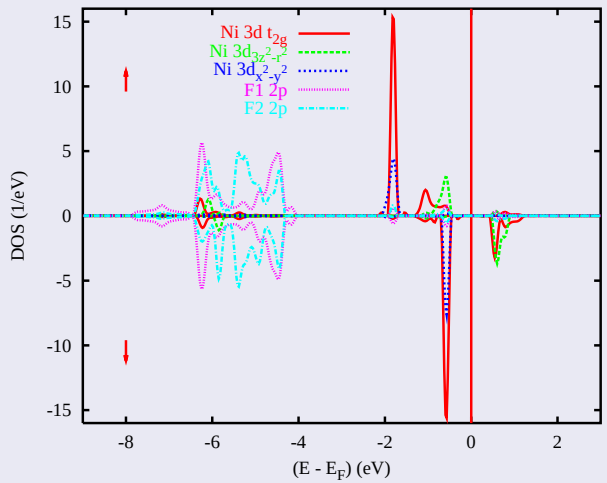

Moments (μ_B)

Ni	1.28
F2	0.04
sublattice	1.38

Results

- moment: $d_{3z^2-r^2}$, $d_{x^2-y^2}$
- $\Delta E_{tot} = -30.5\,\text{mRyd}$

K_2CuF_4

Magnetic Properties

- $T_C = 6.26$ K
- $m = 1.00\,\mu_B$
- magnetic moments $\perp$ c
- 2D spin-wave dispersion
  - $J'/J < 0.00066$
- 3D ($S = \frac{1}{2}$) Heisenberg Model
- + 1% XY-like anisotropy
- $J/k_B = 11.2$ K

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K_2CuF_4

Magnetic Properties

- $T_C = 6.26$ K
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Early XRD (Knox)

- "K_2NiF_4" structure
- $d_{Cu-F_{apex}} < d_{Cu-F_{plane}}$
  - $\sharp$ related Cu-compounds

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K_2CuF_4

Khomskii and Kugel Model

- Heisenberg Hamiltonian
- + Pseudospin Hamiltonian
  - orbital ordering
- compressed octahedra
  - $\nexists$ ferromagnetic order
- antiferrodistortive structure proposed
  - side-centered orthorh.

Early XRD (Knox)

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- $d_{Cu-F_{apex}} < d_{Cu-F_{plane}}$
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K_2CuF_4

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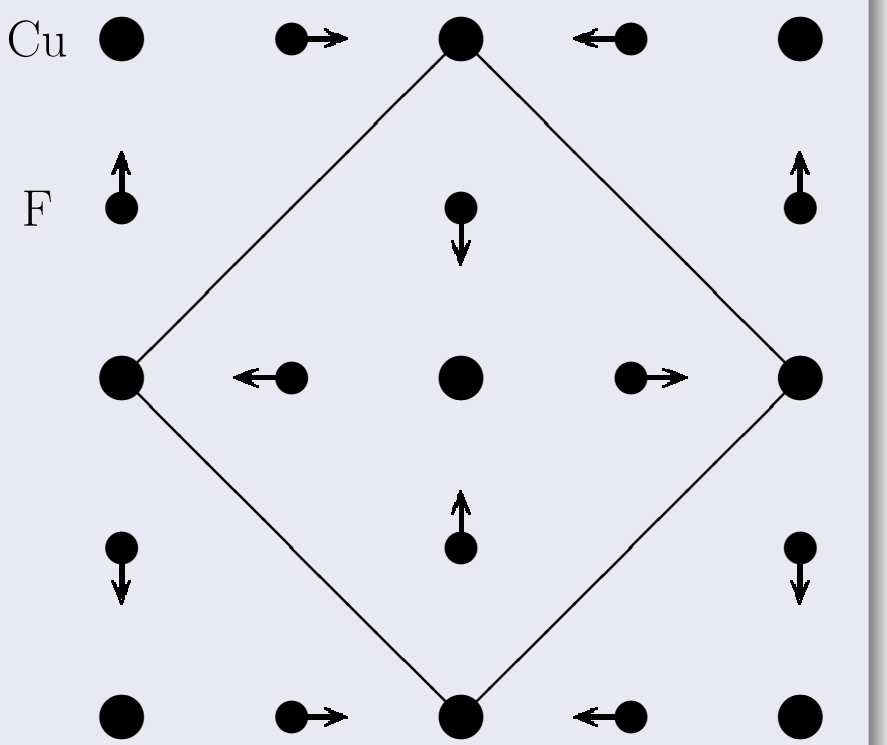
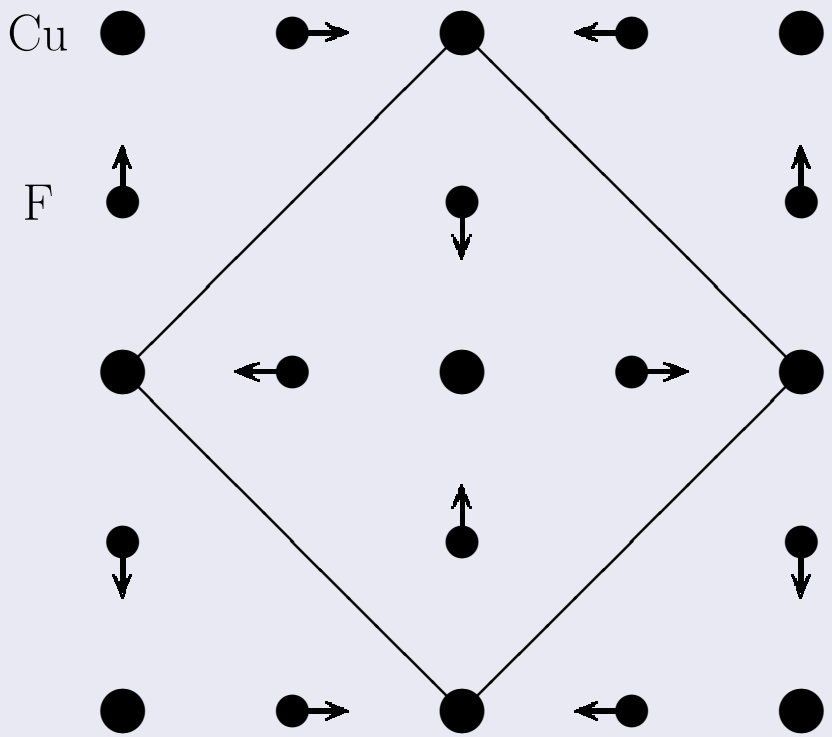
In-Plane Structure



