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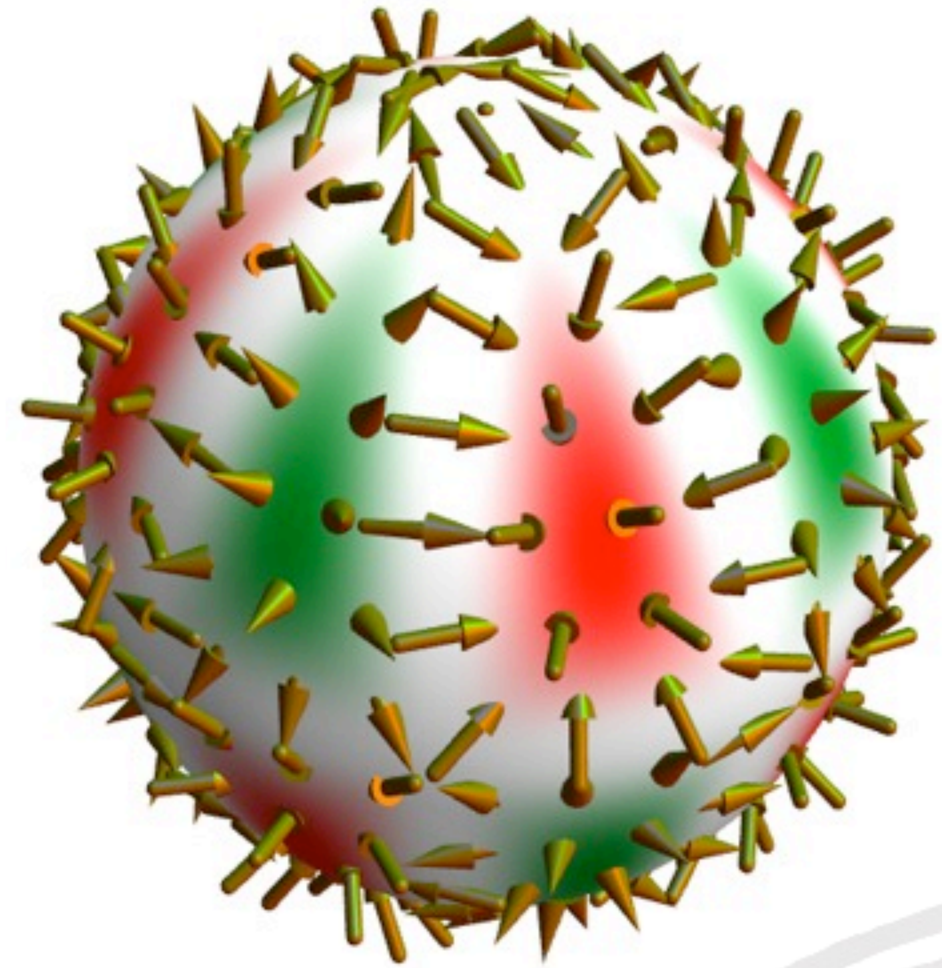

Lars Nordström

Uppsala U, Sweden

DFT+*U* method with LAPW

Electronic Structure with the *Elk* Code - CECAM July 2011

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Outline

- DFT+*U*
  - Double counting
- Tensor moments
- General polarisation of the open shell
- Katt's rules
- Applications
  - URu_2Si_2 & NpO_2 – uncover the hidden order ...
  - Fe pnictides – why low moments?

DFT+*U*

U: $$E_{\mathrm{HF}} = \frac{1}{2} \sum_{abcd} \left[\rho_{ac}\rho_{bd} - \rho_{ad}\rho_{bc} \right] \langle ab|g|cd \rangle$$

where *a*,*b*,*c*,*d* enumerate the orbitals of the correlated atomic shell (*d* or *f*)

Problem:

- Part of the interaction is treated both in DFT and *U*!
- Have to subtract the *Double Counting*.

DFT+U

Electron interaction in terms of Slater parameters

$$\langle ab|g|cd\rangle = \delta(s_a, s_c)\delta(s_b, s_d)(2\ell+1)^2 \sum_{kq} \begin{pmatrix} \ell & k & \ell \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$\times(-)^{m_a+m_b+q} \begin{pmatrix} \ell & k & \ell \\ -m_a & -q & m_c \end{pmatrix} F^{(k)} \begin{pmatrix} \ell & k & \ell \\ -m_b & q & m_d \end{pmatrix}$$

Bare interactions

$$F^{(k)} = \int dr_1 r_1^2 R_\ell^2(r_1) \frac{r_<^k}{r_>^{k+1}} R_\ell^2(r_2) r_2^2 dr_2$$

Screening

$$\frac{r_<^k}{r_>^{k+1}} \rightarrow -(2k+1)\lambda j_k(i\lambda r_<) h_k^{(1)}(i\lambda r_>)$$

DFT+U history

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- Main interest - TM oxides ... (Anisimov et al)
- 90 - localisation: only diagonal elements of ρ
- 95 - distortions: block diagonal elements of ρ
- 00 - magnetic order: full ρ (Solvyev et al)
    - for $l=2$, ρ has dimension 10×10
        - no problem for computer ...
        - but for understanding!
- 03 - spherical averaged interaction (Dudarev et al)

Double counting

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- Around mean field (AMF) (Anisimov et al)
  - H and X in DFT correspond to HF for an unpolarised density matrix (DM)
- Fully localised limit (FLL) (Dudarev et al)
  - Appropriate when DM has eigenvalues zero or one only
- Interpolation between the two (Petukhov et al)
  - Interpolation constant calculated from DM

$$E_{\mathrm{DC}} = \alpha\, E_{\mathrm{DC,FLL}} + (1-\alpha)\, E_{\mathrm{DC,AMF}} \qquad \alpha = \frac{c_{\mathrm{tot}}}{c_{\mathrm{max}}}$$

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Background on actinides

- Abundant itinerant magnetic materials
- Unquenched orbital moments & huge anisotropies
- Interplay: magnetism & superconductivity
- DFT overestimates spin moments ...
- Can be remedied in DFT+ approaches

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Polarisation of open shell

Local density matrix for the correlated shell

$$\rho = (2[\ell])^{-1}\,(n\,\mathbf{1}\otimes\mathbf{1} + m_z\mathbf{1}\otimes\sigma_z + \ldots)$$

$[\ell]\times[\ell]$

2×2

Unpolarised

Spin polarisation

$$[\ell] := 2\ell + 1$$

Higher polarisation terms?

Different kinds of orbital polarisation ...

Combined spin & orbital polarisation ...

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Tensor moments ...

Transformation $\mathbf{w}^{\alpha} \equiv \mathbf{w}^{kpr} = \mathrm{Tr}\, \mathbf{\Gamma}^{kpr} \rho$

Racah (42)

NOVEMBER 1 AND 15, 1942 PHYSICAL REVIEW VOLUME 62

Theory of Complex Spectra. II

GIULIO RACAH
The Hebrew University, Jerusalem, Palestine

Following Dirac's vector model we can also substitute the operator (37) **I** for the double sign which precedes g_k and assume as coefficient of G^k in the exchange interaction between two electrons the expression

$$-[\tfrac{1}{2}+2(\mathbf{s}_1\cdot\mathbf{s}_2)](l_1\|C^{(k)}\|l_2)^2 \sum_r (-1)^r(2r+1)\,W(l_1l_1l_2l_2;rk)(\mathbf{u}_1^{(r)}\cdot\mathbf{u}_2^{(r)}). \qquad (60)$$

It will also be convenient to consider the quantities $(\mathbf{s}_1\cdot\mathbf{s}_2)(\mathbf{u}_1\cdot\mathbf{u}_2)$ as scalar products of "double tensors";[12] a double tensor of the degree (κ, k) is defined as a quantity which behaves as an irreducible tensor of the degree κ with respect to **S** and as an irreducible tensor of the degree k with respect to **L**. The algebra of these double tensors is a trivial extension of the tensor algebra developed in §3; it must be noted only that such a double tensor does not satisfy the commutation rule (23) with respect to **J**, because with respect to **J** it is reducible and may be decomposed in a sum of irreducible tensors, the degrees of which lie between $|k-\kappa|$ and $k+\kappa$. From this point of view the scalar product $(\mathbf{l}\cdot\mathbf{s})$ is the scalar part of the decomposition of the double vector **ls**.

Tensor moments ...

Transformation $$\mathbf{w}^{\alpha} \equiv \mathbf{w}^{kpr} = \mathrm{Tr}\,\mathbf{\Gamma}^{kpr}\rho$$

Racah (42)

even k: density
odd k: current
p=0: charge
p=1: spin
r coupled k & p

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Tensor moments ...

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Racah (42) but with van der Laan & Thole normalisation (95)

even k: density
odd k: current
p=0: charge
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r coupled k & p

jm$_j$-basis:

$$\left\{\mathbf{\Gamma}_t^{kpr}\right\}_{j_1 m_1, j_2, m_2} = \frac{\sqrt{[j_1 j_2]}}{N_{kpr\ell}} (-)^{j_1 - m_1} \begin{pmatrix} j_1 & r & j_2 \\ -m_1 & t & m_2 \end{pmatrix} \begin{Bmatrix} \ell & \ell & k \\ s & s & p \\ j_1 & j_2 & r \end{Bmatrix}$$

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Tensor moments ...

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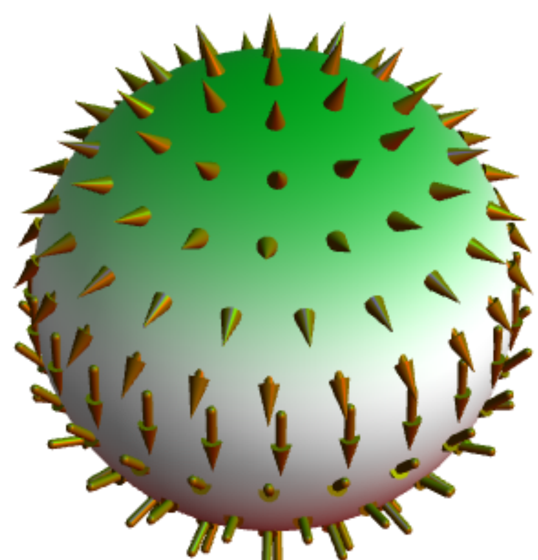

w_0^{211}

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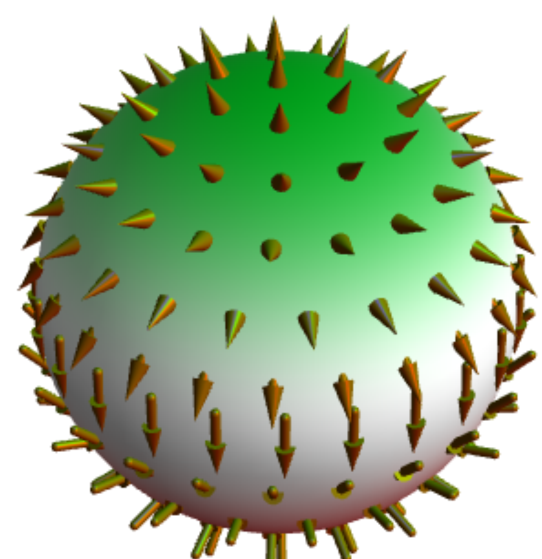
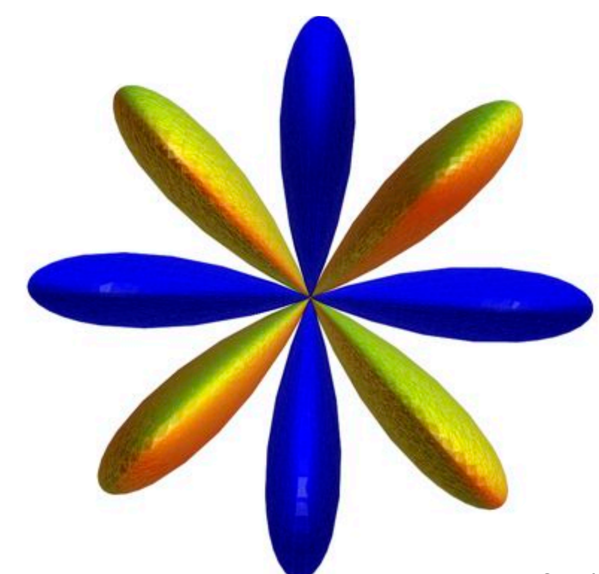


w_0^{211}



w_{40}^{41}

jm$_j$-basis:

$$\left\{\mathbf{\Gamma}_t^{kpr}\right\}_{j_1 m_1, j_2, m_2} = \frac{\sqrt{[j_1 j_2]}}{N_{kpr\ell}} (-)^{j_1 - m_1} \begin{pmatrix} j_1 & r & j_2 \\ -m_1 & t & m_2 \end{pmatrix} \begin{Bmatrix} \ell & \ell & k \\ s & s & p \\ j_1 & j_2 & r \end{Bmatrix}$$

Open shell polarisation

Physical density matrix $\mathrm{Tr}\rho \geq \mathrm{Tr}\rho^2$

with ”polarisation”

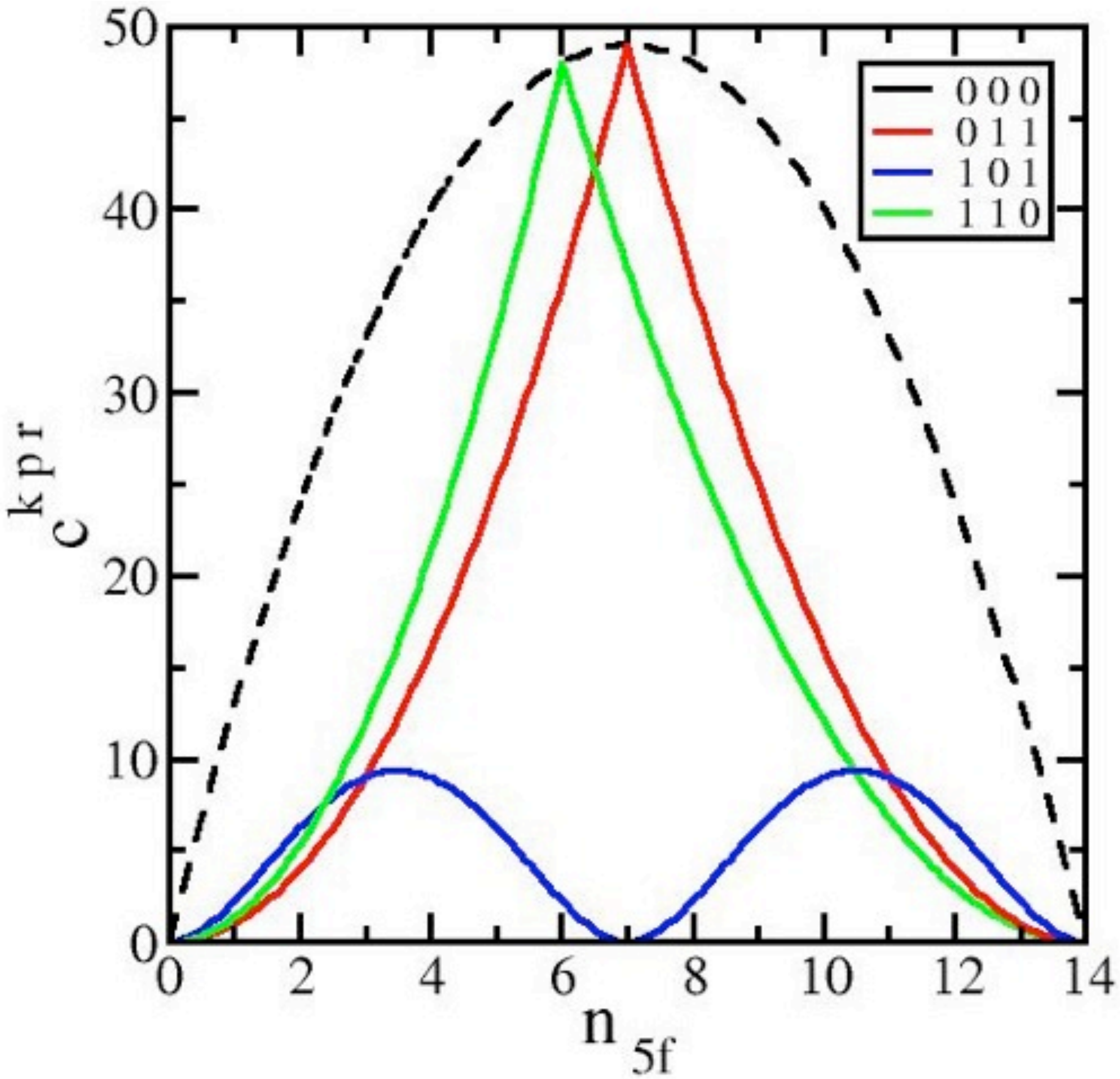
$$c^{kpr} = [kpr]|N_{kpr\ell}|^2\, \mathbf{w}^{kpr} \cdot \mathbf{w}^{kpr}$$

$$\sum_{kpr \neq 000} c^{kpr} \leq nn_h$$

$$(c_{\mathrm{tot}} \leq c_{\mathrm{max}})$$

Open shell polarisation

Physical density matrix $\mathrm{Tr}\rho \geq \mathrm{Tr}\rho^2$



$$\sum_{kpr \neq 000} c^{kpr} \leq n n_h$$

$$(c_{\mathrm{tot}} \leq c_{\mathrm{max}})$$

Reformulation of HF

"GHF" $$E_{\mathrm{HF}} = \frac{1}{2} \sum_{abcd} \left[\rho_{ac}\rho_{bd} - \rho_{ad}\rho_{bc} \right] \langle ab|g|cd \rangle$$

