Determining orbital wavefunctions using core level non-resonant inelastic x-ray scattering

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Theory - calculations

DMFT

DFT

Experiment

Spectroscopy

$k$-dependence: e.g. ARPES, neutron

local: e.g. core-level PES/XAS/IXS

on-site correlations, orbitals, atomic multiplet structure
Inelastic x-ray scattering

Max Planck – PETRA III non-resonant inelastic x-ray scattering

- vector-q dependence gives symmetry
- large transferred q: beyond dipole
  - determination of orbital state
  - spectroscopy and direct imaging
- bulk sensitive, extreme conditions

\[ S(q, \omega) = \sum_f |\langle f | e^{iqr} | i \rangle|^2 \delta(\hbar \omega_i - \hbar \omega_f - \hbar \omega). \]
Non-resonant inelastic x-ray scattering (NIXS) @ N-edge

Inelastic scattering from core electrons: A multiple scattering approach

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Nonresonant Inelastic X-Ray Scattering Involving Excitonic Excitations: The Examples of NiO and CoO
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High multipole transitions in NIXS: Valence and hybridization in 4f systems
Non-resonant inelastic x-ray scattering (NIXS) @ N-edge

NIXS is based on: $q$ dependent multipole selection rules!!

$$S(q, \omega) = \sum_f \left| \langle f | e^{iqr} | i \rangle \right|^2 \delta(\hbar \omega_i - \hbar \omega_f - \hbar \omega).$$

$$S(q, \omega) = \sum_f \left| \sum_k \frac{i^k(2k+1)}{k!} \langle R_f | j_k(qr) | R_i \rangle \right| \sum_{m=-k}^{k} \frac{\langle \phi_f | C^{\phi}_{km} | \phi_i \rangle}{R} \delta(\hbar \omega_i - \hbar \omega_f - \hbar \omega).$$

$d \rightarrow d$: monopole, octupole, hexadecapole

$d \rightarrow f$: dipole, octupole, triakontadipole

Code by M.W. Haverkort, MPI CPfS Dresden
Non-resonant inelastic x-ray scattering (NIXS) @ N-edge

Application to a crystal-field problem at Ce N-edge (4d to 4f)

- The large $|q|$ gives rise to the higher multipole transitions at lower energies!

R.A. Gordon et al., EPL 81, 26004 (2008)
Orientation-dependent x-ray Raman scattering from cubic crystals: natural linear dichroism in MnO and CeO$_2$

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Non-resonant inelastic x-ray scattering (NIXS) @ N-edge

Application to a crystal-field problem at Ce N-edge (4d to 4f)

- The large $|q|$ gives rise to the higher multipole transitions.
- Vector $q$ dependence on a single crystal should give sensitivity to orbital anisotropies ($J_z$ admixture) in analogy to polarization dependence in XAS.
- Simulate NIXS for pure $J_z$ states for vector $q$ "in-plane" and "out-of-plane" at large $|q|$ at the Ce N-edge (4d -> 4f) [code by M.W. Haverkort]
Determining the In-Plane Orientation of the Ground-State Orbital of CeCu$_2$Si$_2$

T. Willers,¹ F. Strigari,¹ N. Hiraoka,² Y. Q. Cai,³ M. W. Haverkort,⁴ K.-D. Tsuei,² Y. F. Liao,² S. Seiro,⁵ C. Geibel,⁵ F. Steglich,⁵ L. H. Tjeng,⁵ and A. Severing¹

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**Non-resonant inelastic x-ray scattering (NIXS) @ N-edge**
Direct bulk-sensitive probe of 5f symmetry in URu$_2$Si$_2$

Martin Sundermann$^a$, Maurits W. Haverkort$^{b,1}$, Stefano Agrestini$^b$, Ali Al-Zein$^{c,2}$, Marco Moretti Sala$^c$, Yingkai Huang$^d$, Mark Golden$^d$, Anne de Visser$^d$, Peter Thalmeier$^b$, Liu Hao Tjeng$^b$, and Andrea Severing$^{a,3}$

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URu$_2$Si$_2$ and the hidden order state


Phase diagram

- $T_{\text{HO}} = 17.5$ K
- $T_{\text{sc}} = 1.5$ K
- $T < T_{\text{HO}}$ small $\mu_{\text{ord}} \leftrightarrow$ parasitic minority phase
- $p \geq 0.7$ GPa at $T_N \approx T_{\text{HO}}$ (LMAF-phase)

