Multipurpose Electronic Structure Database for Correlated Systems

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Collaborators

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Calculated Electronic Properties of Metals

by

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J. F. Janak
A. R. Williams

PERGAMON

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Electronic structure database

http://gurka.fysik.uu.se/ESP/

http://gurka.fysik.uu.se/ESP/

wiki saob eniro seb SAS News (168) work sj ul stockholm ord torrent LK musik SSH

ESP					
Version	Complete list				
A word of causion	Search	Element	Methods	FAQ	Contact

Element: H (Z=1)
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Antal element: 1
Sök!

http://gurka.fysik.uu.se/ESP/

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Computational Materials Science 44, 1042 (2009)

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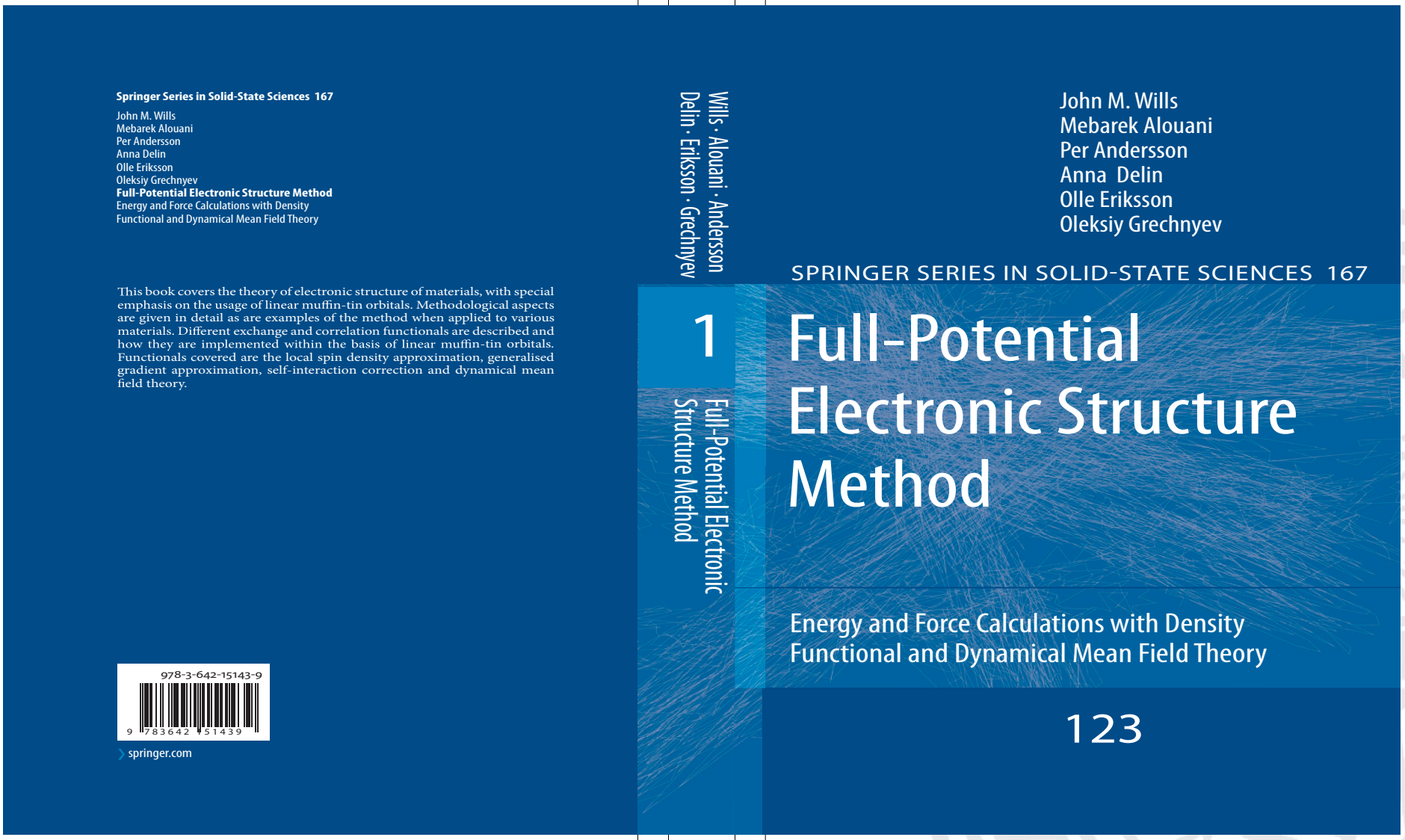
FP-LMTO