Transformation dm to spherical tensors (à la Racah)

one-to-one $\rho \leftrightarrow \mathbf{w}^{\alpha}$

$$\Rightarrow \qquad E_{\mathrm{HF}} = \frac{1}{2} \sum_{\alpha} (J_{\alpha} - K_{\alpha}) \mathbf{w}^{\alpha} \cdot \mathbf{w}^{\alpha}$$

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Cricchio et al, PRB **78**, 100404R (2008)

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DFT

$$\mathcal{H} = -\Delta + V + \xi \ell \cdot \boldsymbol{\sigma} - b_{\mathrm{XC}} \cdot \boldsymbol{\sigma}$$

$$b_{\mathrm{XC}} \approx \frac{1}{2} I_{\mathrm{Stoner}} m_{\mathrm{spin}}$$

$\boldsymbol{\sigma} \quad \mathrm{su}(2)$

$m_{\mathrm{spin}} \quad m_{\mathrm{orb}}$

6 degrees of freedom

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DFT+U

Anisimov, Liechtenstein, Solovyev, Shick ...

$$\mathcal{H} = -\Delta + V + \xi \ell \cdot \boldsymbol{\sigma} - b_{\rm XC} \cdot \boldsymbol{\sigma} - \sum_\alpha B^\alpha \cdot \boldsymbol{\Gamma}^\alpha$$

$$b_{\rm XC} \approx \frac{1}{2} I_{\rm Stoner} m_{\rm spin}$$

$$B^\alpha = K_\alpha \boldsymbol{w}^\alpha$$

$\boldsymbol{\sigma}$ $\quad \mathrm{su}(2)$

$\boldsymbol{\Gamma}^\alpha$ $\quad \mathrm{su}(14)$

$\boldsymbol{w}^\alpha$

$m_{\rm spin}$ $\quad m_{\rm orb}$

6 degrees of freedom

195 dof

DFT+*U* vs Hybrid-DFT

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- Both add exact exchange
- DFT+*U* restricts to the correlated shell
- DC vs reduced DFT
- HDFT: ”screen” everything with 0.25
  - OK for *U* ...
  - But not for higher Slater parameters, that are screened much less (0.7 – 0.9)
- DFT+*U* as a CDFT ...?

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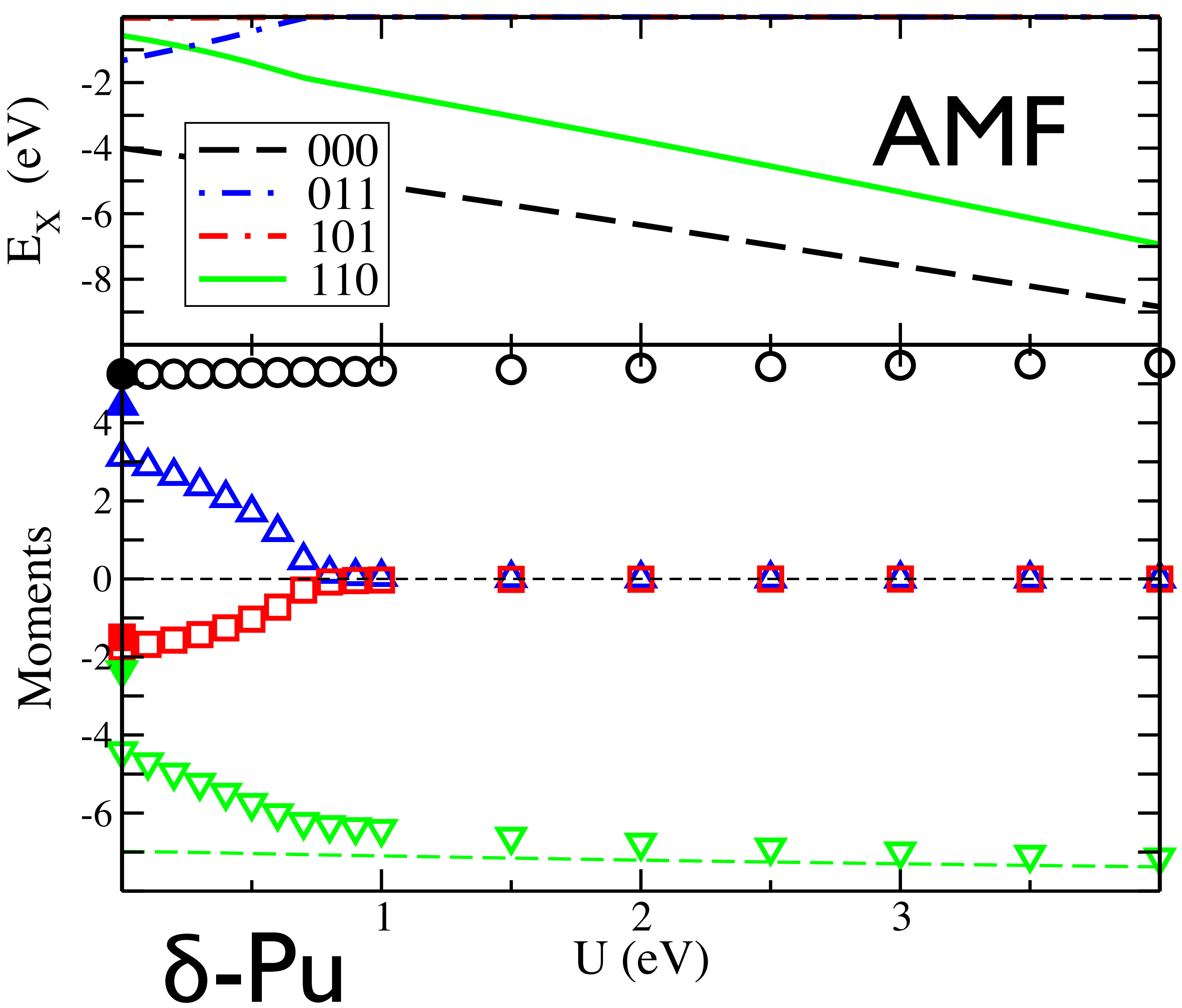
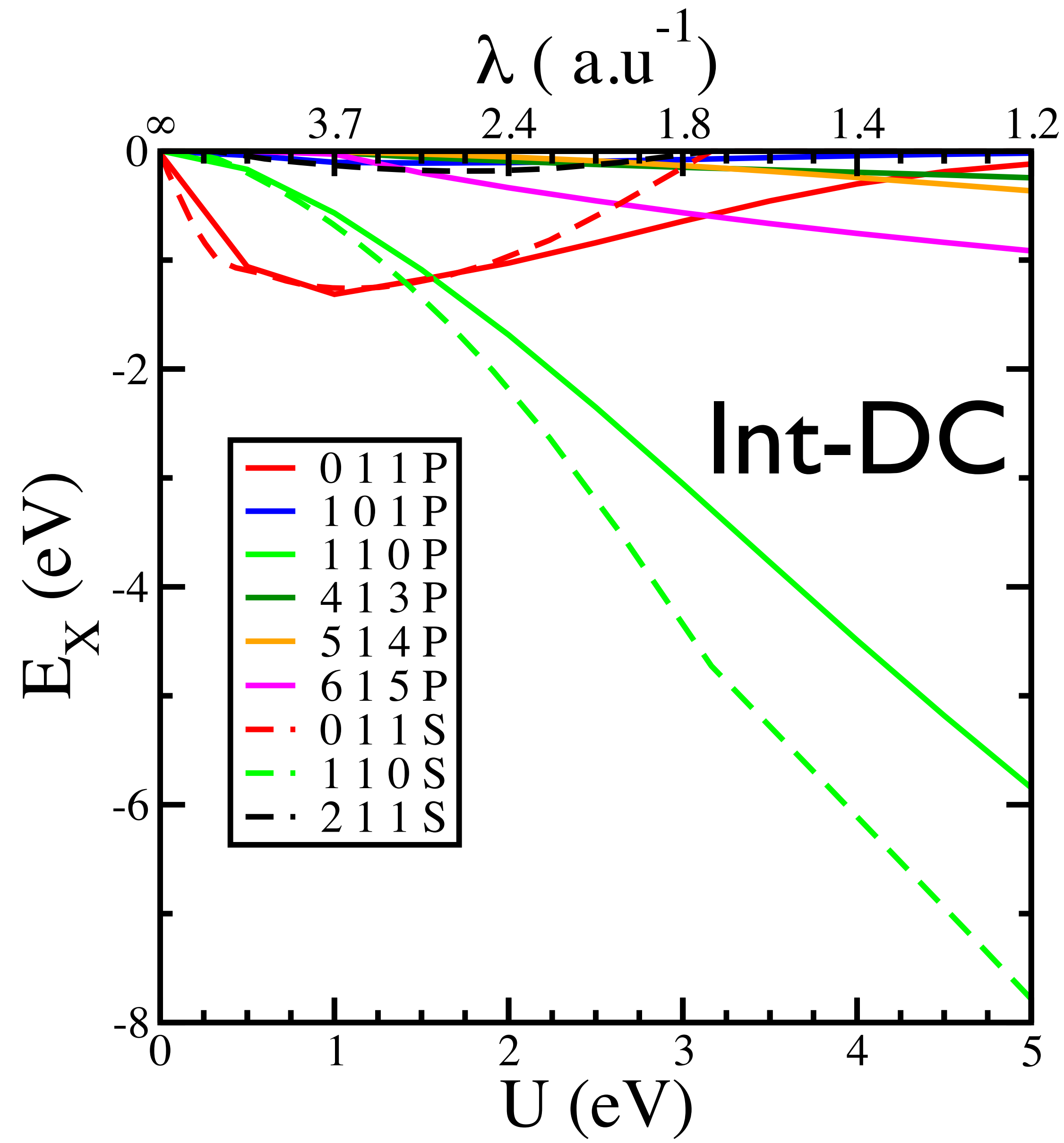
Free parameters ...

- In the fields B^{α} – 4 Slater integrals: $F^{(k)}$
  - Calculate with Yukawa potential $\frac{1}{r}e^{-\lambda r}$
    - One parameter – $U = F^{(0)}$
- Double counting – AMF or FLL?
  - Interpolation scheme by Petukhov *et al*
- Implemented in ELK (FP-APW+*lo*) un-constrained non-collinear elk.sourceforge.net (open source)