**HO phase**

- 2nd order phase transition $\leftrightarrow$ into electronically ordered state
- large loss of entropy ($\approx 1/5 \ln 2$)
- Fermi surface reconstruction
- change of quasiparticle scattering rate
- Fermi surfaces of $HO \approx$ Fermi surface LMAF phase
- Loss of fourfold symmetry

Energy scales

- $\Delta_{\text{hyb}} \approx 13$ meV (150K) opening at $T_{\text{hyb}} \approx 27$K > $T_{\text{HO}}$
- $\Delta_{\text{HO}} \approx 4$ meV (45K) in charge and spin channel
- $\Delta_{\text{res}} \approx 1.6$ meV (18K) in charge and spin channel
Non-resonant inelastic scattering $U\;5d \rightarrow 5f$ of URu$_2$Si$_2$

Isotropic spectrum sum of all CF states

- Spin orbit and Coulomb interaction for localized $U^{4+}\;f^2$ always yield $J = 4$.
- Atomic values Cowan code
- Adjust here reduction factors ($5f-5f$ and $5d-5f \approx 50\%$)
- Relative contributions of spin-orbit and Coulomb interaction determine ratio of $L=3,4,5$ (here 1\%, 14\% and 85 \%).
- FWHM = 0.8 eV Gaussian for resolution FWHM = 1.3 eV Lorentzian for lifetime
- Simulation by Quanty – Haverkort
Non-resonant inelastic x-ray scattering (NIXS) @ N-edge

Application to a crystal-field problem at Ce N-edge (4d to 4f)

- The large $|q|$ gives rise to the higher multipole transitions at lower energies!

Further away from continuum states $\rightarrow$ more excitonic!

R.A. Gordon et al., EPL 81, 26004 (2008)
Non-resonant inelastic scattering $U \, 5d \rightarrow 5f$ of $\text{URu}_2\text{Si}_2$

Isotropic spectrum sum of all CF states

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- FWHM = $0.8eV$ Gaussian for resolution
  FWHM = $1.3 \, eV$ Lorenzian for lifetime
- Simulation by $\text{Quanty} – \text{Haverkort}$
\[
I(\text{FS}_2) = \left| \langle \text{FS}_2 | f^+c | \text{GS} \rangle \right|^2 \\
= |\beta'' \langle \text{cf}^3 | - \alpha'' \langle \text{cf}^4 L | f^+c | \alpha | f^2 \rangle + \beta \langle f^3 L | \rangle |^2 = |\beta'' \alpha - \alpha'' \beta|^2
\]

XAS

\[
\text{ground state problem}
\]

\[
\Delta'' = \Delta : \alpha'' = \alpha, \beta'' = \beta \rightarrow
\]

\[
I(\text{FS}_1) = 1 \quad I(\text{FS}_2) = 0
\]

\rightarrow \text{looks like ionic!}

\[
\text{GS} = \alpha | f^2 \rangle + \beta | f^3 L \rangle
\]
XAS (d → f) final state: e.g. Uranium M-edges

\[ E(\text{cf}^{n+2L}) = (n+2)E_f + \frac{1}{2}(n+2)(n+1)U_{ff} - E_L + E_c - (n+2)U_{cf} \]

\[ E(\text{cf}^{n+1L}) = (n+1)E_f + \frac{1}{2}(n+1)nU_{ff} + E_c - (n+1)U_{cf} \]

\[ \Delta^{\prime\prime} = E(\text{cf}^{n+1L}) - (\text{cf}^n) = \Delta + U_{ff} - U_{cf} \]

\[ U_{ff} \sim U_{cf} \rightarrow \Delta^{\prime\prime} \sim \Delta \rightarrow \text{XAS} \sim \text{ionic} \]

ground state problem

\[ E(\text{fn}^{+1L}) = (n+1)E_f + \frac{1}{2}(n+1)nU_{ff} - E_L \]

\[ E(\text{fn}) = nE_f + \frac{1}{2}n(n-1)U_{ff} \]

\[ \Delta = E(\text{fn}^{+1L}) - (\text{fn}) = E_f - E_L + nU_{ff} \]
**XPS final state**

\[
\begin{align*}
\text{E}(c^{n+1}_f) &= (n+1)E_f + \frac{1}{2}(n+1)nU_{ff} - E_L + E_c - (n+1)U_{cf} \\
\text{E}(c^n) &= nE_f + \frac{1}{2}n(n-1)U_{ff} + E_c - nU_{cf}
\end{align*}
\]

\[\Delta' = \text{E}(c^{n+1}_f) - (c^n) = \Delta - U_{cf}\]

\[\Delta' \text{ is very different from } \Delta \rightarrow \text{XPS : satellites!}\]