K_2CuF_4

In-Plane Structure

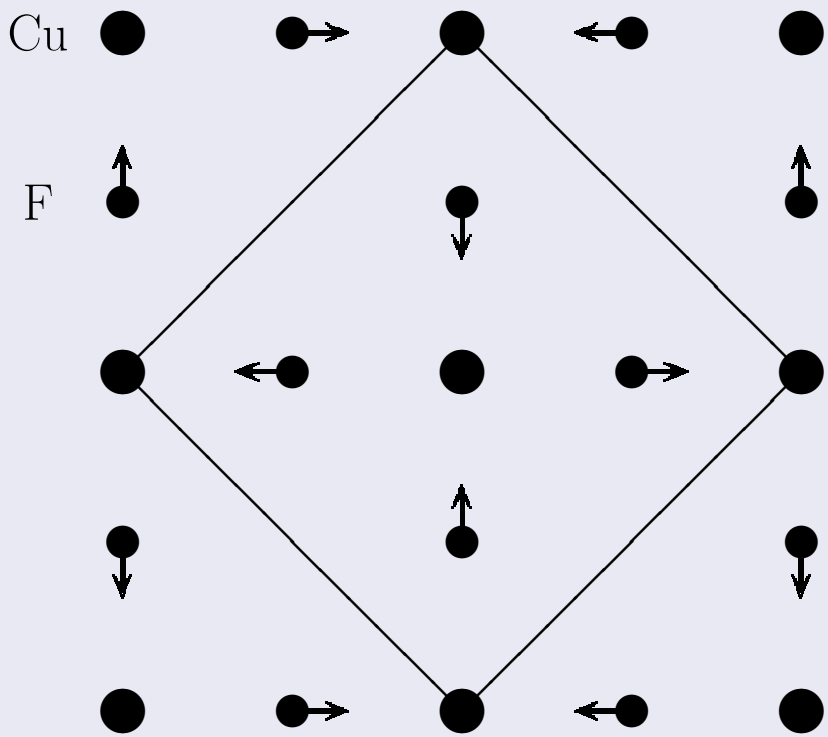


NMR (Le Dang Khoi, Veillet)

- octahedra elongated, long axis $\perp$ c

K_2CuF_4

In-Plane Structure



NMR (Le Dang Khoi, Veillet)

- octahedra elongated, long axis $\perp$ c

XRD (Hidaka et al.)

- Cmca (side-centered orthorh.)
- F at $(\frac{1}{4} - \delta, \frac{1}{4} - \delta, 0)$
  - $\delta = 0.0176$

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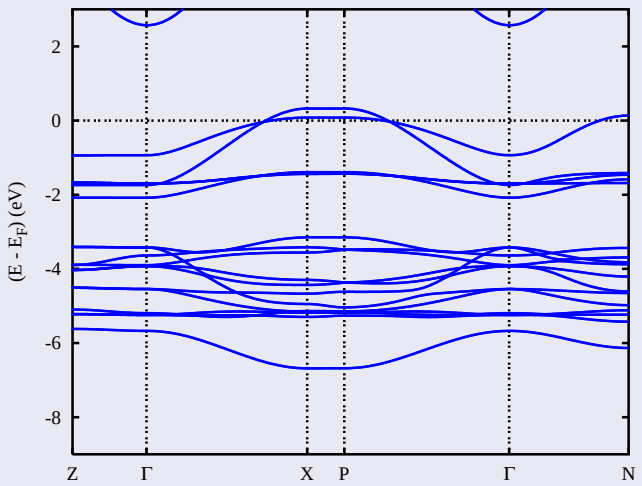
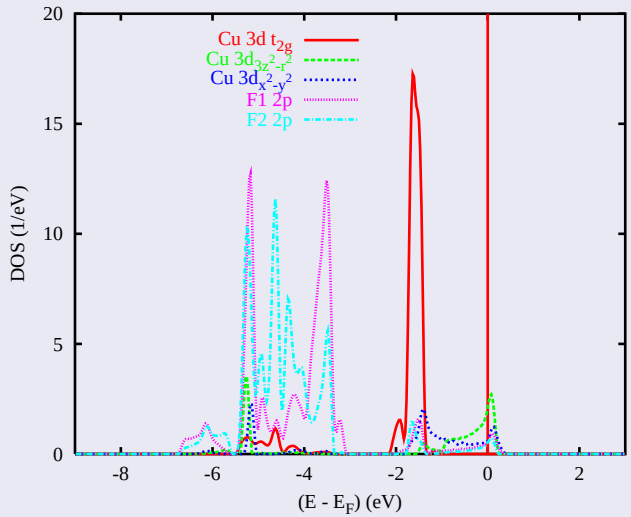
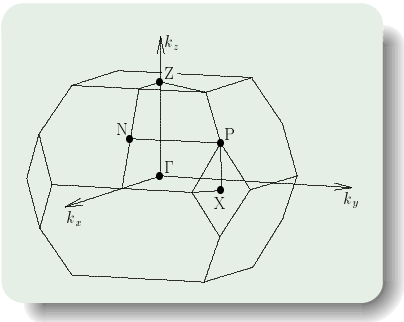
K_2CuF_4: Spin-Degenerate Calculations

Band Structure



Partial DOS



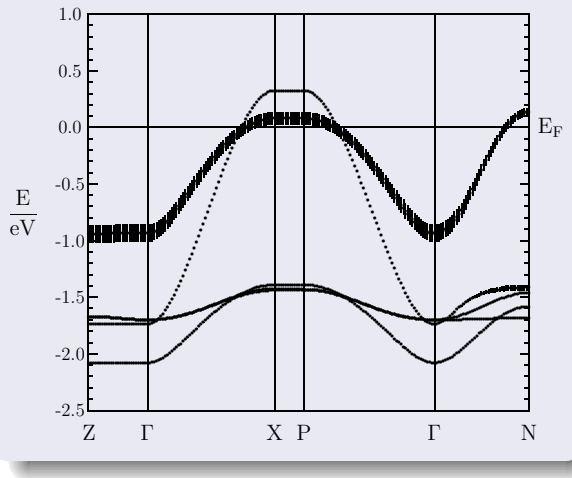


Results

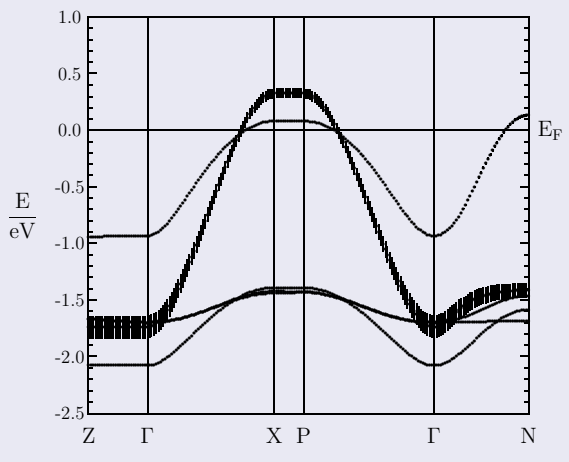
- similar to K_2NiF_4
- *d*-*p* splitting smaller
- electron count!