Non-magnetic Pu

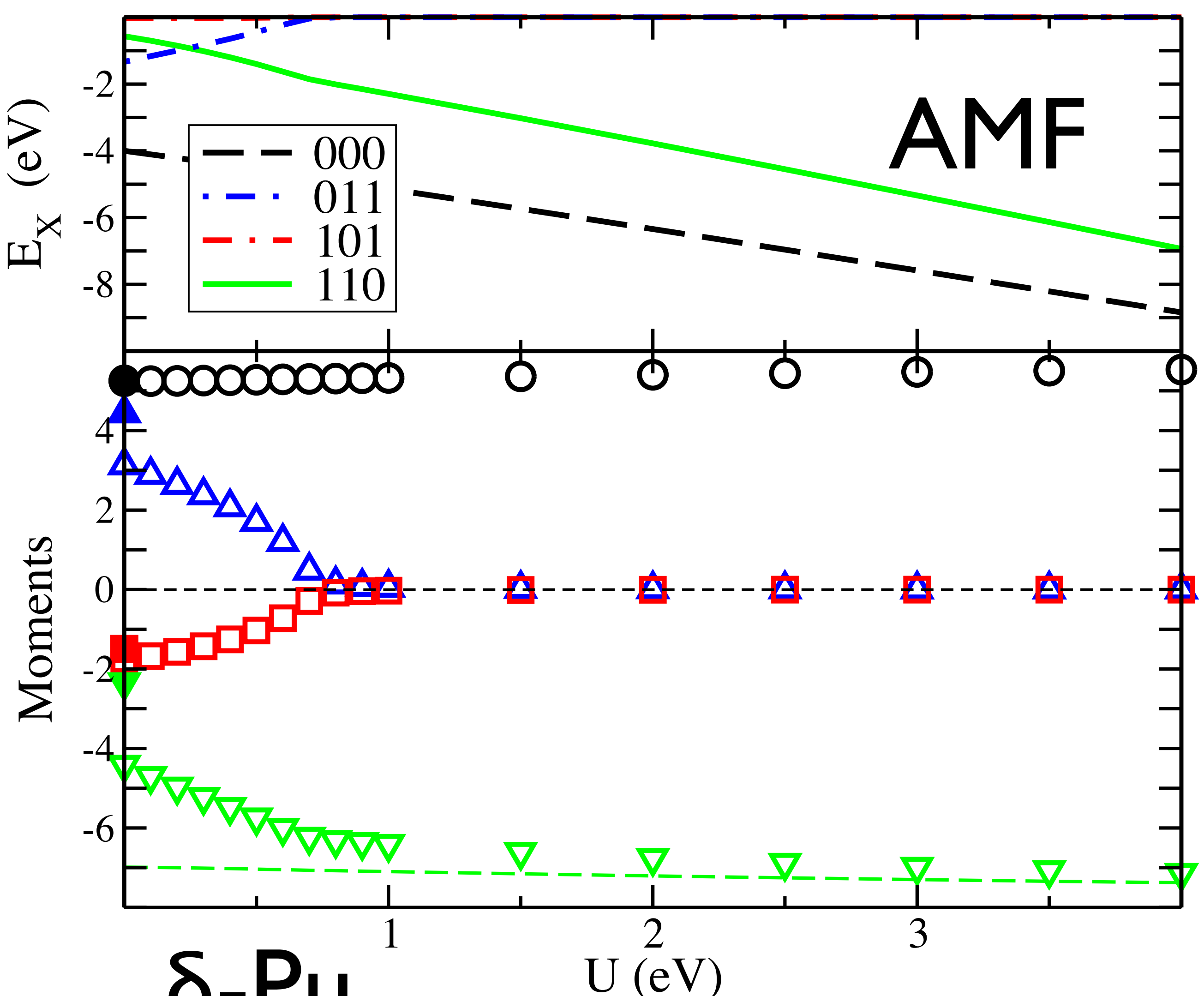




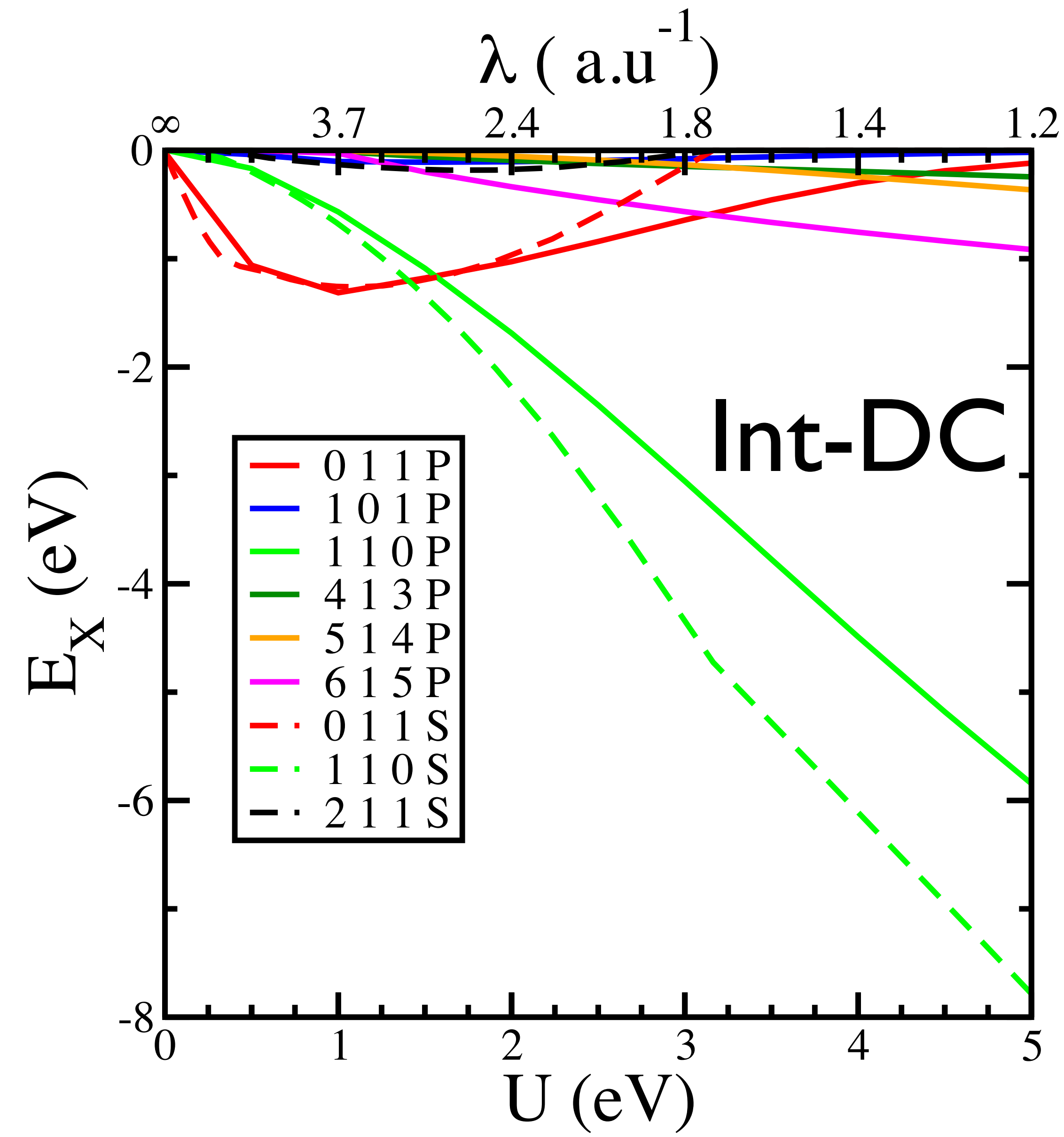
PuS & PuP in NaCl, PM resp FM

Exchange enhanced SOC!

Non-magnetic Pu



δ-Pu

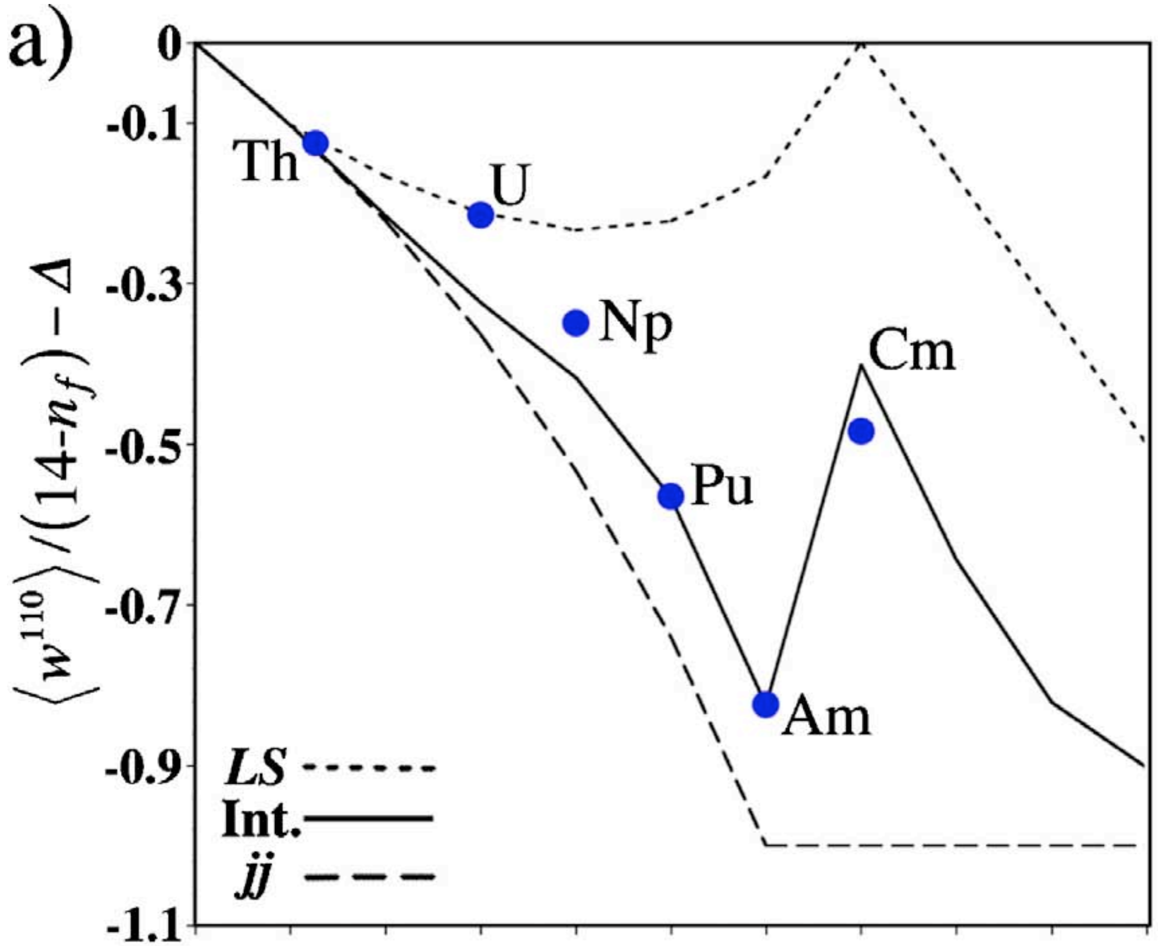


PuS & PuP in NaCl, PM resp FM

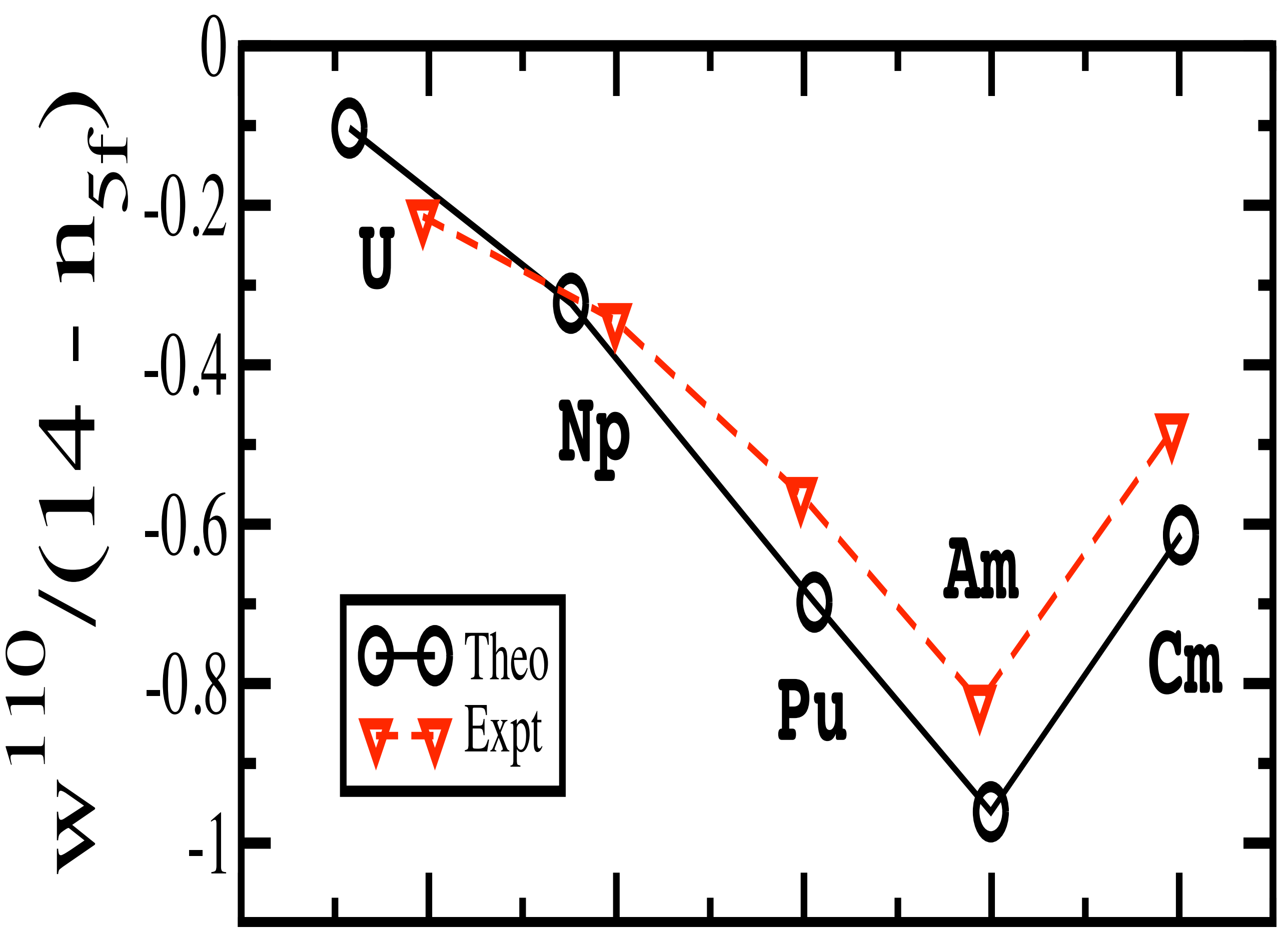
Cricchio *et al*, PRB **78**, 100404(R) (2008) & Bultmark *et al*, PRB **80**, 035121 (2009)

Exchange enhanced SOC!

110 moments



EELS SO-sum rule



present work

from Moore et al, PRB **76**, 073105 (2007)

Polarisation terms

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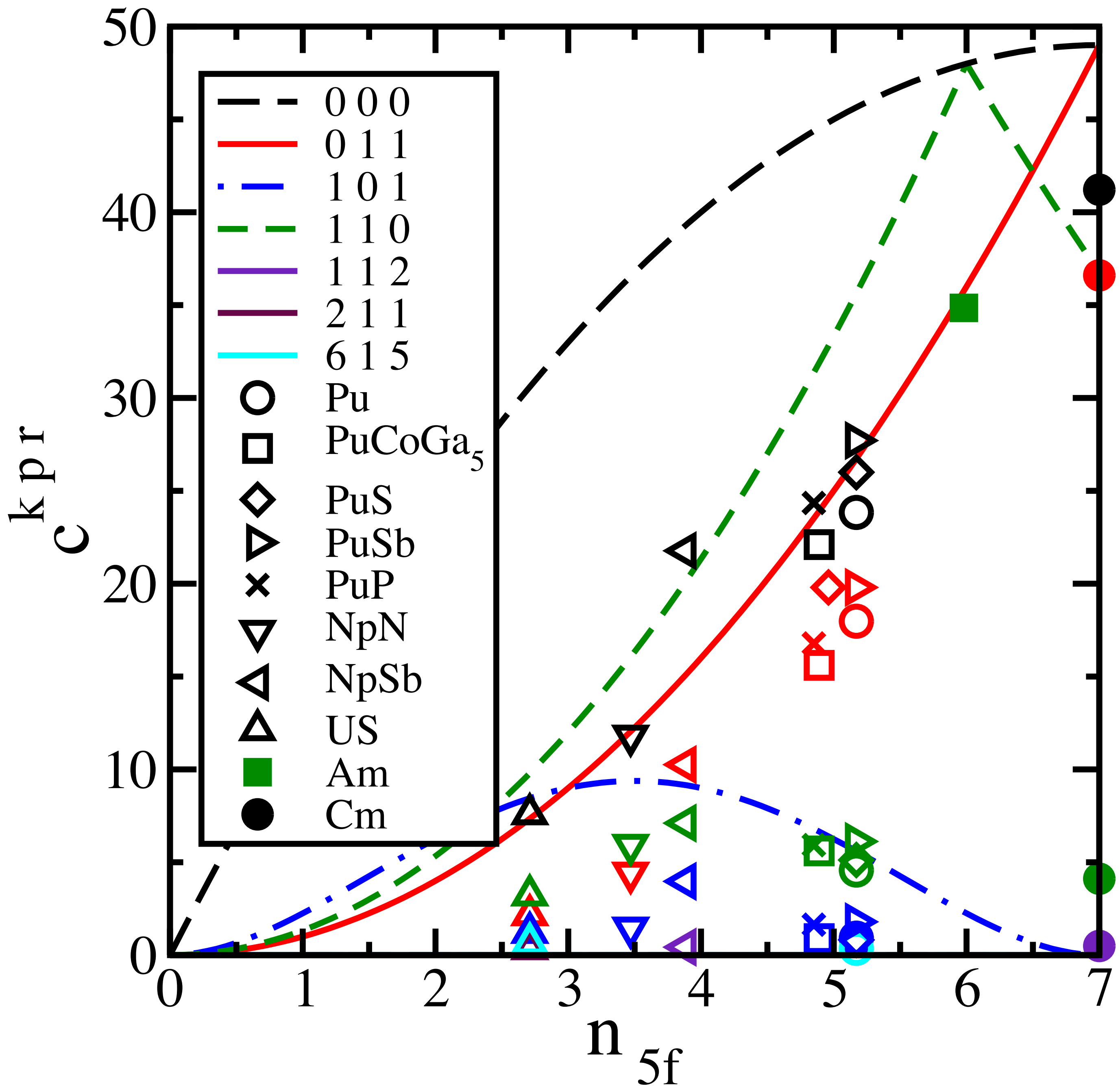
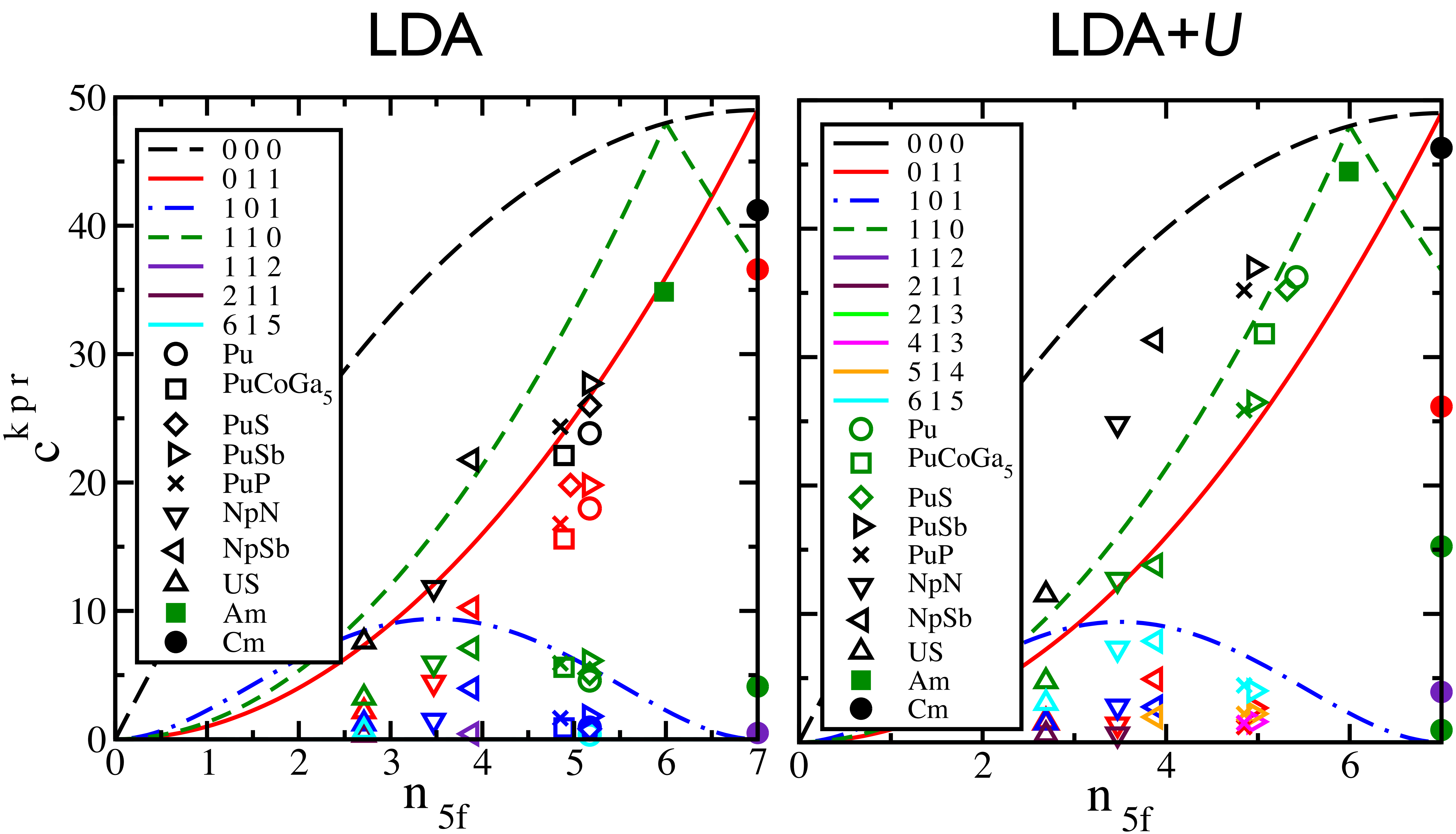
LDA