**ground state problem**

\[
\begin{align*}
\text{E}(f^{n+1}_f) &= (n+1)E_f + \frac{1}{2}(n+1)nU_{ff} - E_L \\
\text{E}(f^n) &= nE_f + \frac{1}{2}n(n-1)U_{ff}
\end{align*}
\]

\[\Delta = \text{E}(f^{n+1}_f) - (f^n) = E_f - E_L + nU_{ff}\]
XAS ($p \rightarrow d$) final state: e.g. Uranium L-edges

\[
\begin{align*}
\text{E}(\text{cd}^{1}f^{n+1}_{\L}) &= (n+1)E_{f} + \frac{1}{2}(n+1)nU_{ff} - E_{L} + E_{c} + E_{d} - (n+1)U_{cf} - U_{cd} + (n+1)U_{df} \\
\Delta'''' &= \text{E}(\text{cd}^{1}f^{n+1}_{\L}) - \text{E}(\text{cd}^{1}f^{n}) = \Delta - U_{cf} + U_{df} \\
\end{align*}
\]

\(U_{df} \sim 0 \Rightarrow \Delta'''' \sim \Delta' \Rightarrow \text{L-XAS} \sim \text{XPS}\)

ground state problem

\[
\begin{align*}
\text{E}(f^{n+1}_{\L}) &= (n+1)E_{f} + \frac{1}{2}(n+1)nU_{ff} - E_{L} \\
\text{E}(f^{n}) &= nE_{f} + \frac{1}{2}n(n-1)U_{ff} \\
\Delta &= \text{E}(f^{n+1}_{\L}) - \text{E}(f^{n}) = E_{f} - E_{L} + nU_{ff} \\
\end{align*}
\]
Non-resonant inelastic scattering $U\,5d \rightarrow 5f$ of $URu_2Si_2$

Isotropic spectrum sum of all CF states

- Spin orbit and Coulomb interaction for localized $U^{4+}\,f^2$ always yield $J = 4$.
- Atomic values Cowan code
- Adjust here reduction factors ($5f-5f$ and $5d-5f \approx 50\%$)
- Relative contributions of spin-orbit and Coulomb interaction determine ratio of $L=3,4,5$ (here 1%, 14% and 85%).
- FWHM = 0.8 eV Gaussian for resolution
- FWHM = 1.3 eV Lorenzian for lifetime
- Simulation by Quanty – Haverkort
NIXS: groundstate $T > T_{HO}$

Energy transfer (eV)

$|q| = 9.6\text{Å}^{-1}$

$J_z$
Simulation of spectra with full multiplet routine
Quanty by M.W. Haverkort

\[ J = 4, \ J_z = \{-4, -3, \ldots, 2, 3, 4\} \]
tetragonal CEF splits \( J = 4 \)
into five singlets and 2 doublets

\[
\Gamma_1^{(1)}(\theta) = \cos(\theta) |0\rangle + \sin(\theta) \sqrt{\frac{1}{2}} (|4\rangle + |-4\rangle) \\
\Gamma_1^{(2)}(\theta) = \sin(\theta) |0\rangle - \cos(\theta) \sqrt{\frac{1}{2}} (|4\rangle + |-4\rangle) \\
\Gamma_2 = \sqrt{\frac{1}{2}} (|4\rangle - |-4\rangle) \\
\Gamma_3 = \sqrt{\frac{1}{2}} (|2\rangle + |-2\rangle) \\
\Gamma_4 = \sqrt{\frac{1}{2}} (|2\rangle - |-2\rangle) \\
\Gamma_5^{(1)}(\phi) = \cos(\phi) |\mp 1\rangle + \sin(\phi) |\pm 3\rangle \\
\Gamma_5^{(2)}(\phi) = \sin(\phi) |\mp 1\rangle - \cos(\phi) |\pm 3\rangle
\]
\[ J = 4, \quad J_z = \{-4, -3, \ldots, 2, 3, 4\} \]