K_2CuF_4: Weighted Bands

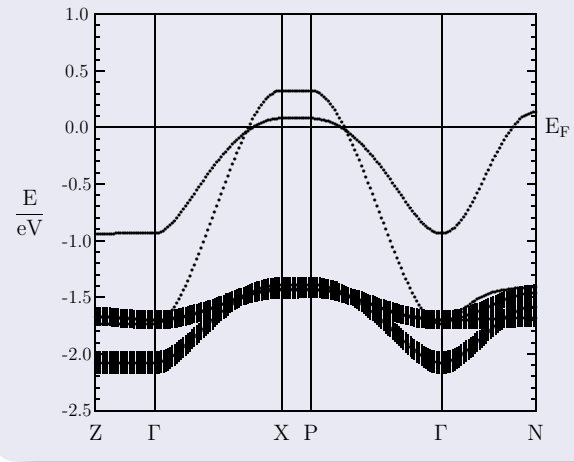
Cu $3d_{3z^2-r^2}$



Cu $3d_{x^2-y^2}$



Cu $3dt_{2g}$



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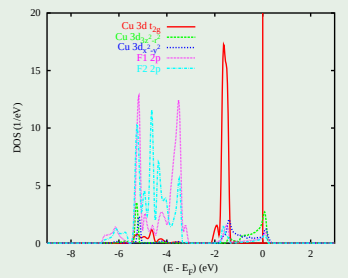
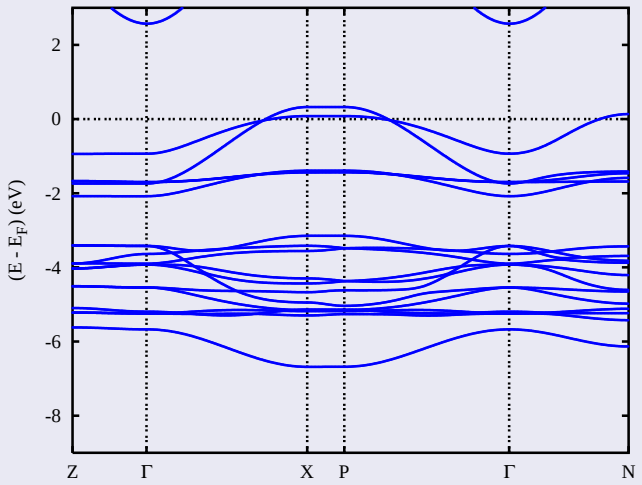


Results

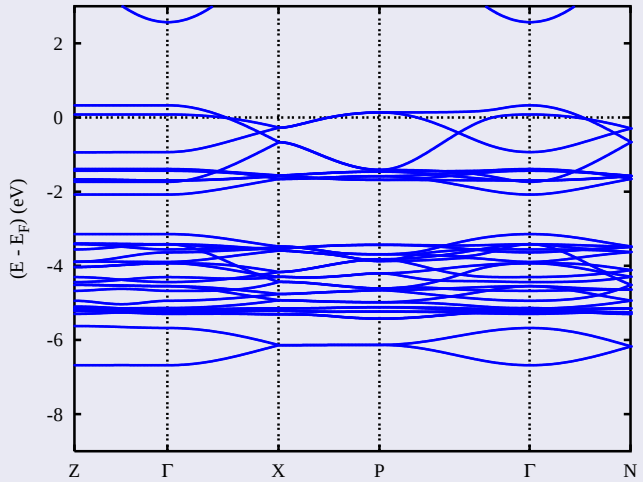
- CEF (t_{2g}/e_g) $\approx$ 1.0 eV
- W($d_{x^2-y^2}$) $\approx$ 2 W($d_{3z^2-r^2}$)
- FS($d_{x^2-y^2}$) $\approx$ FS($d_{3z^2-r^2}$)
- no FS nesting

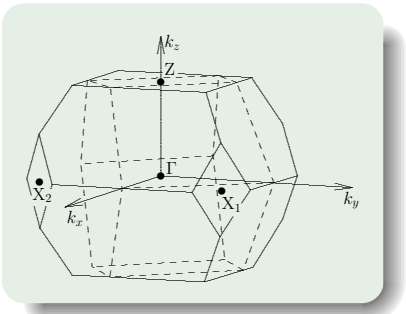
K_2CuF_4: Doubling the Unit Cell

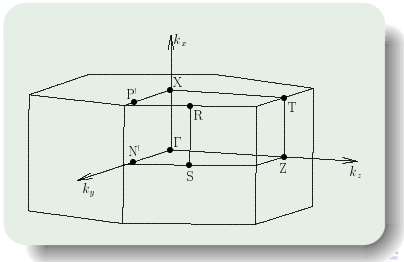
Bands: centered tetragonal



Bands: side-centered orthorh.







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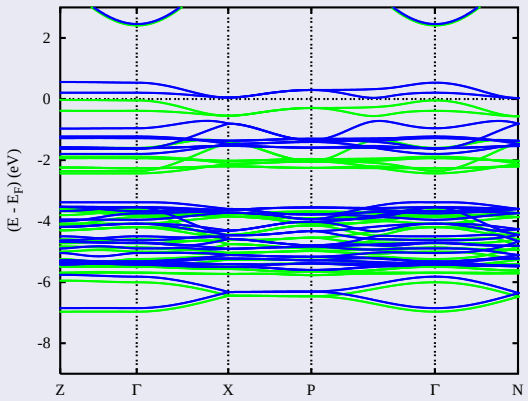
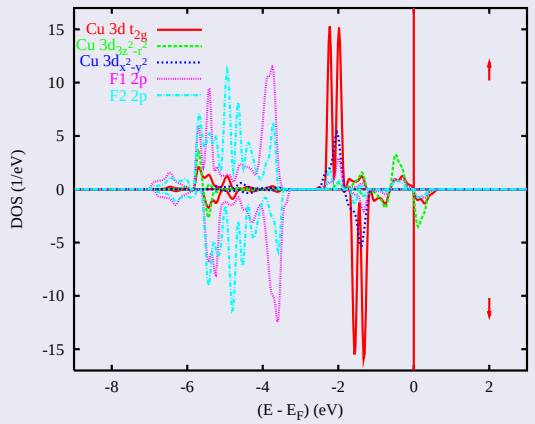
K_2CuF_4: Spin-Polarized Calculations

Band Structure



Partial DOS



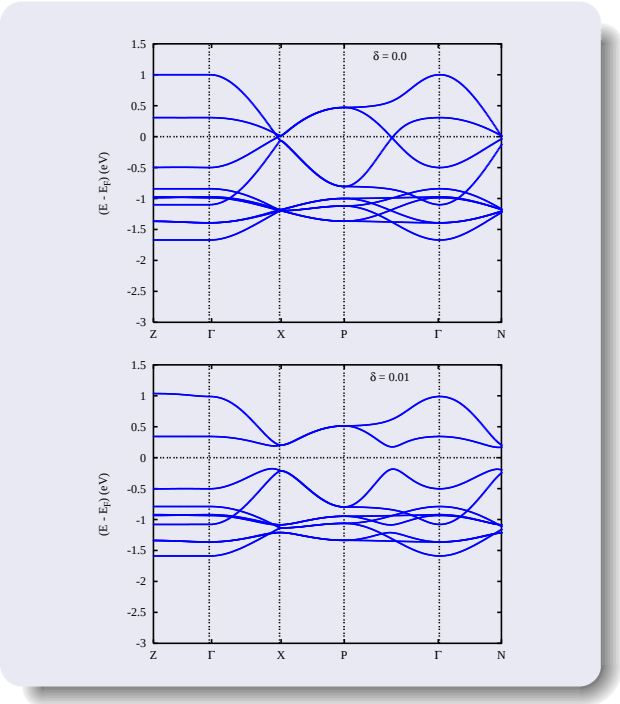
Moments (μ_B)