	WIEN2k-new	FLEUR	RSPt	FPLO_TplusF_soft	FPLO_TplusF	FPLO_default	Abinit_JTH2	Abinit_JTH	Abinit_delta40	GPAW09	GPAW06	QE31	VASPGW	VASP53hard	VASP52	VASP	CASTEP8	CASTEP7	CASTEP-MS	CASTEP-USP	OpenMX	DACAPO	Abinit_FHI
WIEN2k-new	0.0	0.8	0.8	0.9	1.0	3.9	0.6	1.2	1.3	1.5	3.8	1.8	0.8	0.7	1.0	2.1	0.5	2.4	3.4	7.7	2.0	6.2	14.5
FLEUR	0.8	0.0	0.7	0.9	0.9	3.5	0.7	0.8	1.5	1.7	3.4	1.6	1.2	0.9	1.3	1.8	1.0	2.8	3.7	7.8	1.7	6.5	13.8
RSPt	0.8	0.7	0.0	0.9	0.7	3.2	0.7	0.9	1.5	1.7	3.4	1.6	1.2	1.0	1.3	1.9	1.1	3.0	3.9	7.9	1.8	6.5	14.0
FPLO_TplusF_sof	0.9	0.9	0.9	0.0	0.8	3.6	0.9	1.2	1.7	1.9	3.5	1.6	1.3	1.2	1.4	1.9	1.1	2.9	3.7	7.7	1.8	6.4	13.9
FPLO_TplusF	1.0	0.9	0.7	0.8	0.0	3.1	0.9	1.0	1.8	2.0	3.4	1.6	1.3	1.1	1.5	1.9	1.2	3.1	3.9	7.9	1.8	6.4	14.6
FPLO_default	3.9	3.5	3.2	3.6	3.1	0.0	3.6	3.4	4.1	4.2	3.1	3.3	4.0	3.9	4.0	2.8	4.0	5.8	6.2	8.9	3.2	7.2	13.6
Abinit_JTH2	0.6	0.7	0.7	0.9	0.9	3.6	0.0	0.9	1.4	1.6	3.5	1.6	1.0	0.7	1.0	1.9	0.7	2.6	3.6	7.6	1.9	6.2	14.2
Abinit_JTH	1.2	0.8	0.9	1.2	1.0	3.4	0.9	0.0	1.5	1.8	3.2	1.6	1.6	1.4	1.6	1.9	1.3	3.0	3.8	7.9	1.5	6.5	13.4
Abinit_delta40	1.3	1.5	1.5	1.7	1.8	4.1	1.4	1.5	0.0	0.7	3.6	2.2	1.6	1.4	1.7	2.4	1.4	2.5	3.5	7.9	2.3	6.0	14.2
GPAW09	1.5	1.7	1.7	1.9	2.0	4.2	1.6	1.8	0.7	0.0	3.6	2.3	1.9	1.7	1.9	2.5	1.6	2.8	3.7	8.0	2.5	6.4	14.3