tetragonal CEF splits \( J = 4 \)

into five singlets and 2 doublets

\[
\begin{align*}
\Gamma_1^{(1)}(\theta) &= \cos(\theta) |0\rangle + \sin(\theta) \sqrt{\frac{1}{2}} (|4\rangle + |-4\rangle) \\
\Gamma_1^{(2)}(\theta) &= \sin(\theta) |0\rangle - \cos(\theta) \sqrt{\frac{1}{2}} (|4\rangle + |-4\rangle) \\
\Gamma_2 &= \sqrt{\frac{1}{2}} (|4\rangle - |-4\rangle) \\
\Gamma_3 &= \sqrt{\frac{1}{2}} (|2\rangle + |-2\rangle) \\
\Gamma_4 &= \sqrt{\frac{1}{2}} (|2\rangle - |-2\rangle) \\
\Gamma_5^{(1)}(\phi) &= \cos(\phi) |\mp 1\rangle + \sin(\phi) |\pm 3\rangle \\
\Gamma_5^{(2)}(\phi) &= \sin(\phi) |\mp 1\rangle - \cos(\phi) |\pm 3\rangle
\end{align*}
\]

Some ground state suggestions

- Haule & Kotliar (2009)
- Santini & Amoretti (1994), Nagao & Igarashi (2005)
- Nagao & Igarashi (2005), Kuwahara et al. (1997)
- Ohkawa & Shimizu (1999), Sugiyama et al. (1999), Chandra et al. (2013),
NIXS: groundstate \( T > T_{\text{HO}} \)

**GS:** mainly singlet \( \Gamma_1^{(1)}(\approx 90^\circ) \) and/or \( \Gamma_2 \) and some other state, e.g. the doublet \( \Gamma_5^{(1)}(\approx 90^\circ) \) mixed in.
How to set up the energy level diagram of URu$_2$Si$_2$??

**Kramers doublet** $f^3$

- $\Gamma_1^{(1)}$ $f^2\varepsilon^1$
- $\Gamma_2$ $f^2\varepsilon^1$
- $\Gamma_5^{(1)}$ $f^2\varepsilon^1$

**GS**: mainly singlet $\Gamma_1^{(1)}(\approx 90^\circ)$ and/or $\Gamma_2$ and some other state e.g. the doublet $\Gamma_5^{(1)}(\approx 90^\circ)$ mixed in.

- Below $T \approx 27$ K
- $\Delta_{hyb} \approx 150$ K $\approx 13$ meV

STM Park *et al.*

- $\approx 13$ meV
- $\approx \text{meV}$
Topological Kondo Insulators

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A New Exotic State in an Old Material: a Tale of SmB₆¹

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Topological insulator in higher orbital systems. The special attention is given to the already existing f-orbital materials [30], such as CeNiSn, Ce₃Bi₄Pt₃, YbB₁₂, and SmB₆. These materials, which are called Kondo insulators, have all the necessary features needed for realizing topological behavior: strong spin–orbit coupling, strong electron–electron interactions, and orbitals with opposite parity (see table).
Topological Kondo Insulators

Maxim Dzero,1,2 Jing Xia,3 Victor Galitski,4,5 and Piers Coleman6,7


Figure 3

Showing (a) topologically trivial band insulator with $Z_2 = +1$ (b) band-crossing of even and odd parity states at an odd number of high symmetry points leads to a topological insulator with $Z_2 = -1$. Each band crossing generates a Dirac cone of spin-momentum locked surface states.
Figure 4
(a) If we ignore the effects of topology in a conventional Kondo insulator, the interaction can be turned on adiabatically. When the interactions are turned on, the lower band is pushed into the upper band. Two bands of the same parity will always repel one-another and will not cross when the interactions are turned on. (b) When interactions are turned on in a topological insulator, they can lead to band-crossing and a topological phase transition. Here, interactions cause an f-band to push up into a d-band. Since the two bands have opposite parity, they do not hybridize at the high symmetry point so band-crossing occurs, leading to a topological phase transition.
always finite resistivity, even in purest samples

metallic surface states, topologically protected ?!