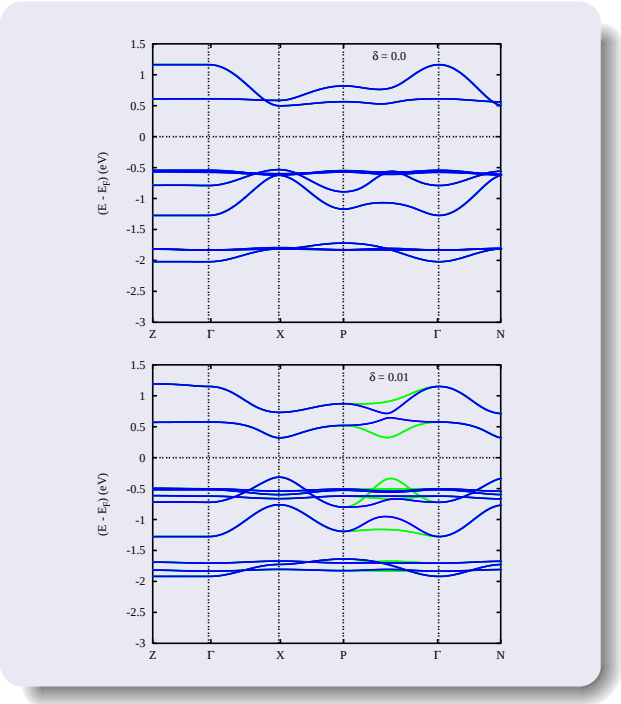
Cu	0.70
F1	0.08
F2	0.06
sublattice	1.00

Results

- moment: $d_{3z^2-r^2}$, $d_{x^2-y^2}$
- $\Delta E_{tot} = -6.5\,\text{mRyd}$

K_2NiF_4: Orbital and Magnetic Order





Conclusion

- FS nesting
- instability
  - $\delta \neq 0$

or

  - $m \neq 0$

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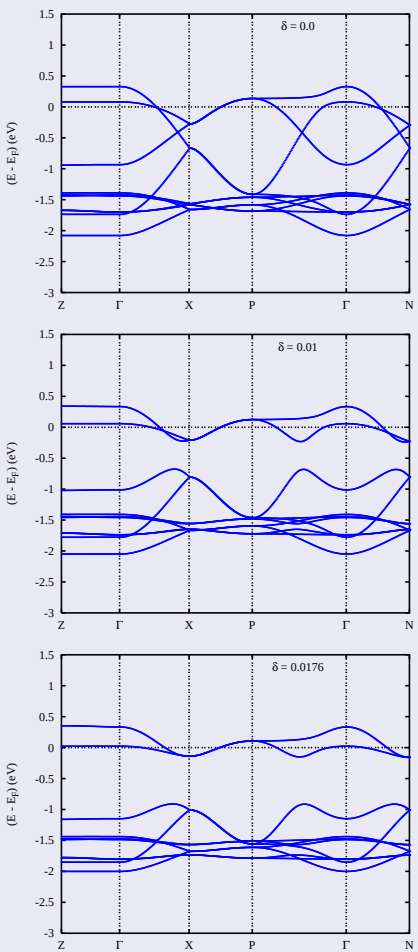
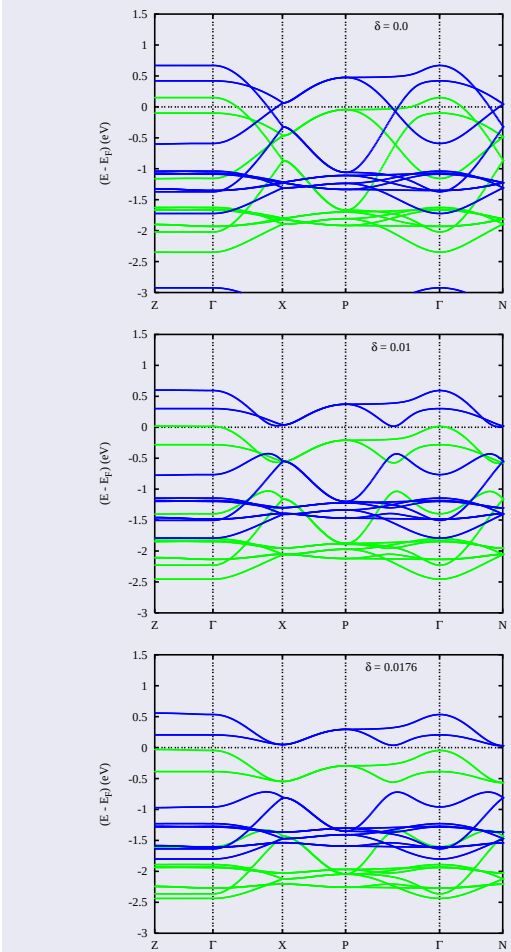
K_2CuF_4: Orbital and Magnetic Order



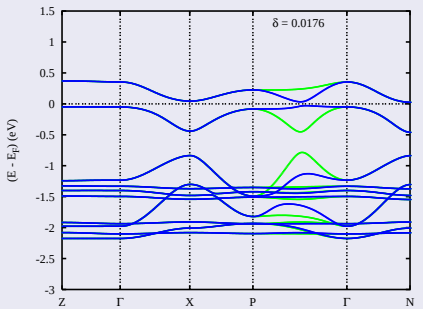


Conclusion

- no FS nesting
- instability
  - $\delta \neq 0$

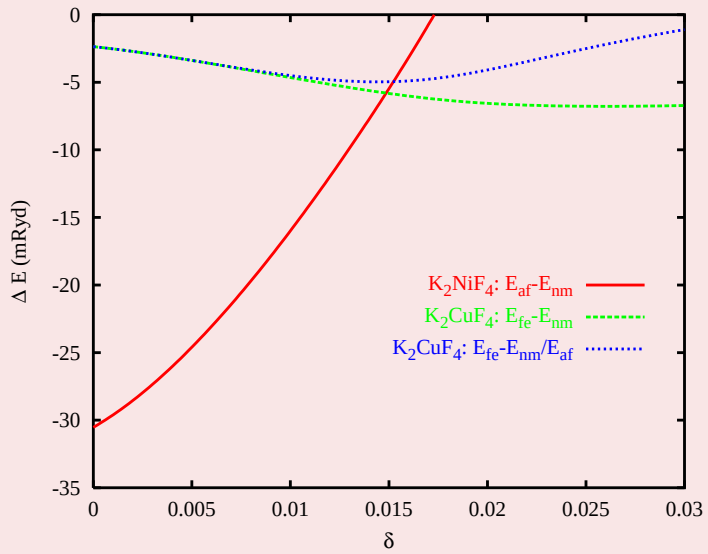
and

- $m \neq 0$

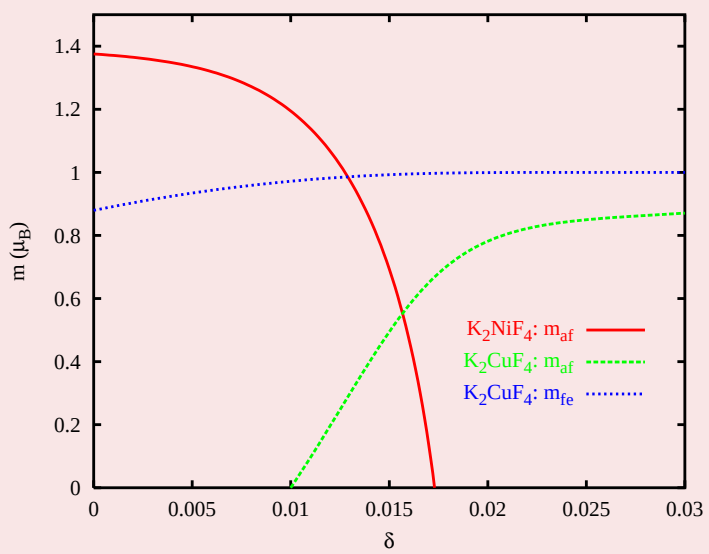


K_2NiF_4 and K_2CuF_4: Energies and Moments

Total Energies



Magnetic Moments



VE, K.-H. Höck, JP:CM **5**, 2987 (1993)
U. Schwingenschlögl, VE, JMMM **312**, L11 (2007)