GPAW06	3.8	3.4	3.4	3.5	3.4	3.1	3.5	3.2	3.6	3.6	0.0	2.9	4.0	3.7	3.9	2.8	3.8	5.6	5.6	8.6	3.0	7.6	13.0
QE31	1.8	1.6	1.6	1.6	1.6	3.3	1.6	1.6	2.2	2.3	2.9	0.0	1.9	1.8	1.9	1.5	1.7	3.3	3.7	7.4	1.8	5.9	14.1
VASPGW	0.8	1.2	1.2	1.3	1.3	4.0	1.0	1.6	1.6	1.9	4.0	1.9	0.0	0.8	1.2	2.1	0.8	2.6	3.6	8.1	2.2	6.1	15.1
VASP53hard	0.7	0.9	1.0	1.2	1.1	3.9	0.7	1.4	1.4	1.7	3.7	1.8	0.8	0.0	0.5	1.8	0.8	2.6	3.5	7.8	2.1	6.3	14.5
VASP52	1.0	1.3	1.3	1.4	1.5	4.0	1.0	1.6	1.7	1.9	3.9	1.9	1.2	0.5	0.0	1.7	1.0	2.8	3.8	8.0	2.3	6.8	14.5
VASP	2.1	1.8	1.9	1.9	1.9	2.8	1.9	1.9	2.4	2.5	2.8	1.5	2.1	1.8	1.7	0.0	2.1	3.5	4.1	7.8	1.7	6.1	13.3
CASTEP8	0.5	1.0	1.1	1.1	1.2	4.0	0.7	1.3	1.4	1.6	3.8	1.7	0.8	0.8	1.0	2.1	0.0	2.2	3.2	7.6	2.0	5.6	14.7
CASTEP7	2.4	2.8	3.0	2.9	3.1	5.8	2.6	3.0	2.5	2.8	5.6	3.3	2.6	2.6	2.8	3.5	2.2	0.0	2.3	6.8	3.4	5.7	14.8
CASTEP-MS	3.4	3.7	3.9	3.7	3.9	6.2	3.6	3.8	3.5	3.7	5.6	3.7	3.6	3.5	3.8	4.1	3.2	2.3	0.0	7.6	3.9	6.0	14.3
CASTEP-USP	7.7	7.8	7.9	7.7	7.9	8.9	7.6	7.9	7.9	8.0	8.6	7.4	8.1	7.8	8.0	7.8	7.6	6.8	7.6	0.0	8.2	11.0	13.5
OpenMX	2.0	1.7	1.8	1.8	1.8	3.2	1.9	1.5	2.3	2.5	3.0	1.8	2.2	2.1	2.3	1.7	2.0	3.4	3.9	8.2	0.0	6.4	13.6
DACAPO	6.2	6.5	6.5	6.4	6.4	7.2	6.2	6.5	6.0	6.4	7.6	5.9	6.1	6.3	6.8	6.1	5.6	5.7	6.0	11.0	6.4	0.0	18.4
Abinit_FHI	14.5	13.8	14.0	13.9	14.6	13.6	14.2	13.4	14.2	14.3	13.0	14.1	15.1	14.5	14.5	13.3	14.7	14.8	14.3	13.5	13.6	18.4	0.0