**Figure S1. Temperature regimes of the SmB$_6$ transport and valence.** The three main transport regimes of SmB$_6$ illustrated by comparison of resistivity/conductivity$^1$, Hall coefficient$^{2,3}$ and bulk valence$^4$ and magnetic susceptibility$^5$: (I) low temperature low carrier “in-gap state” regime below 4K, (II) intermediate metallic-to-insulating transition regime with negative Hall coefficient, and (III) high temperature poor-metal regime with positive Hall coefficient above 60K. Multiple low temperature resistivity profiles are plotted to illustrate the variation of the low temperature residual conduction found in the literature. A further subdivision of each regime into two sub-regimes is readily apparent from the various profiles.
4f-5d inversion: intermediate 4f valence

Note:
SmB$_6$ mixed-valent: homogenous in space but inhomogenous in k-space
Fe$_3$O$_4$ mixed-valent: inhomogenous in space but homogenous in k-space
Temperature dependence of the samarium oxidation state in SmB$_6$ and Sm$_{1-x}$La$_x$B$_6$

J. M. Tarascon, Y. Isikawa (*), B. Chevalier, J. Etourneau, P. Hagenmuller and M. Kasaya

Fig. 1. — Lattice parameter temperature dependence of the cubic unit cell of SmB$_6$ (experimental) and of the hypothetical hexaborides Sm$^{2+}$B$_6$ and Sm$^{3+}$B$_6$ (calculated).

Fig. 3. — Average samarium valence temperature dependence in SmB$_6$ between 300 K and 4.2 K.
SmB$_6$ : an intermediate valence system

SmB$_6$ : an intermediate valence system

**Bulk and surface electronic properties of SmB$_6$: A hard x-ray photoelectron spectroscopy study**
Y. Utsumi,$^{1, \dagger}$ D. Kasinathan,$^1$ K.-T. Ko,$^1$ S. Agrestini,$^1$ M. W. Haverkort,$^{1, \dagger}$ S. Wirth,$^1$ Y.-H. Wu,$^2$ K.-D. Tsuei,$^2$ D.-J. Kim,$^3$ Z. Fisk,$^3$ A. Tanaka,$^4$ P. Thalmeier,$^1$ and L. H. Tjeng$^1$

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**Graphical Abstract**

- **5 K**
  - f$^6$ J=0
  - Intensity (arb. units)
    - Sm 3d$_{3/2}$
    - Sm 3d$_{5/2}$

- **300 K**
  - f$^6$ J=0
  - f$^6$ J=1
  - Intensity (arb. units)
    - Binding energy (eV)
What entropy drives the valence change in SmB$_6$?

• Lattice ??
  -- lattice shrinks in going from 5 to 140 K
  -- lattice expands from 140 K to 300 K, but valence still keeps increasing although there is more room for the bigger Sm$^{2+}$

• Spin !!
  -- Sm$^{2+}$ $^7$F$_0$ (J=0, singlet) to Sm$^{3+}$ $^6$H$_{5/2}$ (J=5/2, sextet)

• Similarities with Yb Kondo/heavy-fermion systems
  -- Yb valence increases from low T to high T, e.g. Yb$^{2.8+}$ to Yb$^{2.9+}$
  -- YbInCu$_4$: sudden expansion of lattice upon cooling !

Sm$^{2+}$ f$^6$ J=0: even number of electrons $\rightarrow$ hybridization gap model
How to set up the energy level diagram of SmB$_6$?

energy separation much smaller than hopping integral (to get valence close to 2.5+)

Problems:
• from low T to high T: valence move always towards 2.5+
• lattice expansion with T tends to lower the f$^6$ energy
How to set up the energy level diagram of SmB$_6$??

- $f^6$ ($^7F_1$)
- $f^6$ ($^7F_0$) with $\Delta, \varepsilon_f$ connected, 40 meV
- $f^5 L^1 (^6H_{7/2})$ with 150 meV
- $f^5 L^1 (^6H_{5/2})$
Energy level diagram in intermediate valent SmB$_6$

\[ \begin{align*}
&\text{Sm}^{2+} f^6 \\
&\text{Sm}^{3+} f^5
\end{align*} \]
quartet GS

hybridization gap *may* open

doublet GS

hybridization gap *will* open
Ground state of the Sm $4f^5$ configuration of SmB$_6$: $\Gamma_7$ or $\Gamma_8$?