Outline

1. Cool-down
2. Full-Potential ASW Method
3. A Short Walk Through Dimensions
   - Where are the Moments?
   - How to Build a Spin-Ladder
   - Greetings from High-T_c
   - A Recipe Against Frustration

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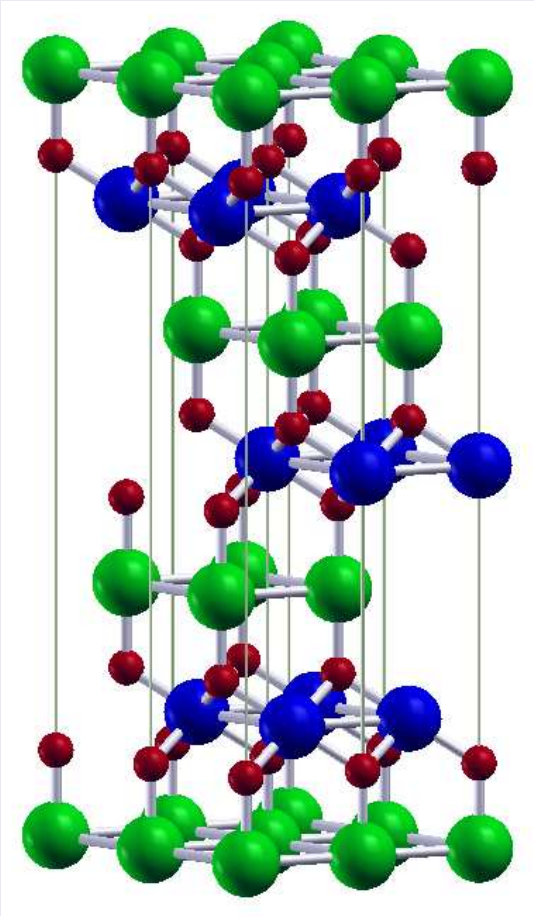
$CuFeO_2$

Delafossite Structure



Basics

- semiconductor
- AF interactions
- triangular lattice

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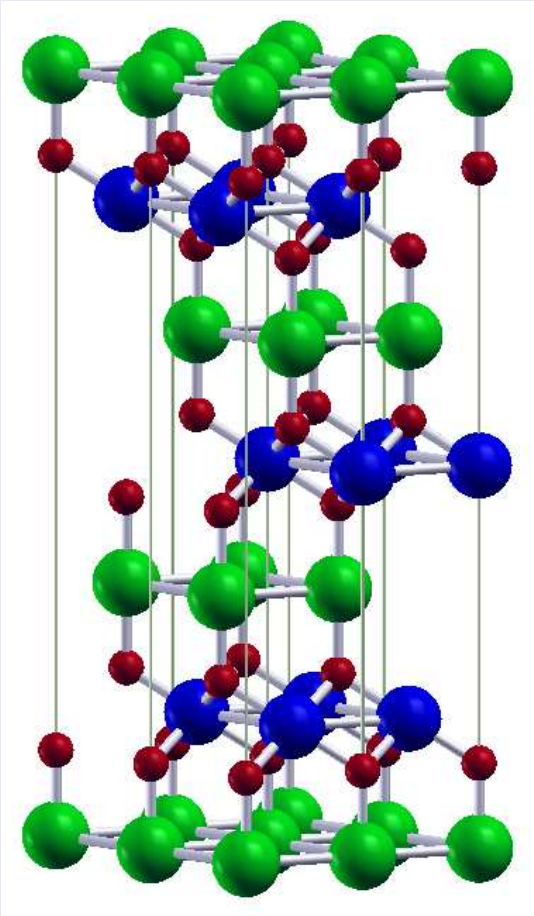

Basics

- semiconductor
- AF interactions
- triangular lattice

Open Issues

- frustration vs. long-range order
- role of Cu 3*d* orbitals?
- role of Fe 3*d* and O 2*p* orbitals?

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$CuFeO_2$

Previous Neutron Data

- $T_{N_1} = 16\,\mathrm{K}$, $T_{N_2} = 11\,\mathrm{K}$
- $\Theta_{CW} = -90\,\mathrm{K}$
- magnetic supercells
- no structural distortion
- $m_{Fe^{3+}} = 4.4\,\mu_B$

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Band Calculations

- rhombohedral structure
- $m_{Fe} = 0.9\,\mu_B$, $m_{Fe} = 3.8\,\mu_B$
- $E_g = 0$ in LDA, GGA
- $\sharp$ PES, XES

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New Neutron Data

- magnetic supercells
- monoclinic structure below 4 K

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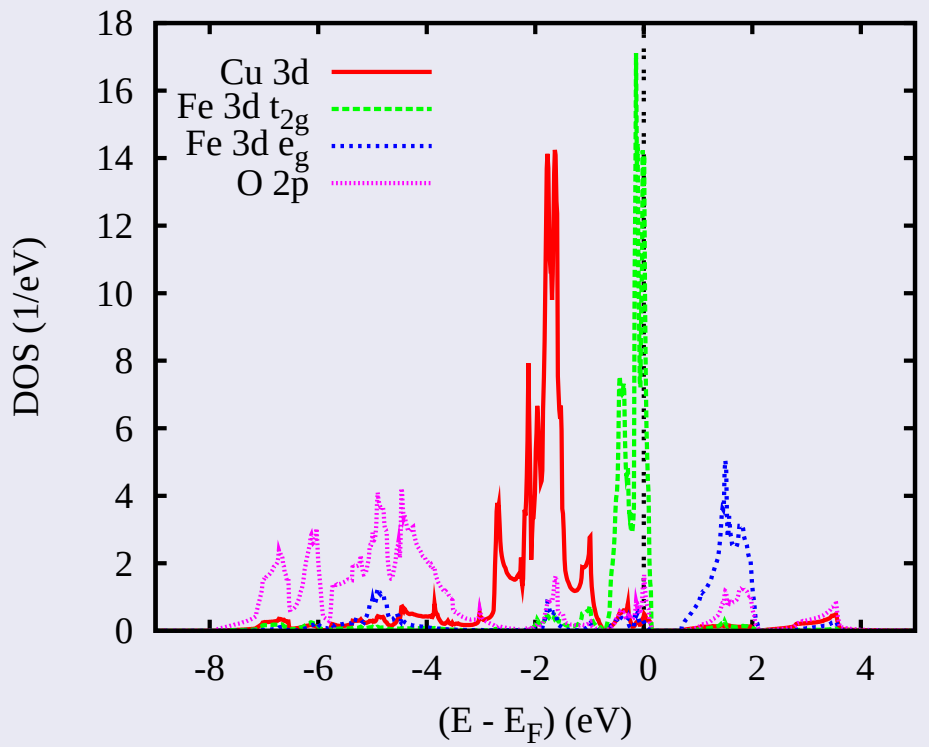
Open Issues

- spin-state of Fe?
- influence of monoc. structure?