Polarisation terms



Time reversal symmetry

First: enhance spin orbit coupling
$\Rightarrow$ 110

$$\begin{pmatrix}
-\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$

5/2

7/2

Time reversal symmetry

First: enhance spin orbit coupling
$\Rightarrow$ 110

$$\begin{pmatrix}
-\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
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0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$

Second: break time reversal symmetry
$\Rightarrow$ 615

$$615_0 \sim \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1
\end{pmatrix}$$

$$615_4 \sim \begin{pmatrix}
0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}$$

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for extended systems:

Hund's rules

HI. Saturate spin polarisation – 011

HII. Optimise polarisation 101

Induced polarisations

110 & 112

HIII. Let $w^{110} < 0$

Katt's rules

KI. Saturate spin-orbit polarisation – 110

KII. Optimise polarisation 615 (617)

Induced polarisations:

415 & 505 (none)

KIII. Polarise 011, if possible

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Cricchio *et al*, EPL (2011)

DFT+*U*

In terms of polarisation

$$E_{\mathrm{X}} = -\frac{1}{4}\sum_{kpr} A_k c^{kpr}$$

$$A_k = \sum_{n'} B^{(\ell)}_{kn'} F^{(n')} = \sum_{n} C^{(\ell)}_{kn} E^{(n)}$$

In terms of Racah parameters

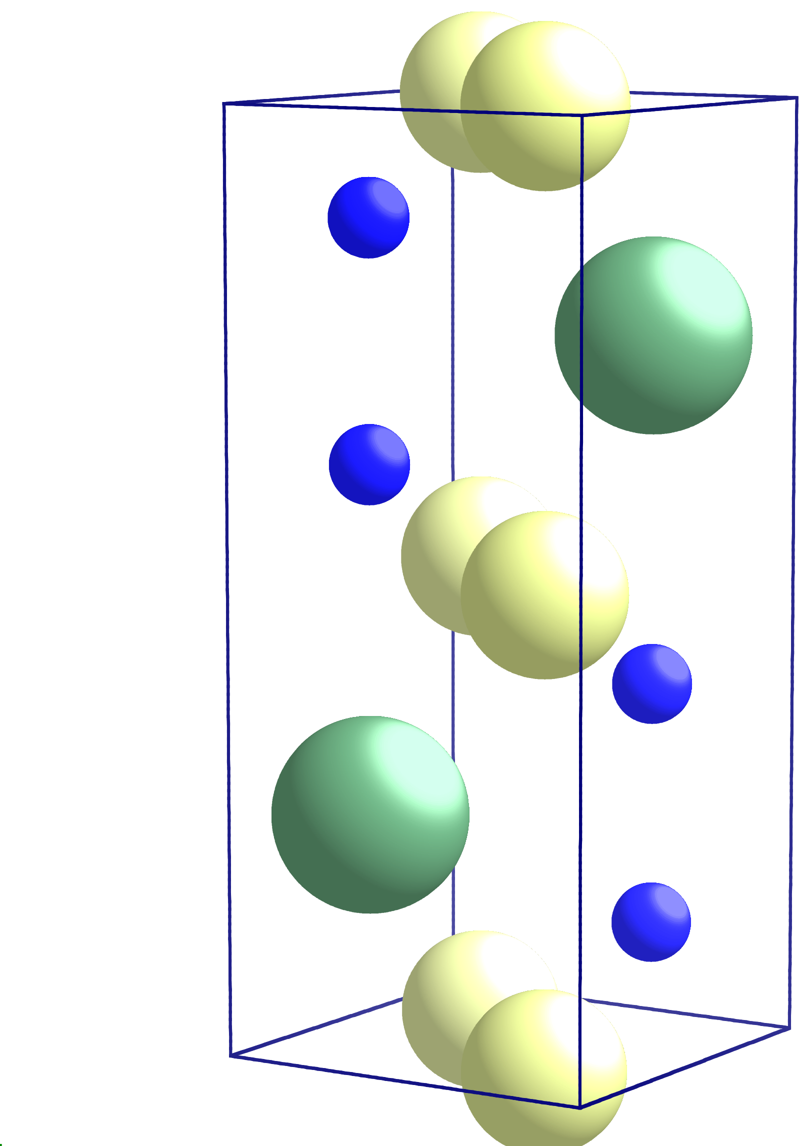
U-J *aJ* E^2 E^3

$$D^{(3)} = \begin{pmatrix} 1 & -\frac{2}{45} & -\frac{1}{33} & -\frac{50}{1287} \\ 0 & \frac{14}{405} & \frac{7}{297} & \frac{350}{11583} \\ 0 & \frac{1}{2025} & -\frac{1}{3267} & \frac{175}{1656369} \\ 0 & \frac{1}{135} & \frac{2}{1089} & -\frac{175}{42471} \end{pmatrix} \Rightarrow C^{(3)} = \frac{1}{7}\begin{pmatrix} 1 & 9 & 0 & 0 \\ 1 & 0 & 0 & 33 \\ 1 & 2 & 286 & -11 \\ 1 & 0 & 0 & 0 \\ 1 & 2 & -260 & -4 \\ 1 & 0 & 0 & -9 \\ 1 & 2 & 70 & 7 \end{pmatrix}$$

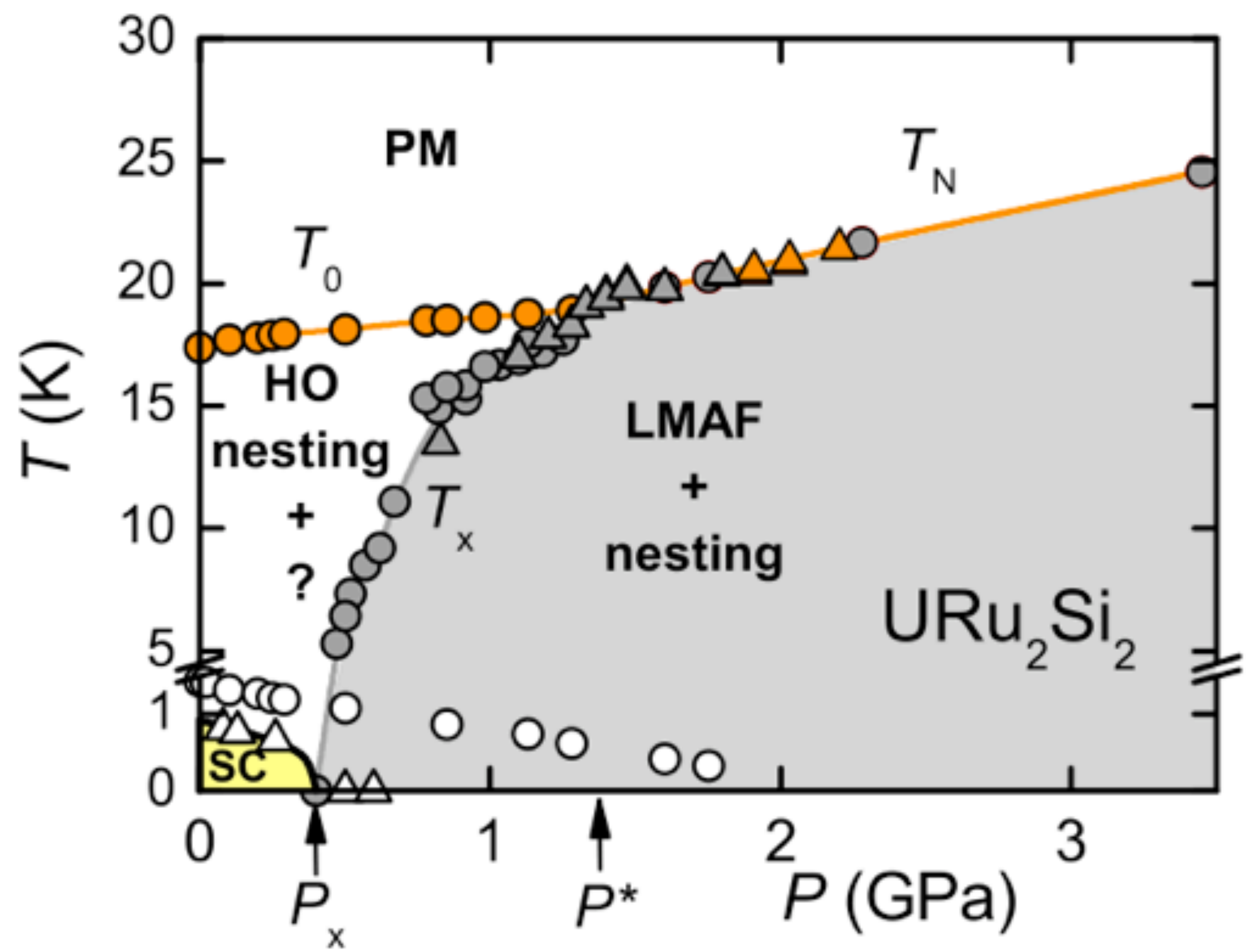
Hidden order

URu_2Si_2 heavy fermion material

Palstra *et al*, 1985



bct



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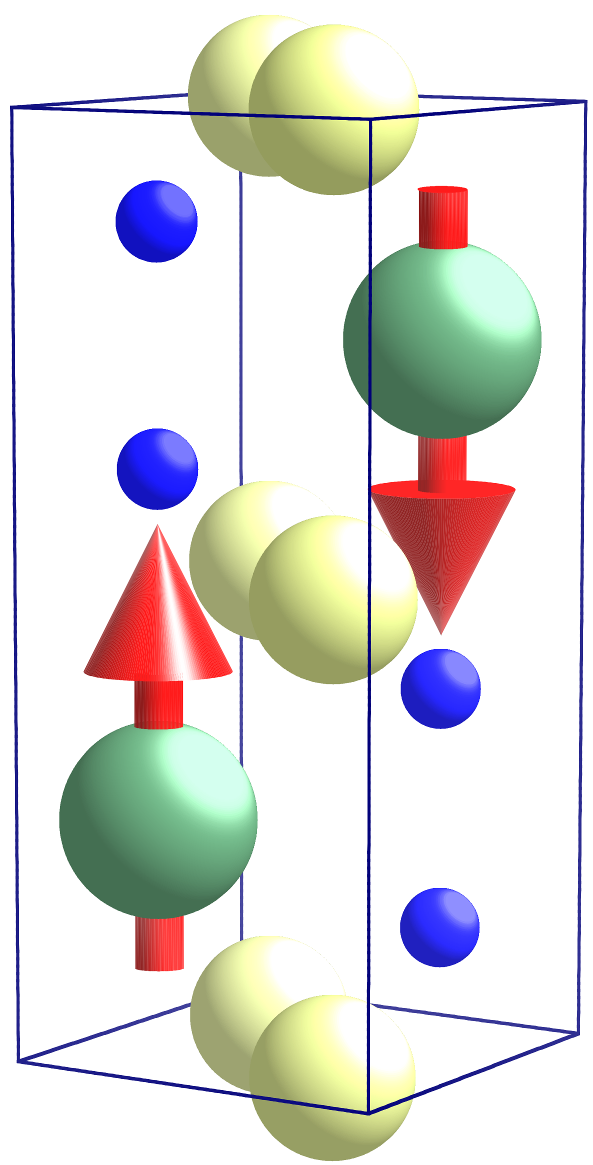
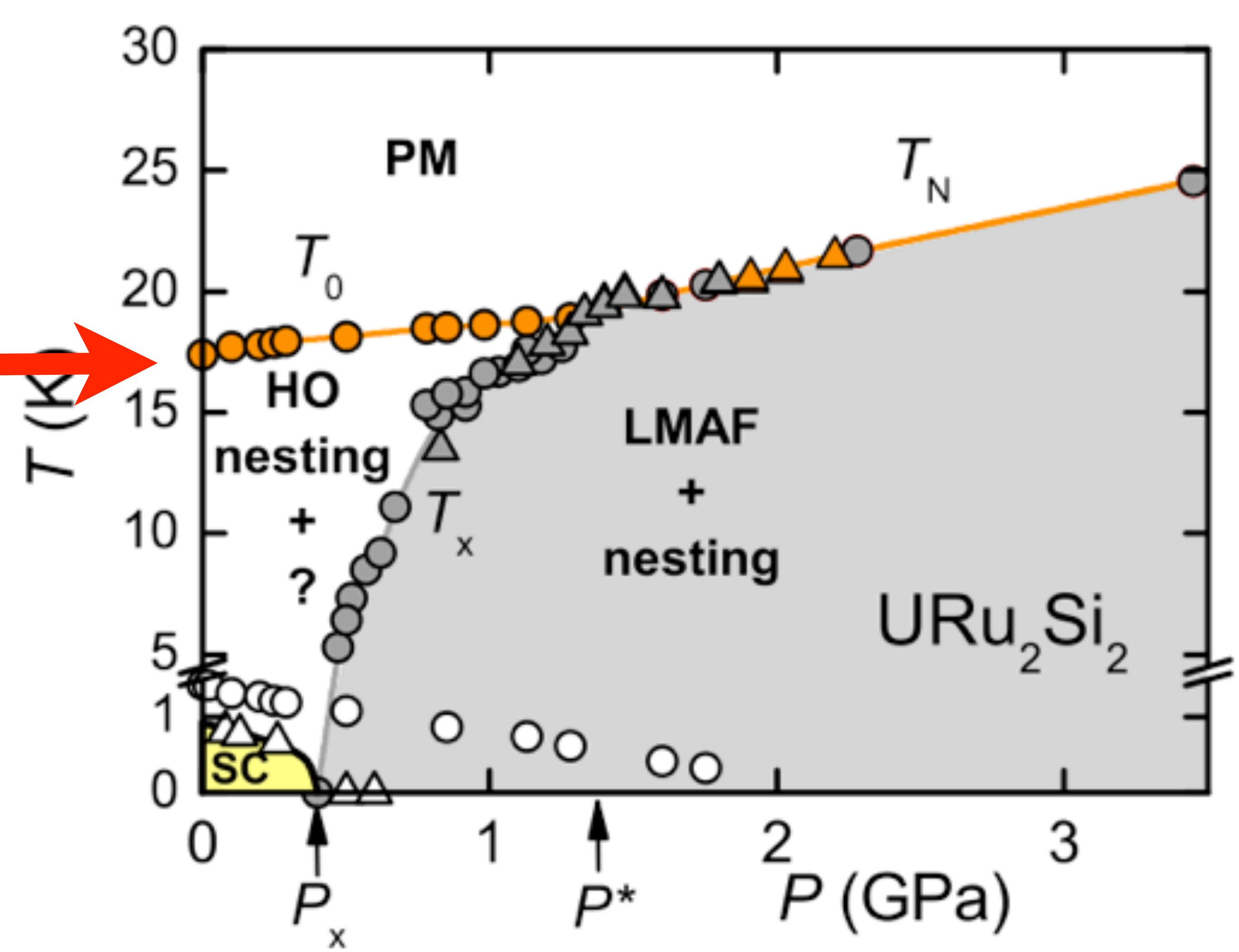
Palstra *et al*, 1985