Consequences: spin-texture of topological surface states
Consequences: spin-texture of topological surface states

FIG. S2. Bandstructure without hybridization (a) and phase diagram (b) for the $\Gamma_7$ model defined in Eq. (S10) and (S8) with $t_d^{(1)} = 1$, $t_d^{(2)} = -0.2$, $t_7^{(1)} = -0.03$, $t_7^{(2)} = 0.02$, and $\epsilon_7 = -3$. The two different spin textures (c–d) in phases I and II, respectively, are shown for hybridization parameters $(V_7^{(1)}, V_7^{(2)}) = (0.3, 0)$ and $(V_7^{(1)}, V_7^{(2)}) = (0.1, 0.1)$, respectively. Due to the negative eigenvalue of the restricted spin operator for $f$ electrons (Eq. (14)), the spin direction is reversed around all HSPs when compared to Fig. 1. Note that the

FIG. 3 (color online). Band structure without hybridization (a) and phase diagram (b) for the $\Gamma_8$ model defined in Eq. (9) with $t_d^{(1)} = 1$, $t_d^{(2)} = -0.2$, $t_8^{(1)} = -0.03$, $t_8^{(2)} = 0.02$, and $\epsilon_8 = -3$. The two spin textures [(c),(d)] in phases I and II, respectively, are realized for the hybridization parameters $(V_8^{(1)}, V_8^{(2)}) = (0.3, 0.07)$ and $(V_8^{(1)}, V_8^{(2)}) = (-0.1, 0.1)$, respectively.
Can core level NIXS solve the SmB$_6$ symmetry problem??
The quartet ground state of CeB₆

Sundermann, Lee, Fisk, Tjeng, Severing et al.
EPL, 117 (2017) 17003
Core level NIXS on SmB$_6$

$\text{Sm}^{2+} f^6$ $\text{Sm}^{3+} f^5$

$J=1, n=3$ $\approx 35\text{meV}$

$J=0, n=1$

$J=7/2, n=8$

$\approx 150\text{meV}$

$J=5/2, n=6$

$\Gamma_6, \Gamma_8, \Gamma_7$
Core level NIXS on SmB$_6$

The $\Gamma_8$ forms the ground state of the Sm $4f^5$ configuration of SmB$_6$.
Band Symmetries of Mixed-Valence Topological Insulator: SmB$_6$

Chang-Jong Kang$^1$, Junwon Kim$^1$, Kyoo Kim$^1$, Jeongsoo Kang$^2$, Jonathan D. Denlinger$^3$, and Byung Il Min$^1$*

\[ \text{[\[\zeta00\][\[1/2\zeta0\][\[\zeta\zeta0\]][\[\zeta\zeta\zeta\]]]} \]

\( E - E_F \) (eV)

\( \Gamma, X, M, \Gamma \)

\( \Delta_7, X_7^- \)

\( \Gamma_7^- \)

\( d_{e_g}, \Gamma_7, \Gamma_8^{(1)}, \Gamma_8^{(2)}, R_7^- \)

\( \Gamma_8^- \)

\( M_6^-, M_7^- \)

\( R_8^- \)
Band Symmetries of Mixed-Valence Topological Insulator: SmB$_6$

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![Graph showing DOS vs Energy](image)
Band structure finds a $\Gamma_7$ (and a gap) but our experiment finds a $\Gamma_8$
Core level NIXS on SmB$_6$

Full $\Gamma_8$ polarization for the Sm 4f$^5$ configuration
- Hardly any mixing in of the $\Gamma_7$
- Extremely narrow 4f bands
- Low energy properties of SmB$_6$ are built up from $\Gamma_8$ states
Fractional Parentage

G.A. Sawatzky and R. Green

4f band formation: $f^6(A, J=0) + f^5(B, J=5/2) \leftrightarrow f^5(A, J=5/2) + f^6(B, J=0)$
Fractional Parentage

G.A. Sawatzky and R. Green

4f band formation: $f^6(A, J=0) + f^5(B, J=5/2) \leftrightarrow f^5(A, J=5/2) + f^6(B, J=0)$

huge reduction factors to the one-electron 4f band width !!!