Electronic Properties of $CuFeO_2$

Partial Densities of States



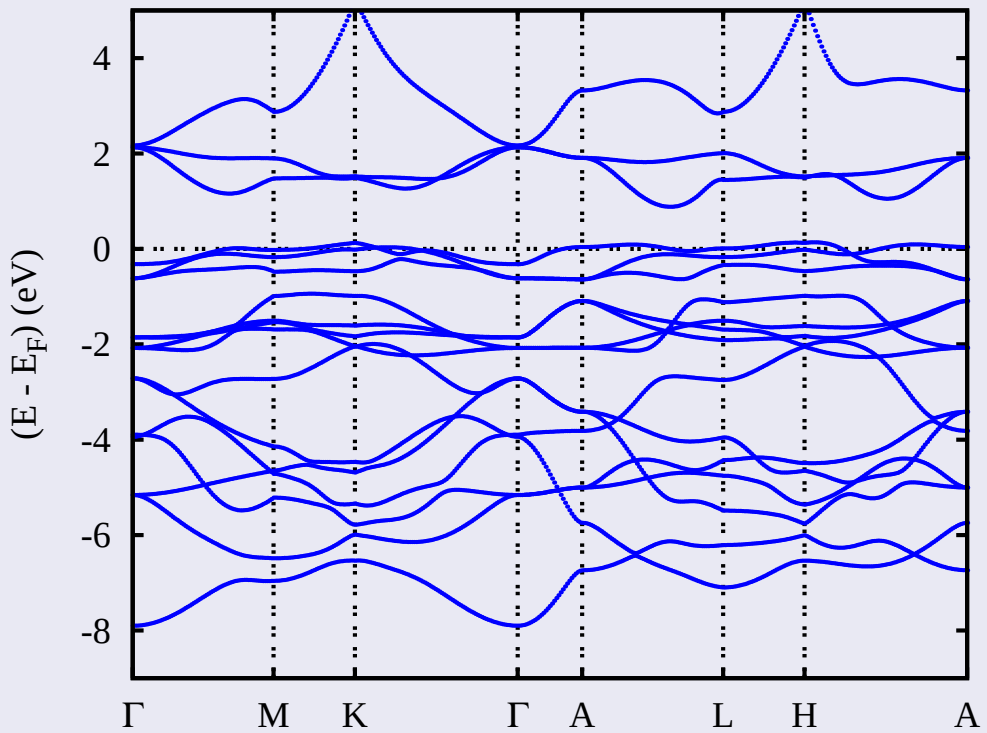
Results

- Fe 3*d*-O 2*p* hybridization
- FeO_6 octahedra: Fe 3*d* $\Rightarrow$ t_{2g} and e_g
- Cu $4d^{10}$ (Cu^{1+})
- Fe 3*d* t_{2g}
  - sharp peak at E_F

VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

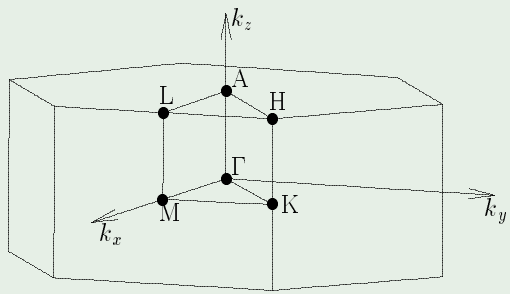
Electronic Properties of $CuFeO_2$

Band Structure



Results

- quasi-2D
- single band crossing E_F



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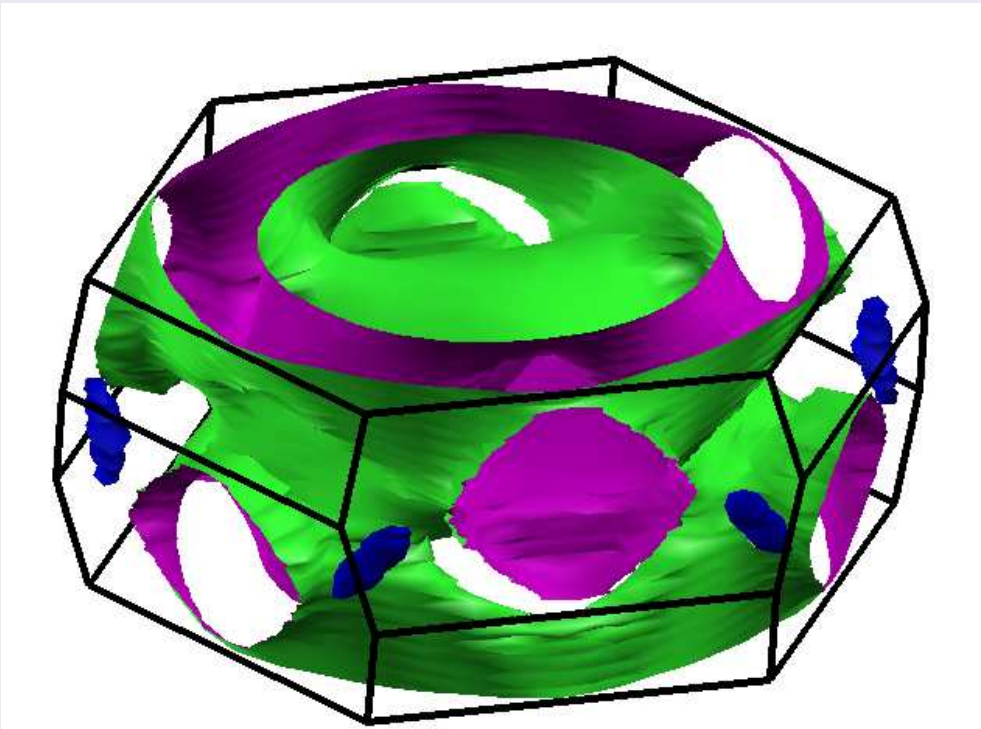
Electronic Properties of $CuFeO_2$

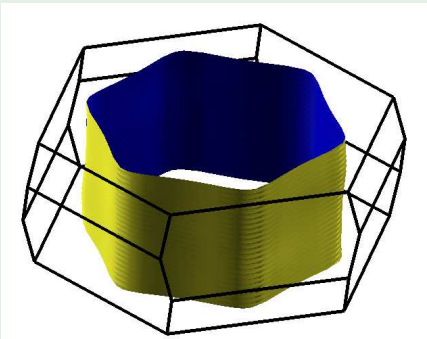
Fermi Surface



Results

- strongly 3D

FS $PdCoO_2$



VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

Magnetic Properties of $CuFeO_2$

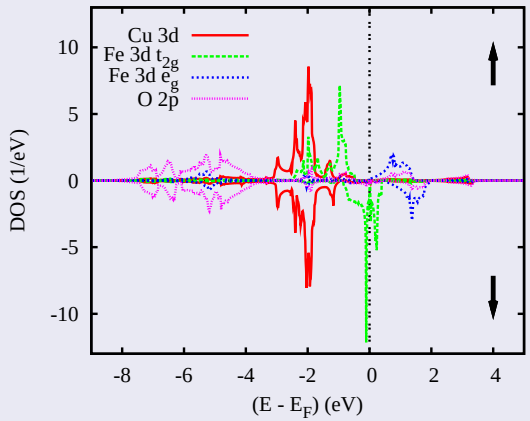
Total Energies (mRyd/f.u.), Magn. Moms. (μ_B), Band Gaps (eV)

structure	magn. order	ΔE	m_{Fe}	m_{O}	E_g
rhomb.	spin-deg.	0.0			-
rhomb.	ferro (LS)	-16.7	1.03	-0.02	-
rhomb.	ferro (IS)	-12.0	2.02	-0.02	-
rhomb.	ferro (HS)	-19.2	3.73	0.21	-