Delta values between codes and potential sets, subdivided according to all-electron (yellow), PAW

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People we have to ‘beat’

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New 2D materials

Search criteria: Only high-symmetry compounds are considered that yield square or hexagonal in-plane structures, packing ratios in the range 0.15–0.50 are selected, large gaps (> 2.4 Å) between crystallographic planes along the c axis. Electronic structures of all 92 compounds provided. Examples: Graphene, BN, TM-halides, TM-disulphides/selenides/telurides, Bi2Te3 and other TI systems, ...Cu_2S.....

PRX **3**, 031002 (2013)

Possible high temperature superconductors

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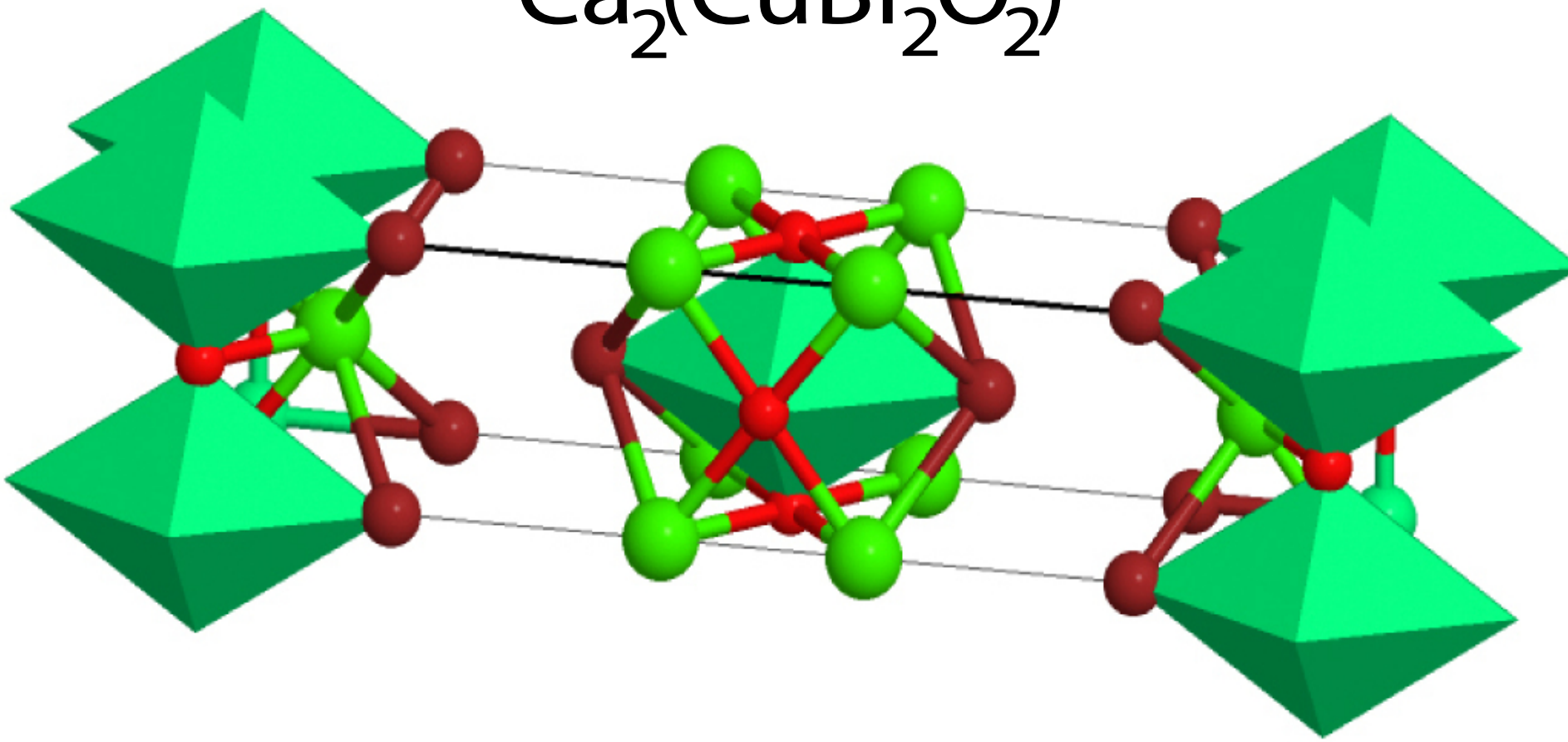
Data-mining criterion-structure