bct



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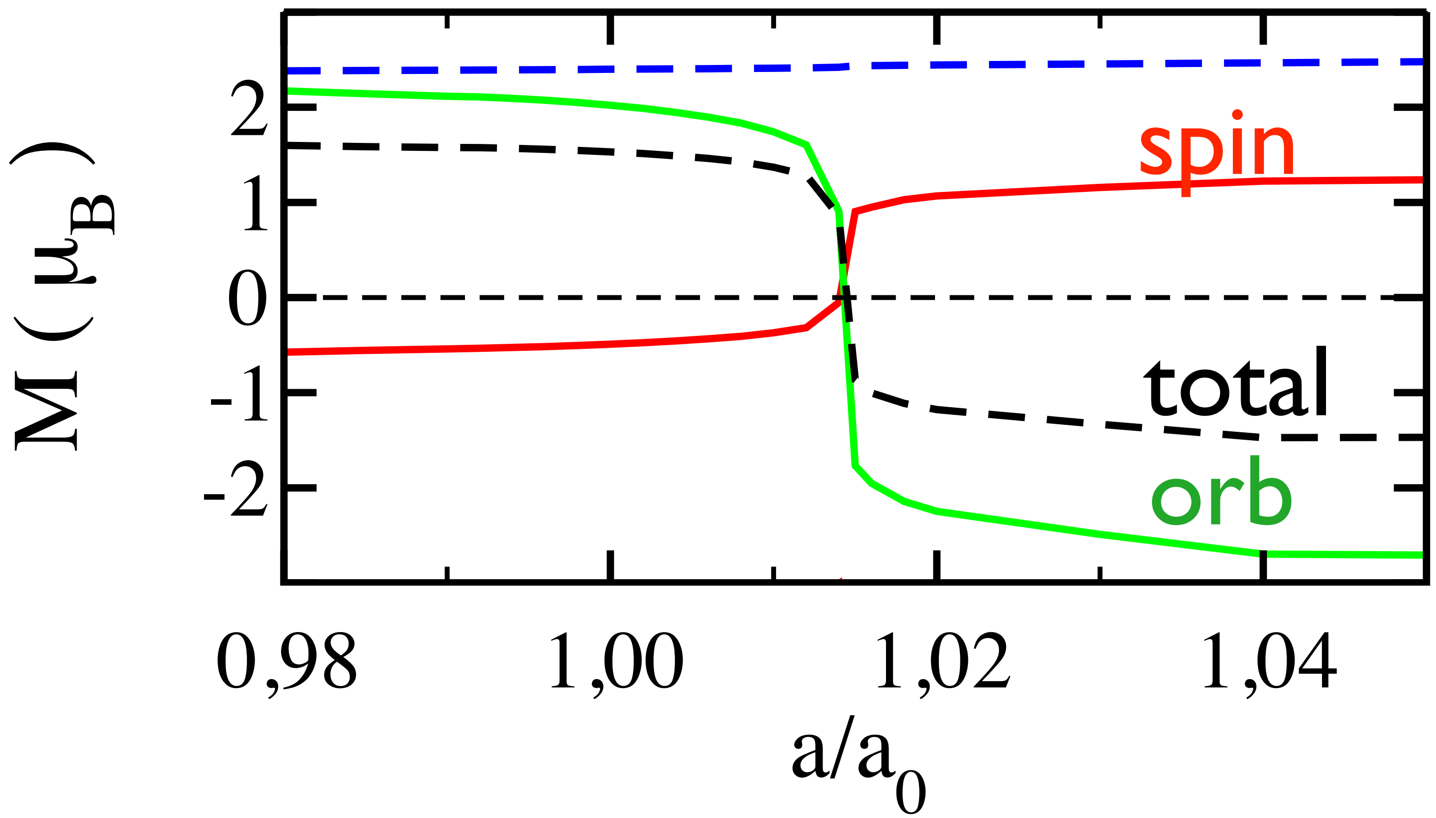
DFT+*U* calculation



Pressure: mainly decrease in *a*

U = 1 eV

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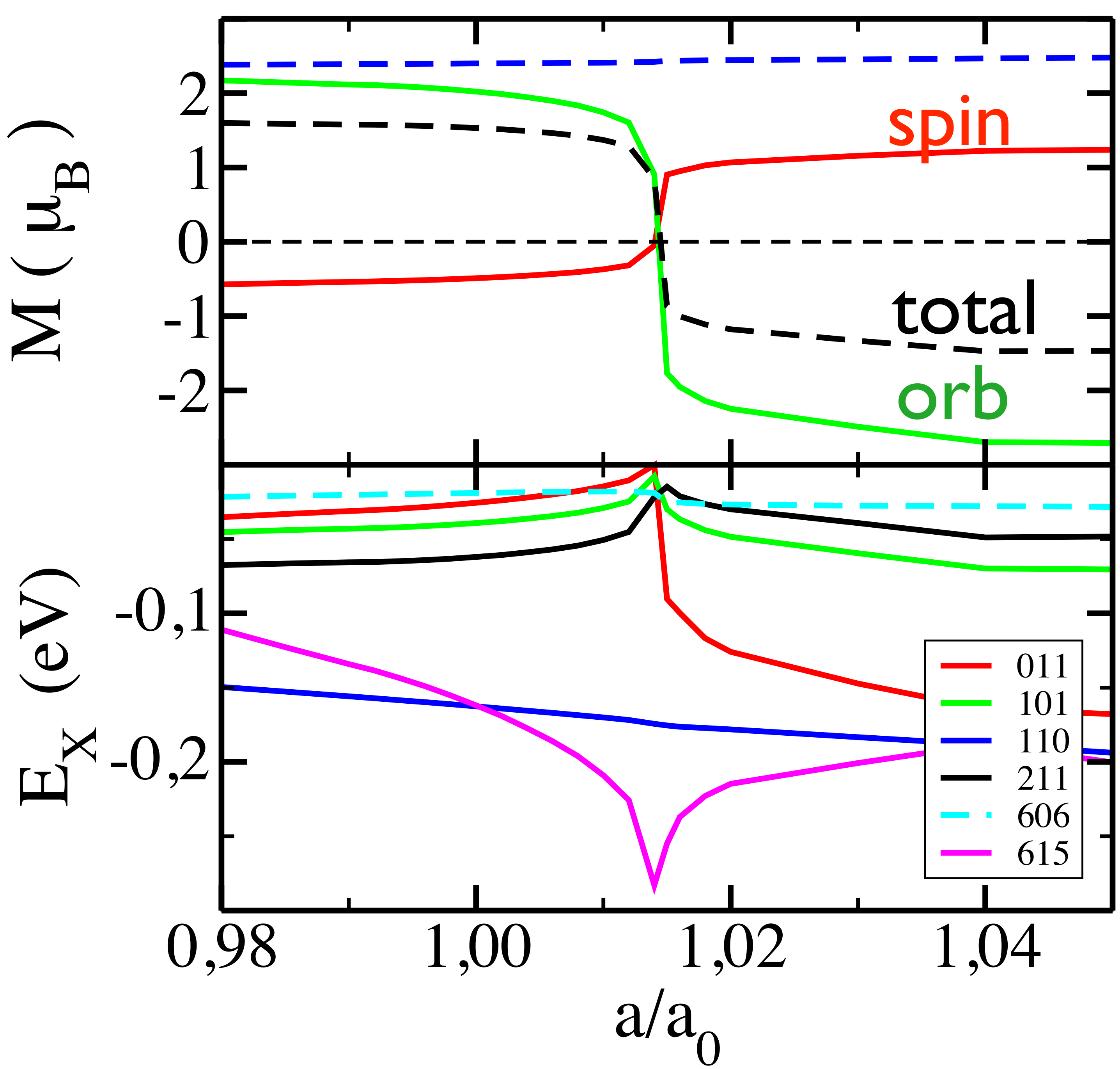
DFT+*U* calculation



Pressure: mainly decrease in *a*

U = 1 eV

Divergence in 615 exchange energy – kills SP!

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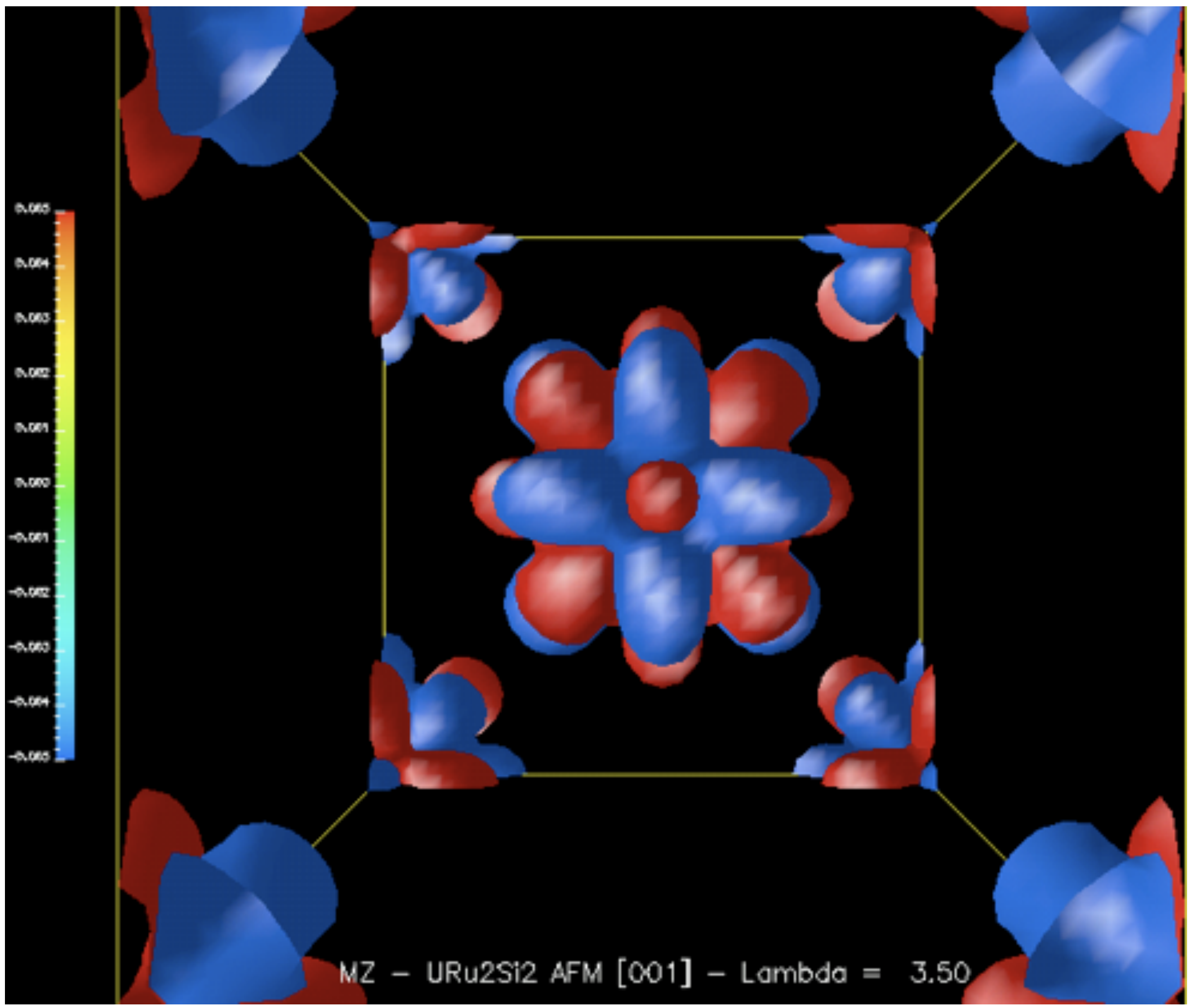
DFT+*U* calculation