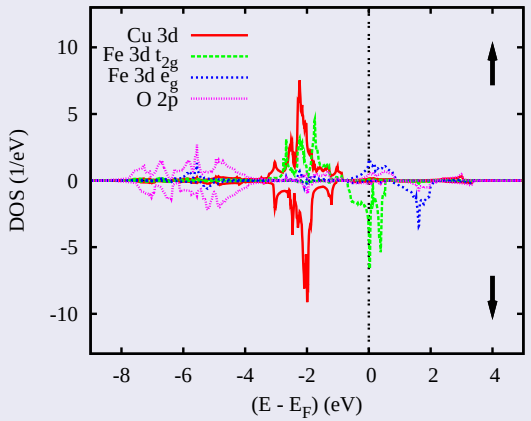
VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

Magnetic Properties of $CuFeO_2$

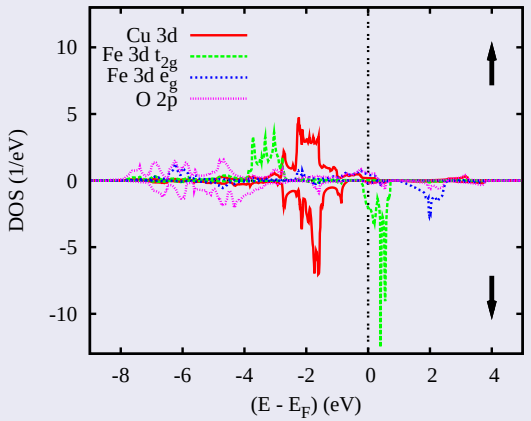
LS Ferromagnet



IS Ferromagnet



HS Ferromagnet



Results

- LS, IS, HS in rhombohedral structure
- HS: O 2*p* polarization via Fe 3*d* e_g

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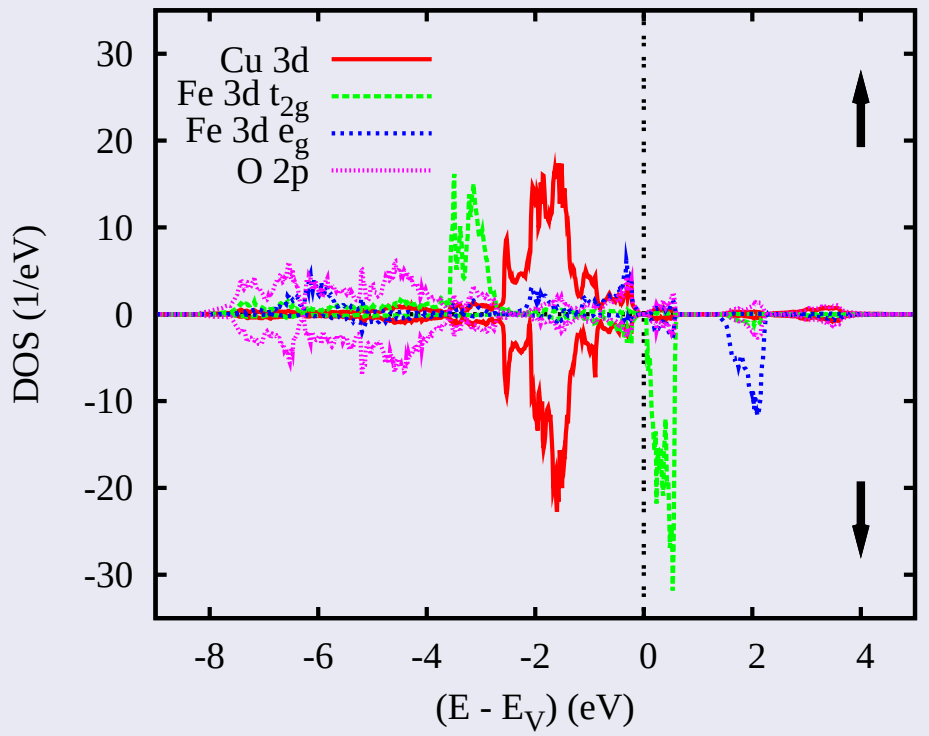
monoc.	spin-deg.	−6.0			-
monoc.	ferro (LS)	−21.5	1.04	−0.02	-
monoc.	ferro (IS)	−19.0	2.08	−0.02	-
monoc.	ferro (HS)	−32.0	3.62	0.19	-

VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

Magnetic Properties of $CuFeO_2$

Antiferromagnet



Results

- monoc. structure
- Fe^{3+} HS
- O 2*p* polarization via Fe 3*d* e_g
- $E_g > 0$ in GGA

VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

Magnetic Properties of $CuFeO_2$

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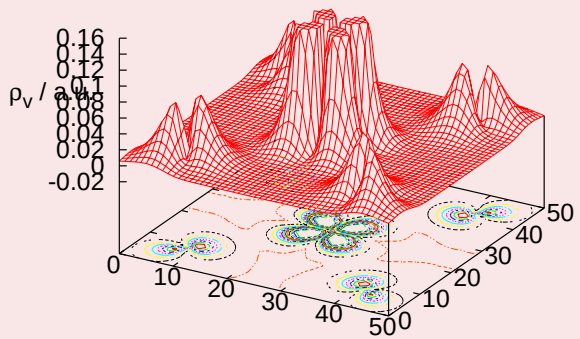
monoc.	ferro (HS)	-32.0	3.62	0.19	-
monoc.	antiferro	-46.0	± 3.72	± 0.08	0.05

VE, R. Frésard, A. Maignan, Phys. Rev. B **78**, 052402 (2008)

A Short Walk: Fundamental Principles

A Short Walk: Fundamental Principles

La_2BaCuO_5 Moments



A Short Walk: Fundamental Principles

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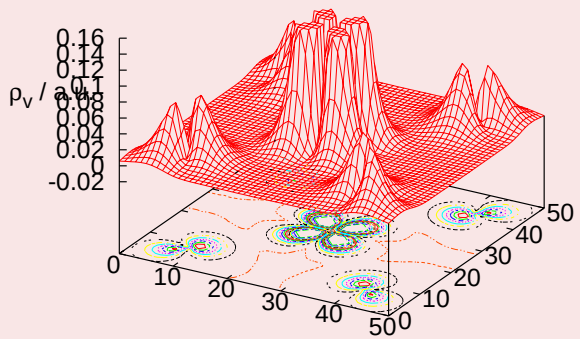
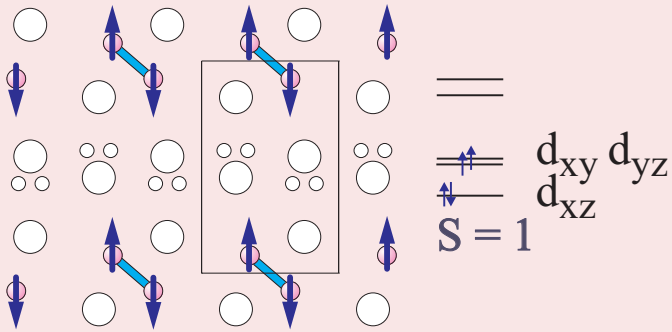