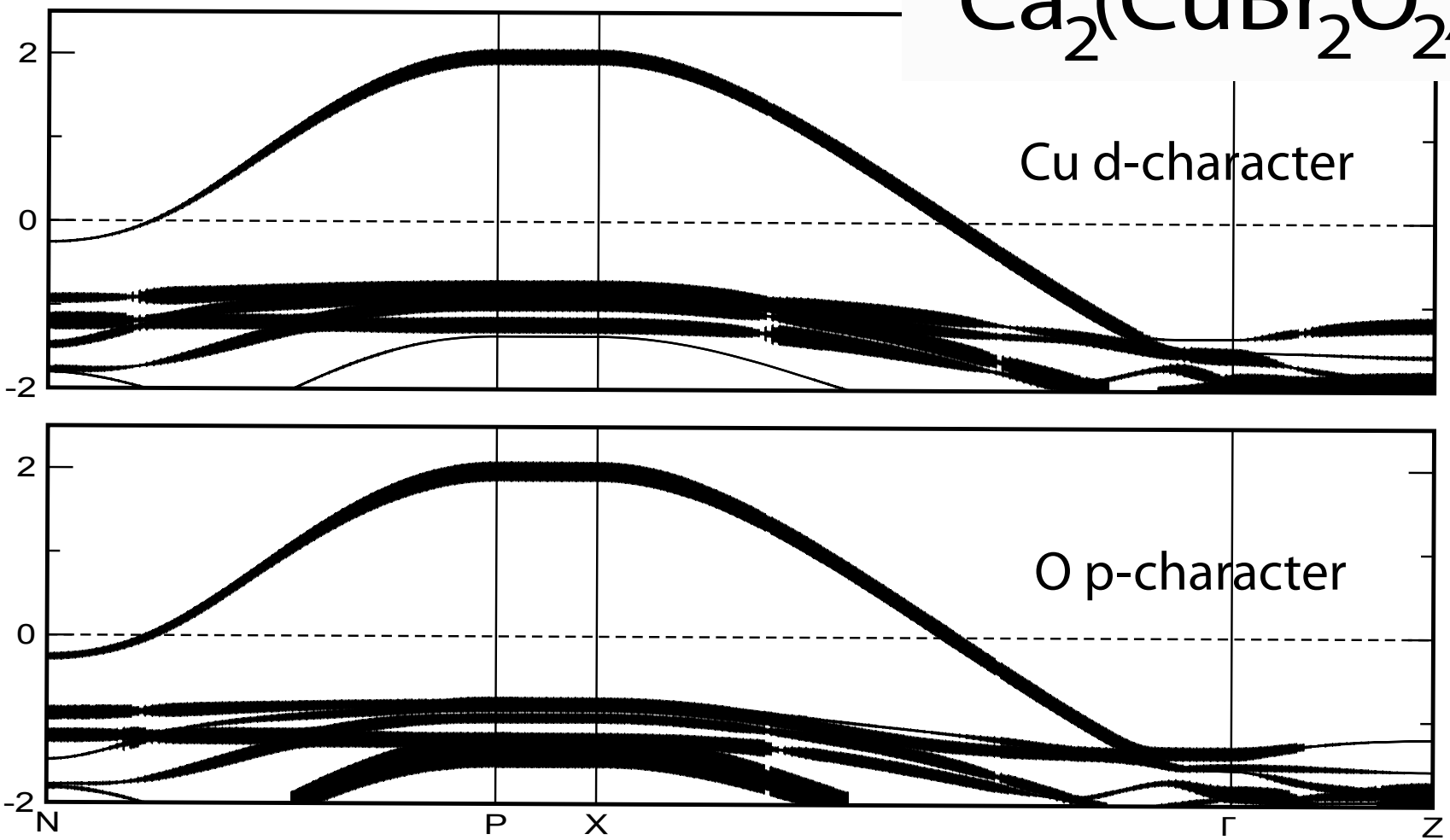
$Ca_2(CuBr_2O_2)$



Computational Materials Science 67 282 (2013)