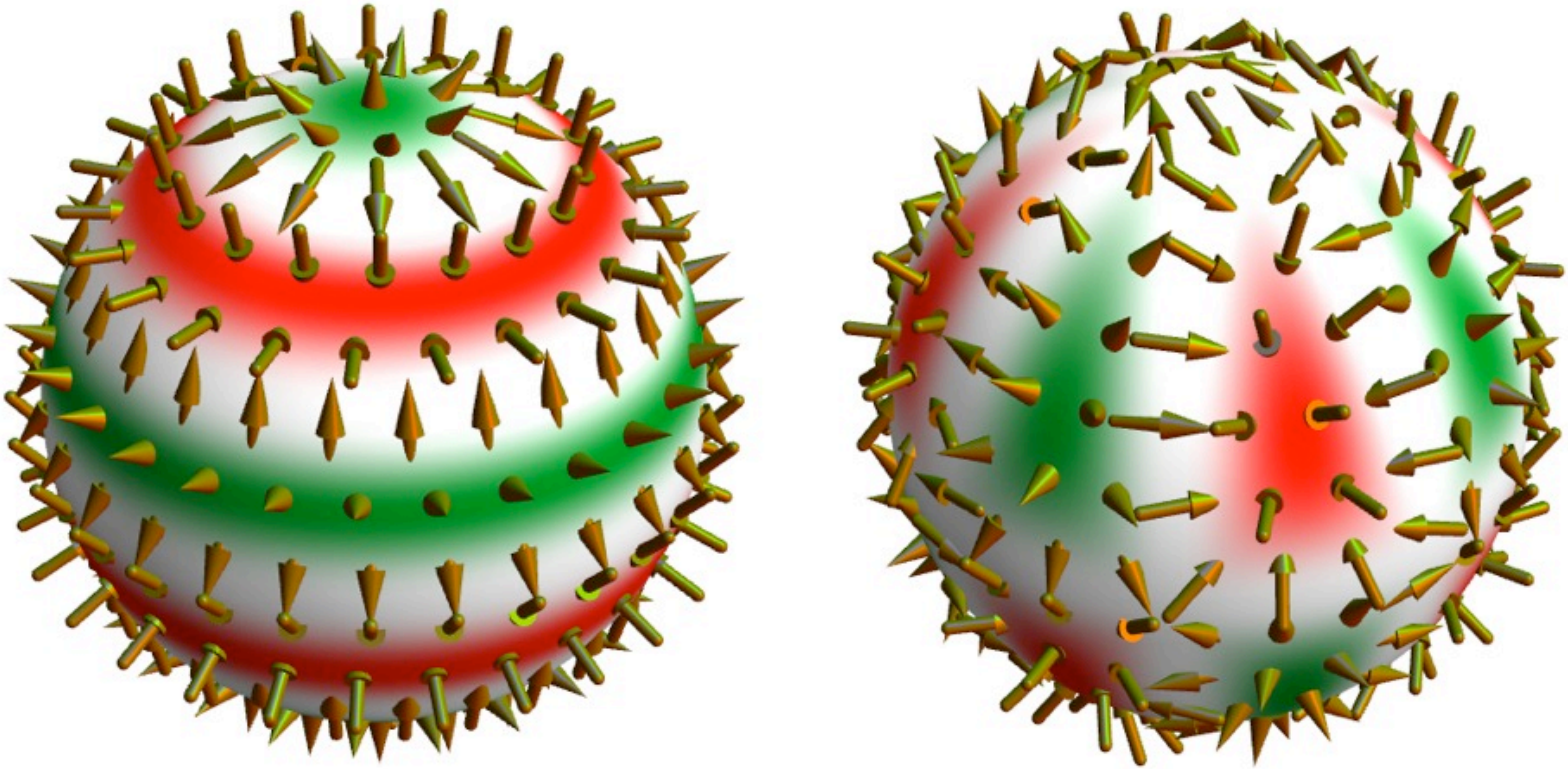
m_z density
blue pos & red neg

Pressure: mainly decrease in *a*

U = 1 eV

Divergence in 615 exchange energy – kills SP!

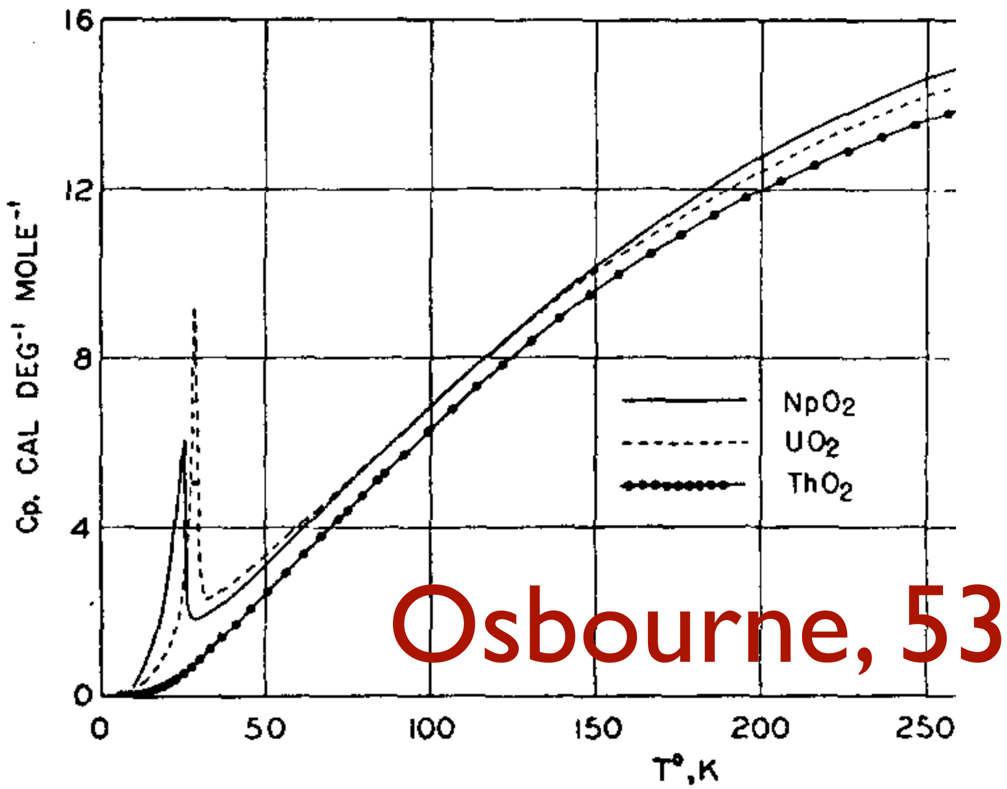
Triakontadipole moments



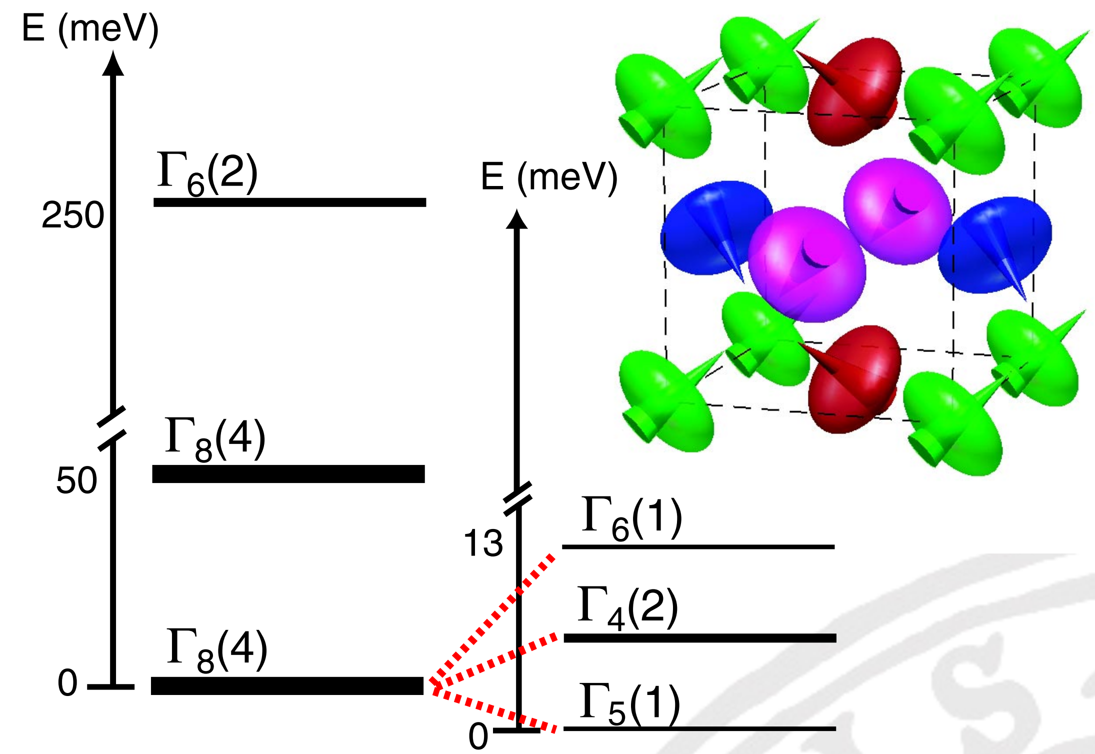
The hidden order

Cricchio *et al.* PRL **103**, 107202 (09)

Hidden order: NpO_2



Osbourne, 53



Magnani *et al*, 08

- 2nd order transition at T_o=26 K
  - but no moments
  - AF-I 3**k** type ordering
- Suggestions: rank 2, 3 and 5 ...
- Triakontadipoles from localized CF picture
  - consistent with INS

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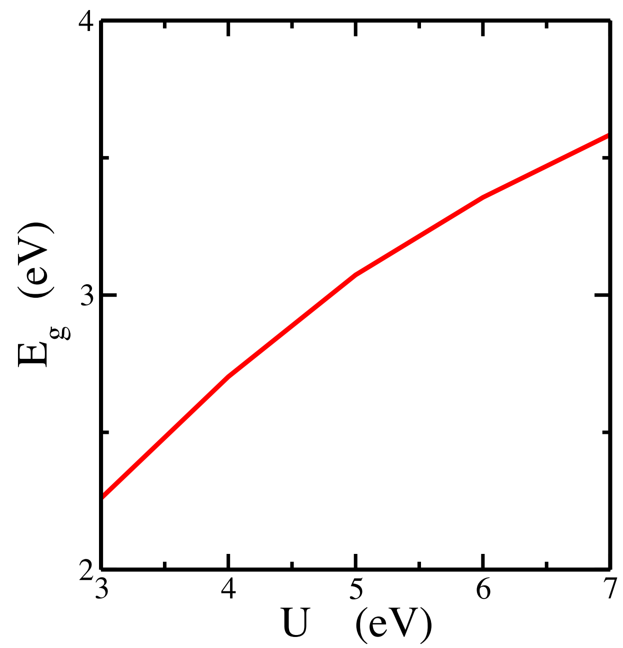
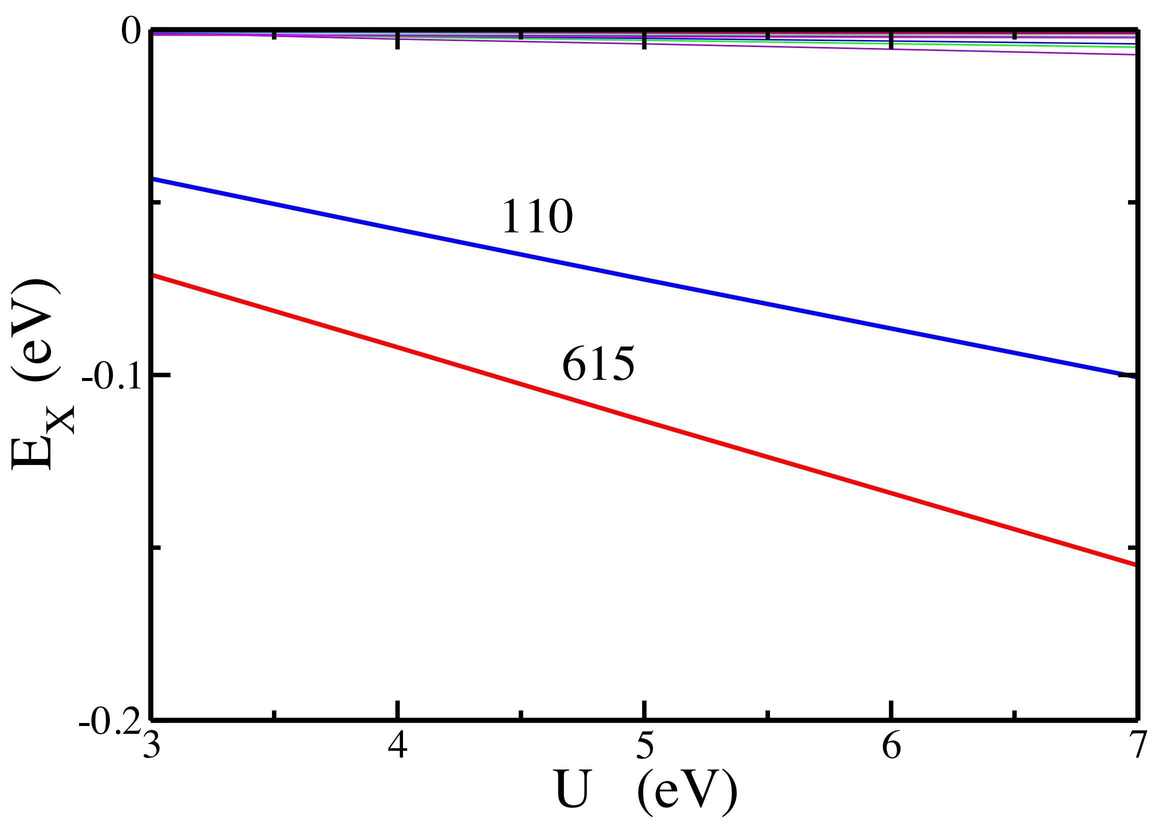
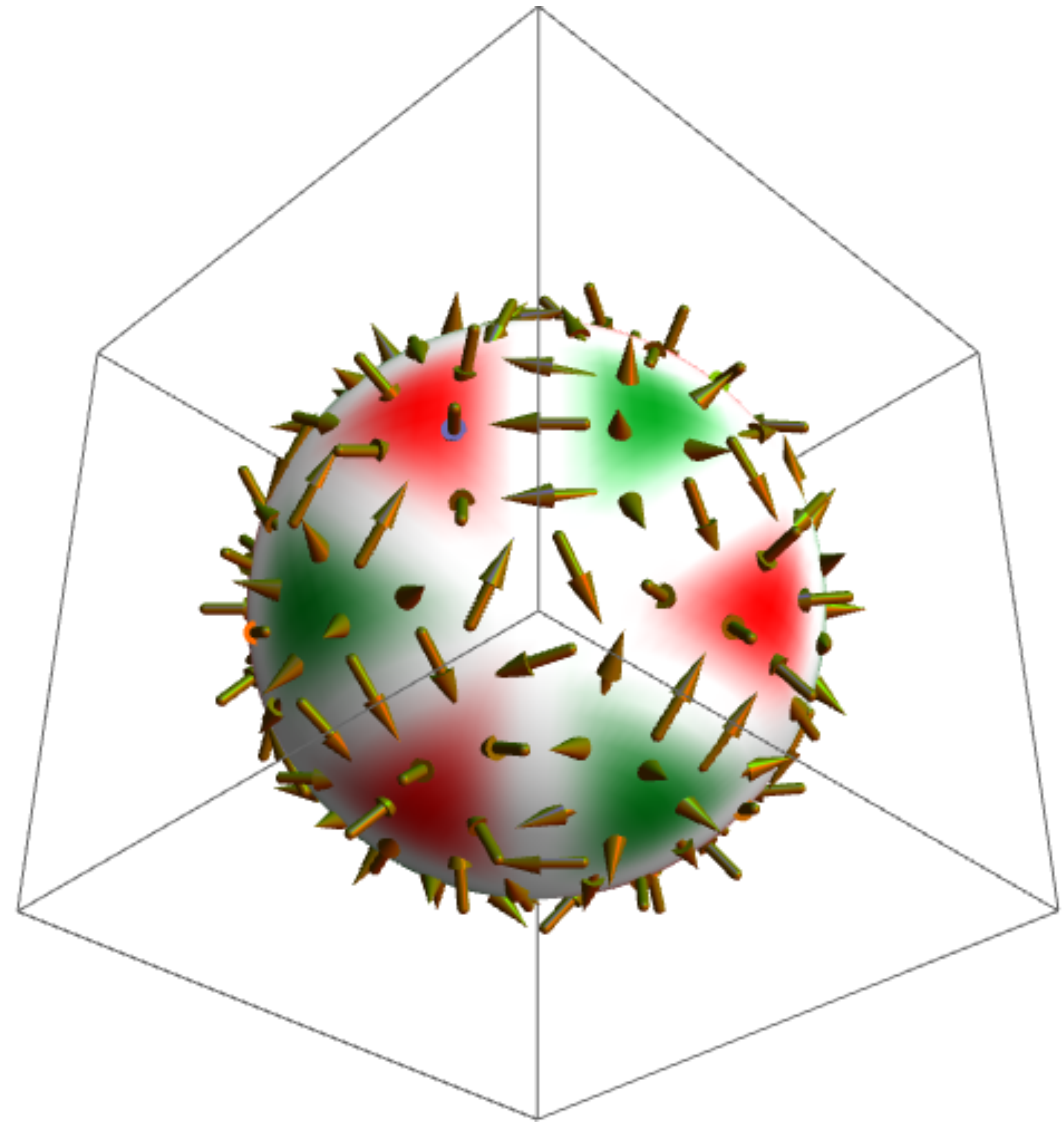
Hidden order: NpO_2