La_2RuO_5 Orbitals



A Short Walk: Fundamental Principles

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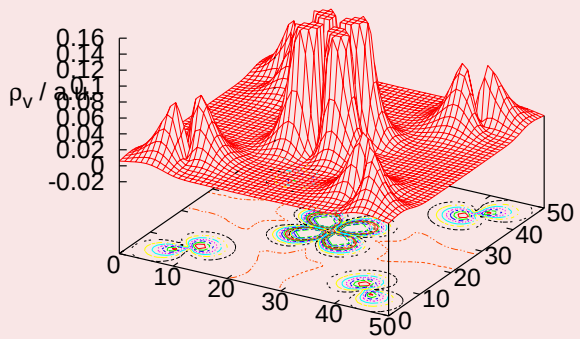

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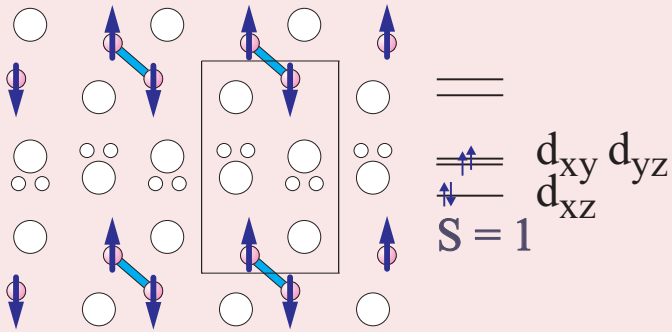
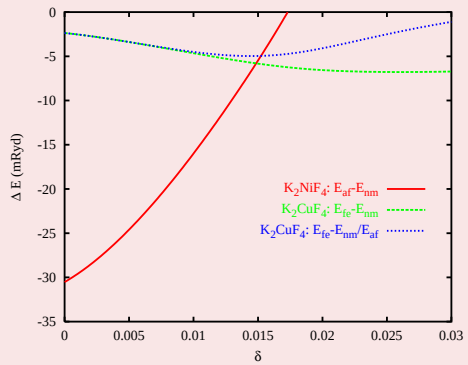


K_2NiF_4, K_2CuF_4 Symmetry



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A Short Walk: Fundamental Principles

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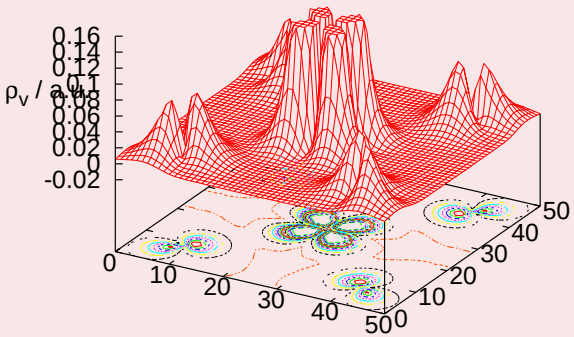

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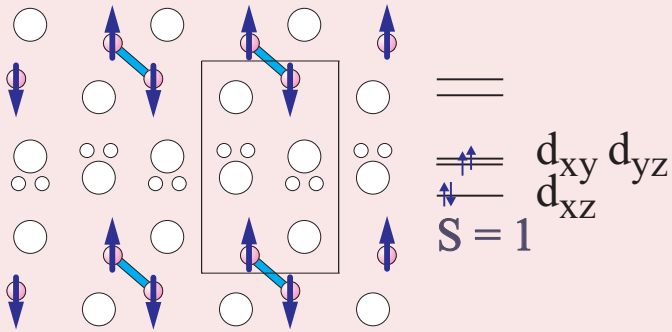

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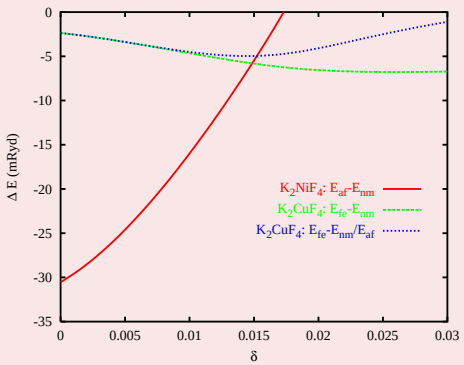
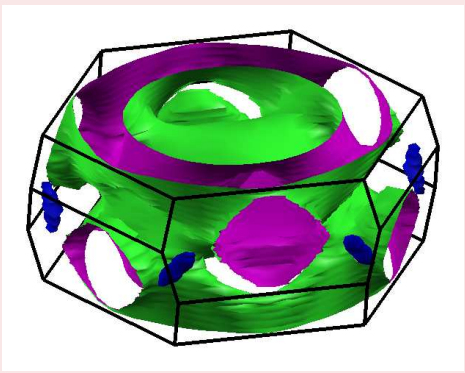


$CuFeO_2$ Structure



Acknowledgments

Caen

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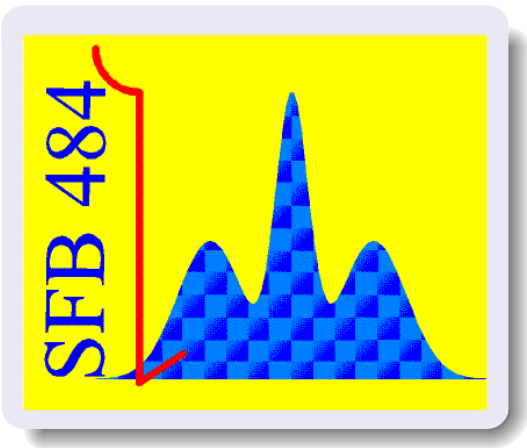
A. Maignan, C. Martin

Darmstadt

P. C. Schmidt

Halle

S. G. Ebbinghaus



Augsburg

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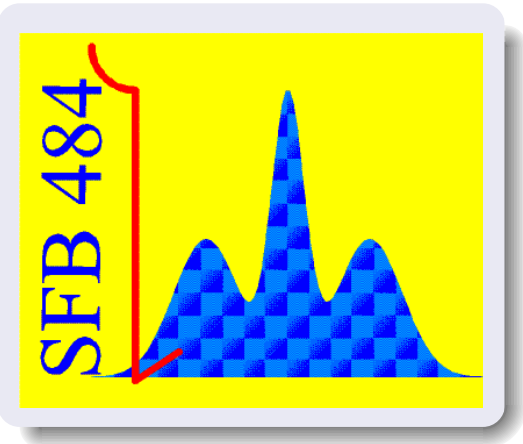

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Vienna

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