LDA+*U*:

- **3k** lowest
- insulator
- no moment







local magnetization at one of four sites

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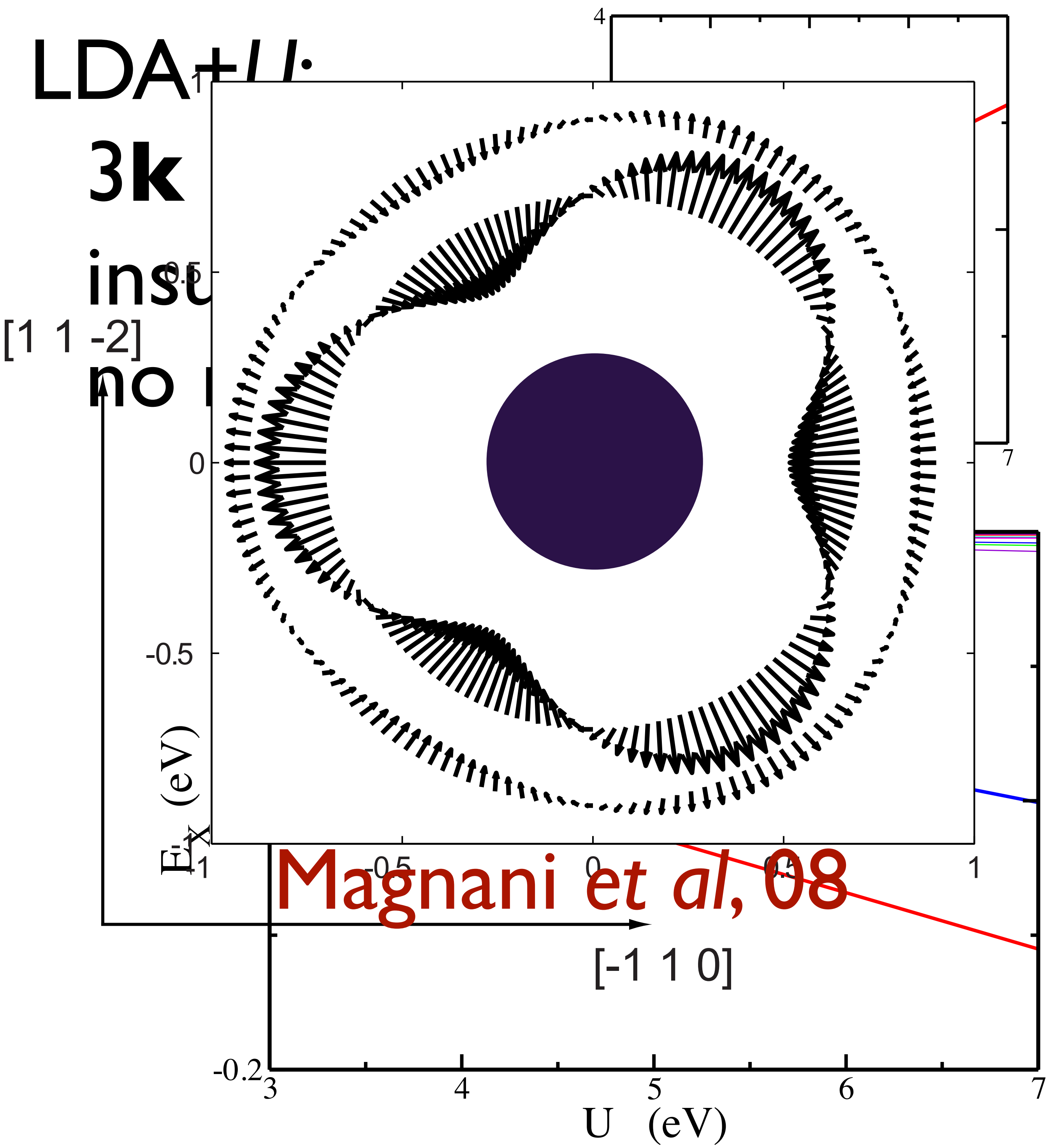
Hidden order: NpO_2

LDA+*U*:

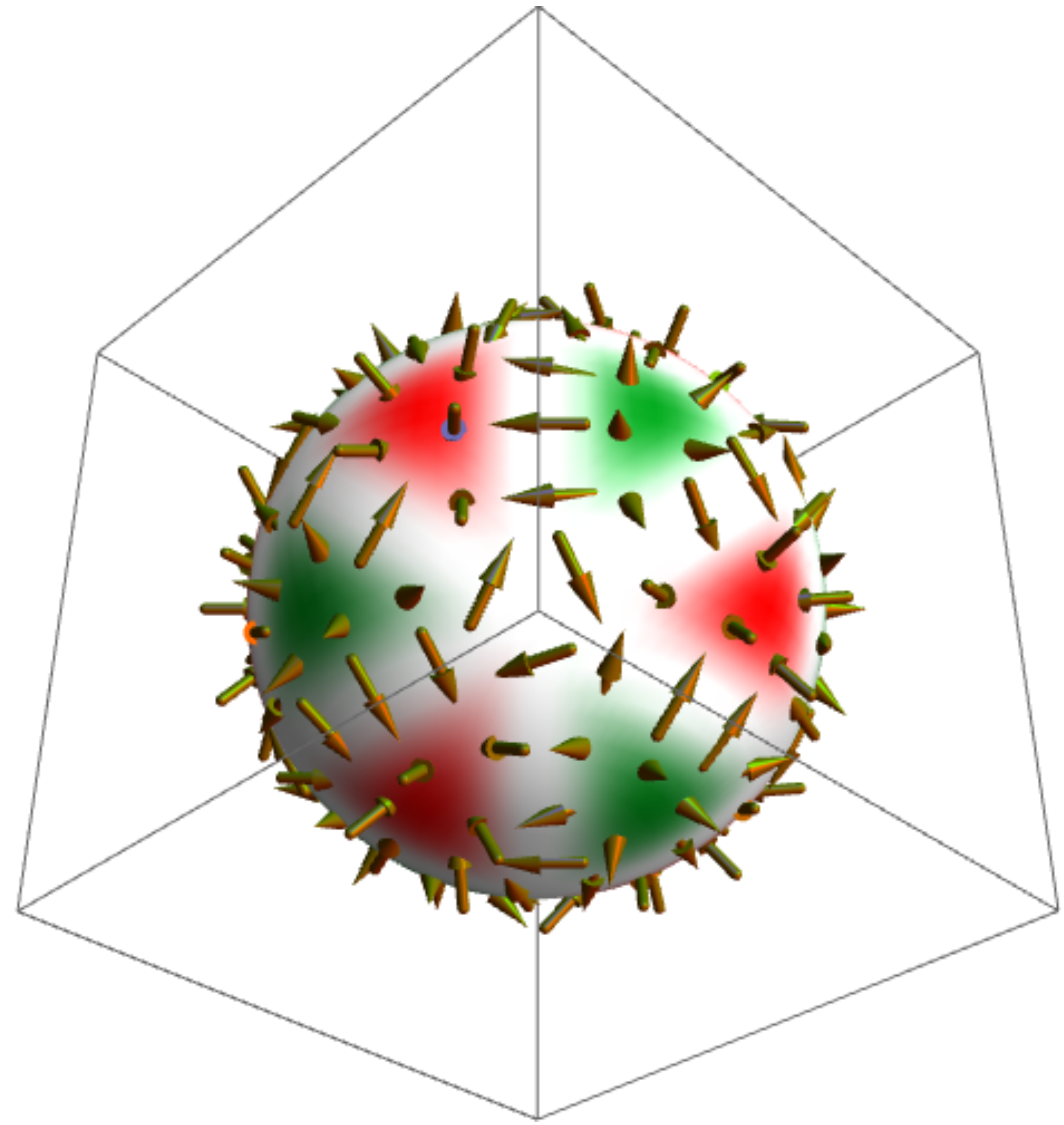
3k

insu

no

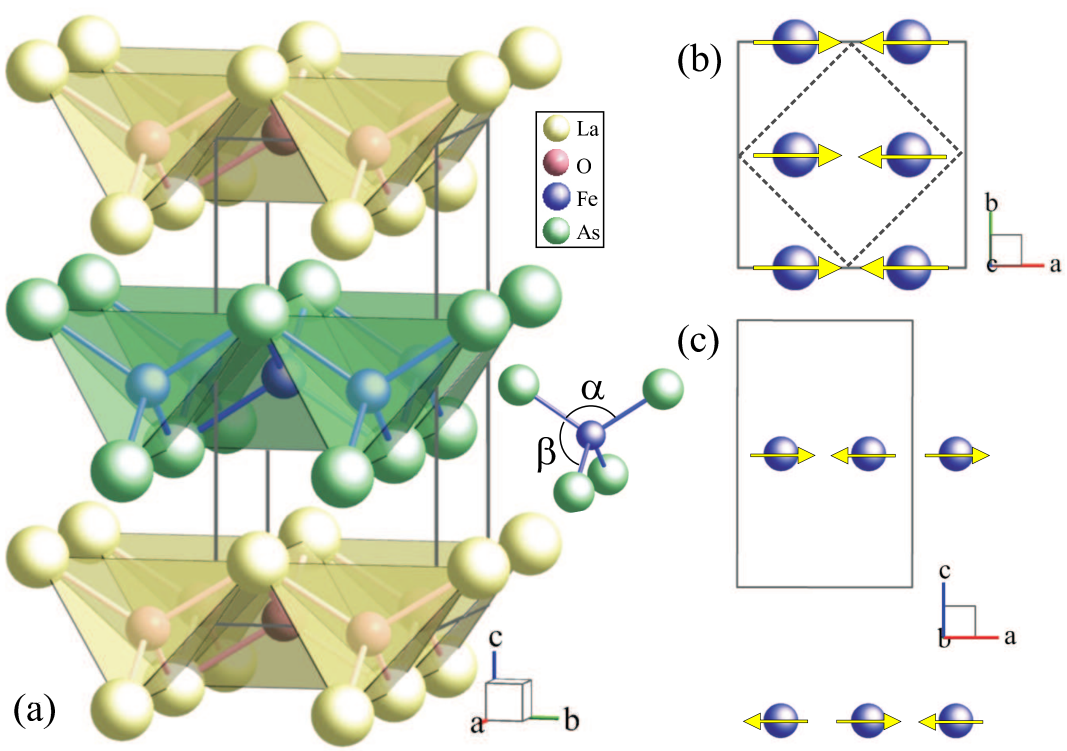


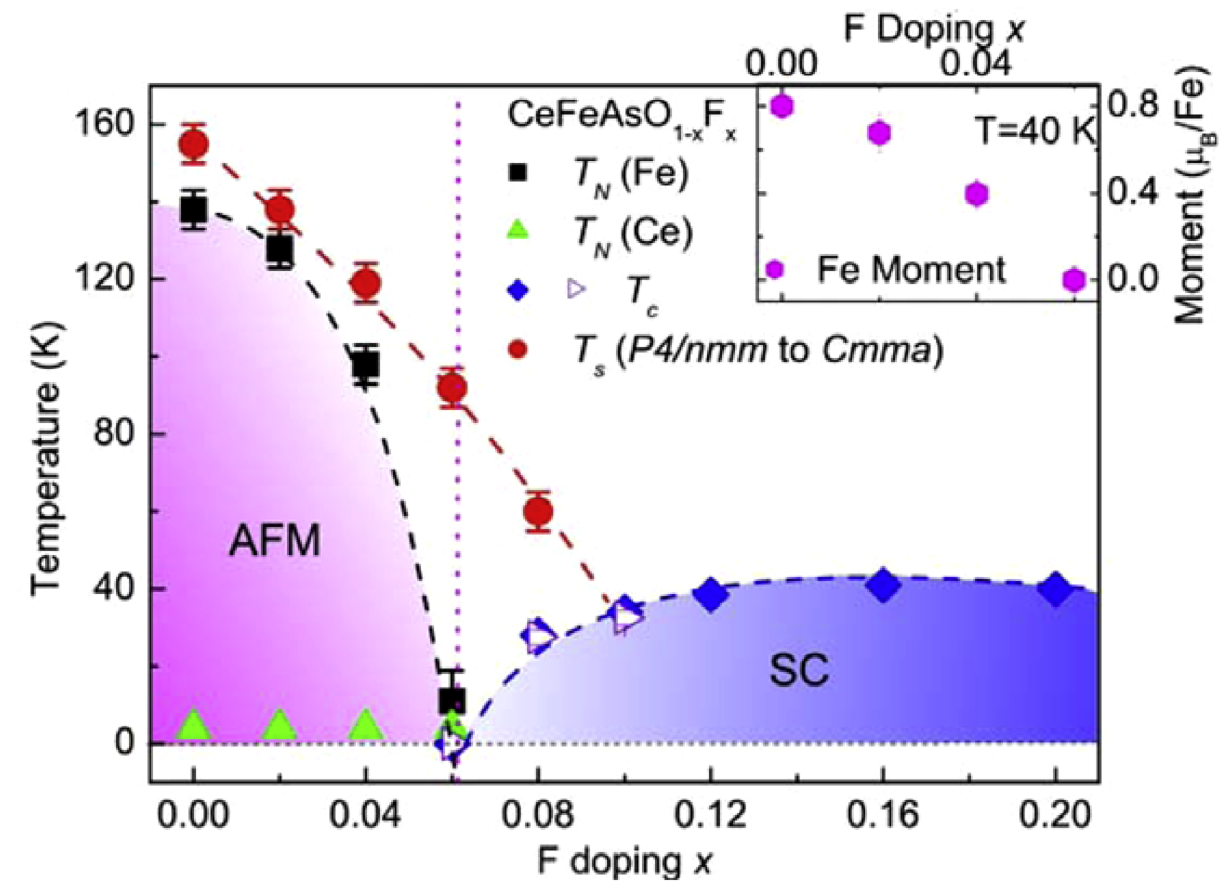
Magnani *et al*, 08



local magnetization at one of four sites

Fe-pnictides

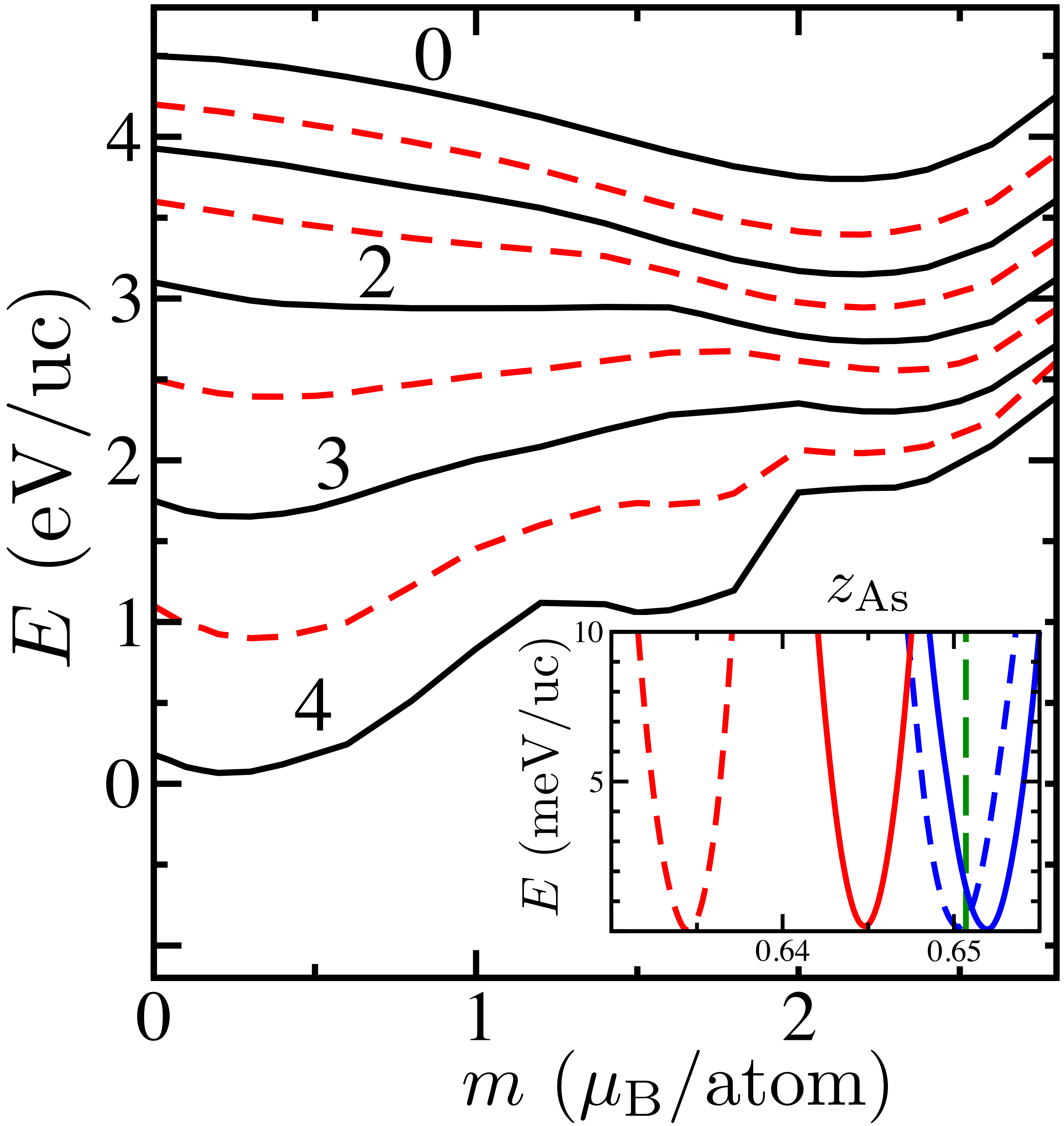




- FeAs layers
- SC under doping – up to 60 K …
- AF in parent compounds
- Correlated electrons?
  - Not understood: Small moments & FeAs bonds

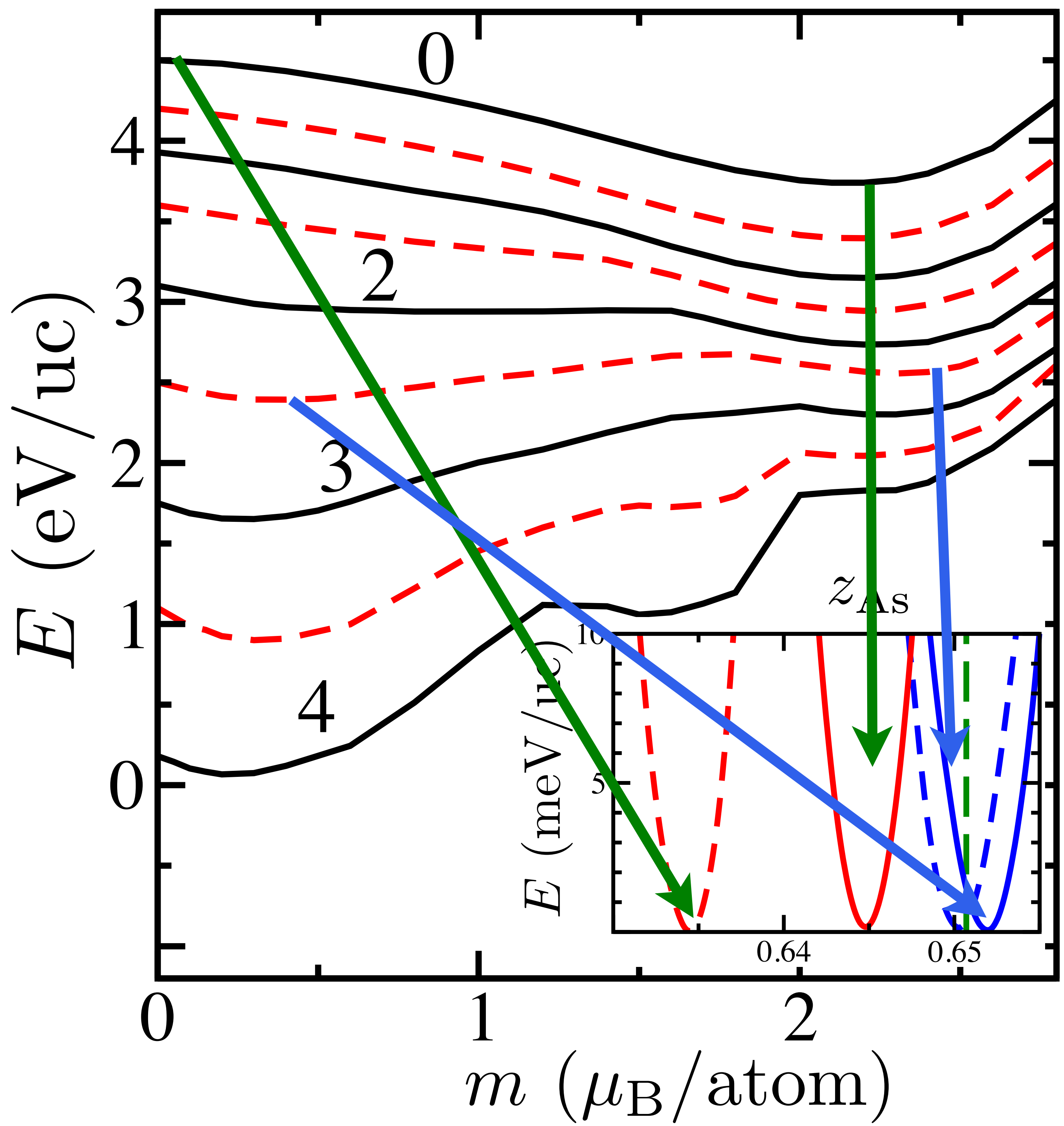
Small moments

DFT+*U*

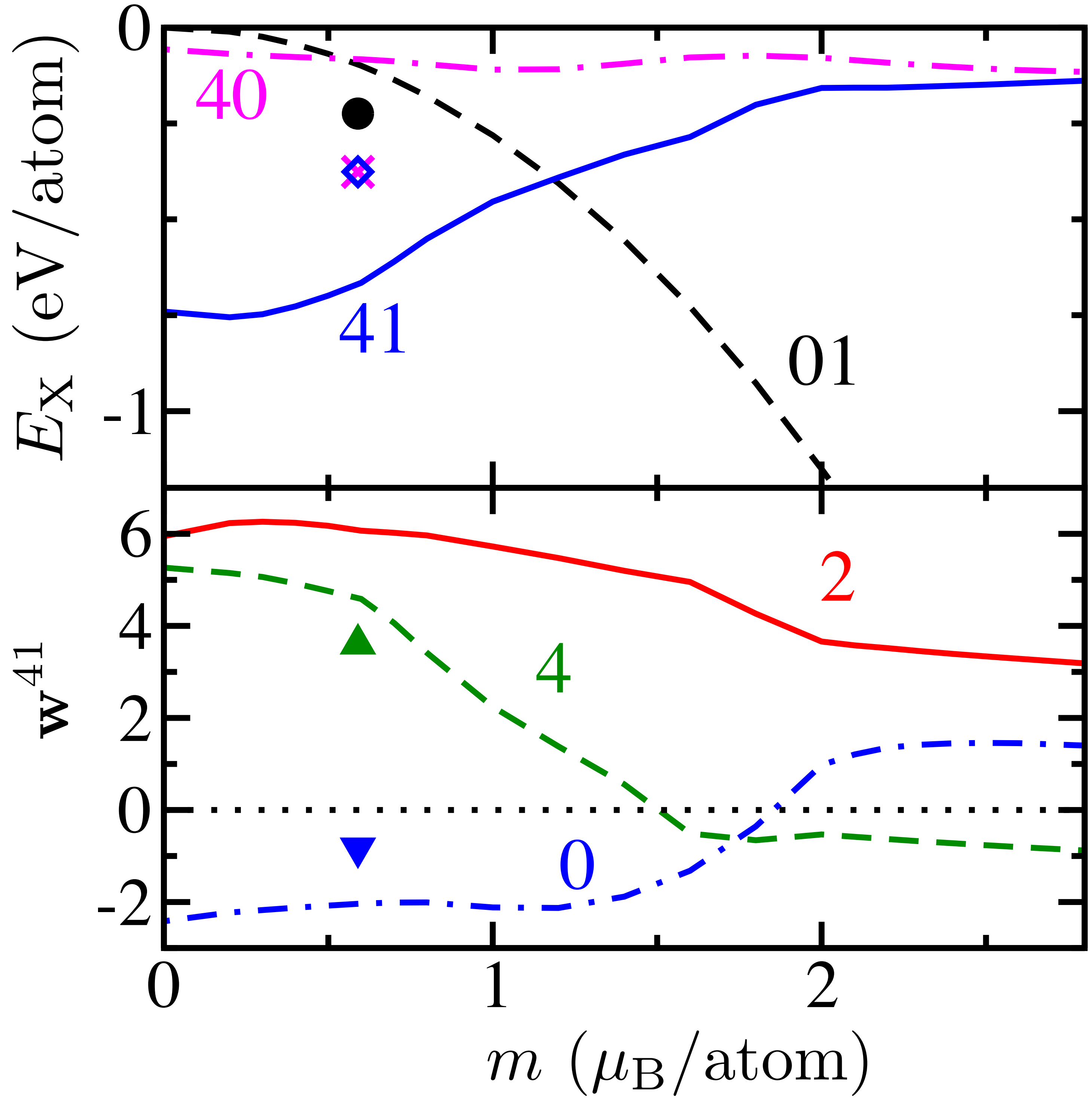


Small moments

DFT+U



Tensor moments



Contribution to DM

$$\Gamma^{41}_{20} = \begin{pmatrix} 2\sqrt{5} & 0 & 0 & 0 & 0 \\ 0 & -2\sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{15} \\ 0 & 0 & 0 & \sqrt{15} & 0 \end{pmatrix} \otimes \sigma_z$$

$$xz \quad zy \quad xy \quad x^2 - y^2 \quad z^2$$

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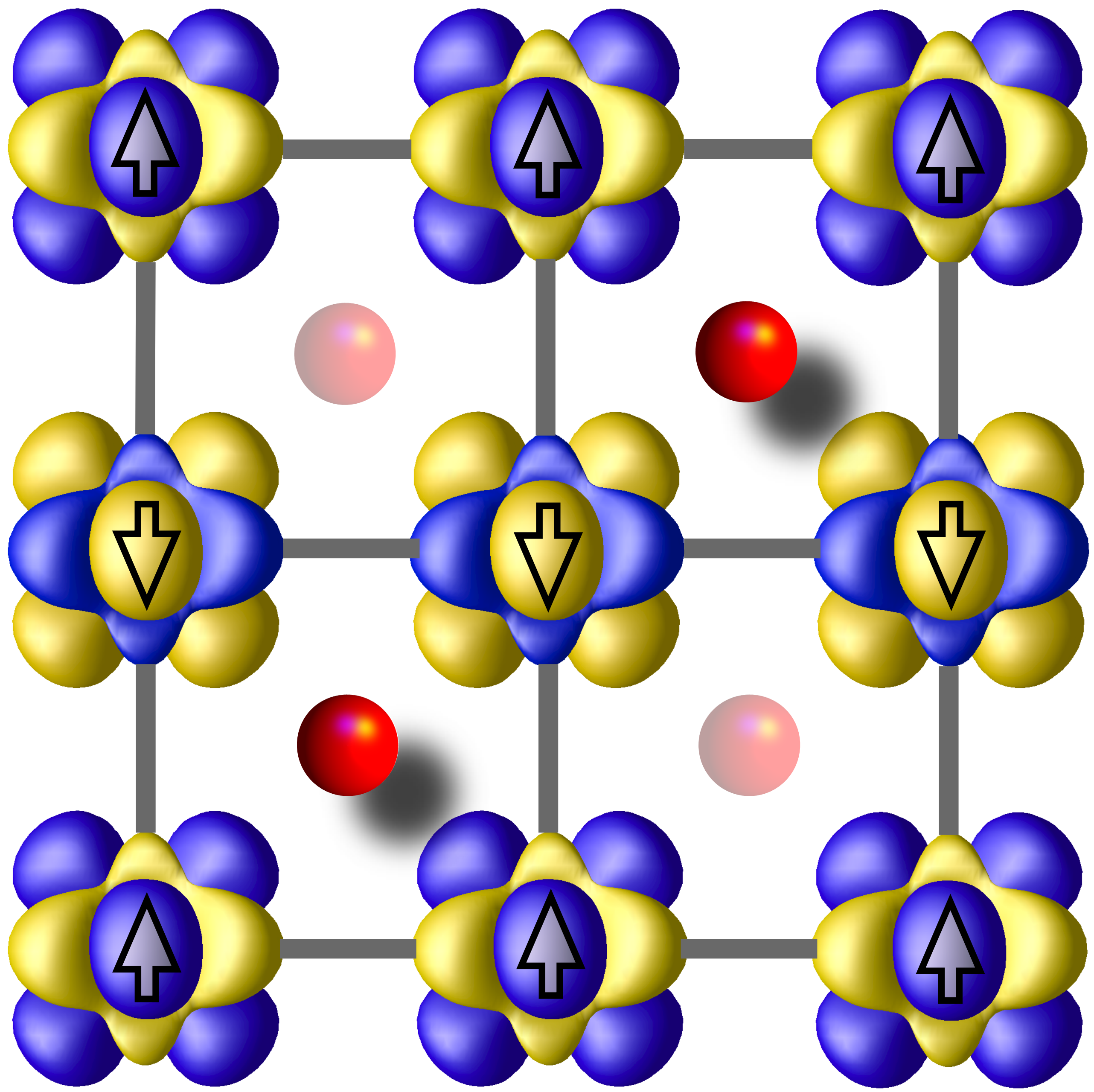
Magnetization density



Cricchio *et al.* PRB **81**, 140403(R) (10)

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Summary

- Brief description of DFT+*U*
- Reformulated (scr) exchange – tensor moments
- Unexpected exchange channels dominate
- Hidden order in URu_2Si_2 & NpO_2 – triakontadipole
  - Katt's rules to substitute Hund's in actinides
- Multipoles play a role in undoped FeAs
  - Small moments
  - FeAs bonding distance

Epilogue

- What about Kondo and Mott and these guys ...?
  - Dynamic effects are important
  - Our static MF approach overestimates the effect

- BUT
  - The energies involved are large
  - Agreement with experiments is compelling
    - Reduced spin moments & Hidden order etc

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THE SWEDISH RESEARCH COUNCIL
The Swedish Research Council

Collaborators

Francesco Cricchio
Oscar Grånäs
Fredrik Bultmark