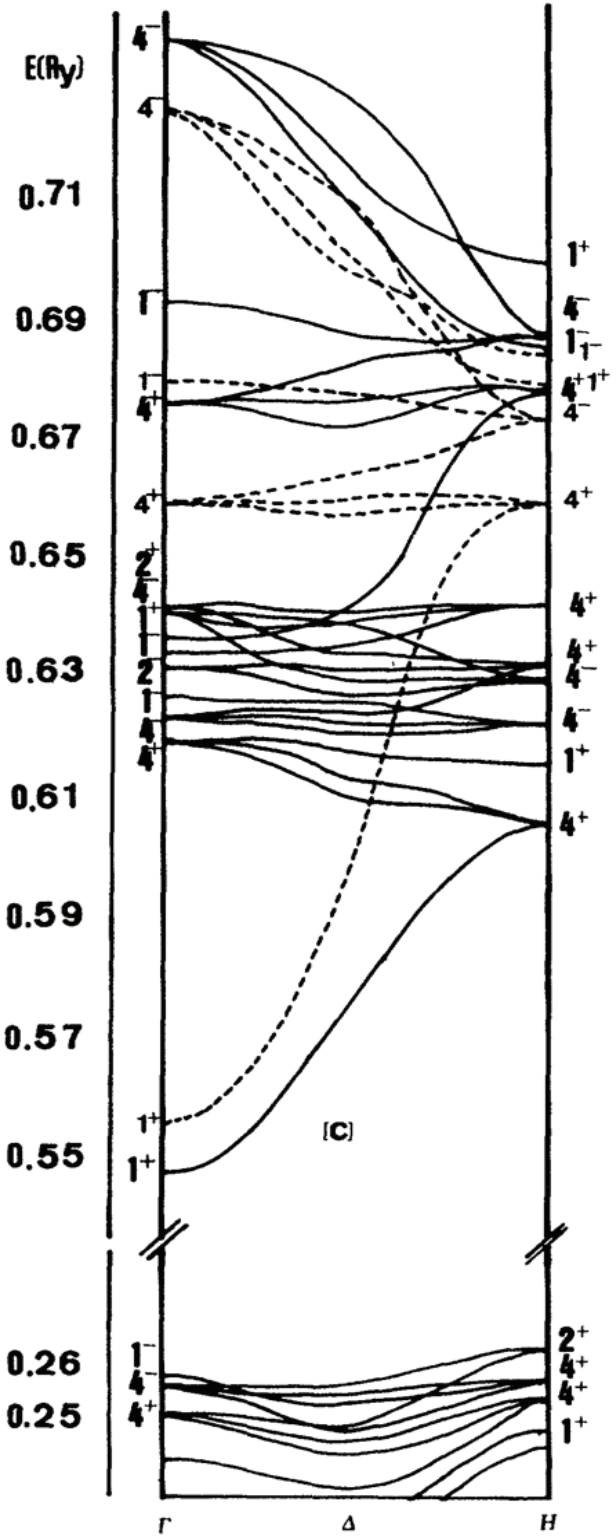
Data-mining criterion-bands/bonds

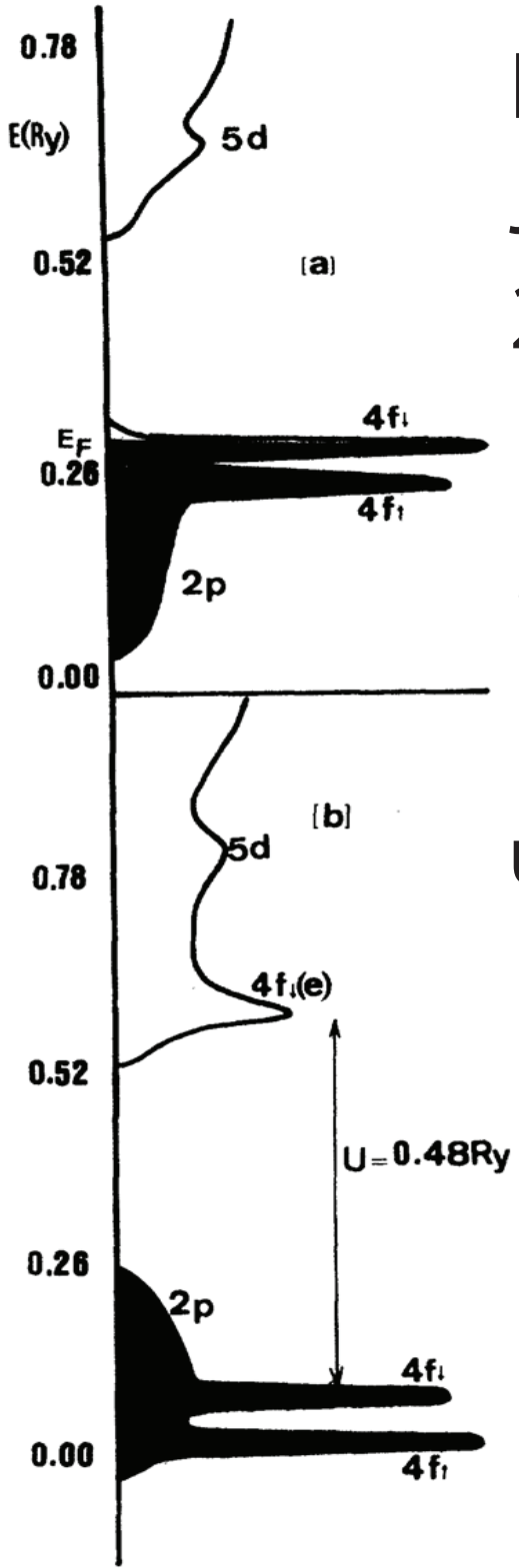
$Ca_2(CuBr_2O_2)$



Computational Materials Science 67 282 (2013)

Correlation effects





F. Lopez-Aguilar and J. Costa-Quintana, PRB 29, 5986 (1984).

$$U(r) = U \sum (1/2 - \langle n_\nu \rangle) |\beta_\nu\rangle\langle\beta_\nu|$$

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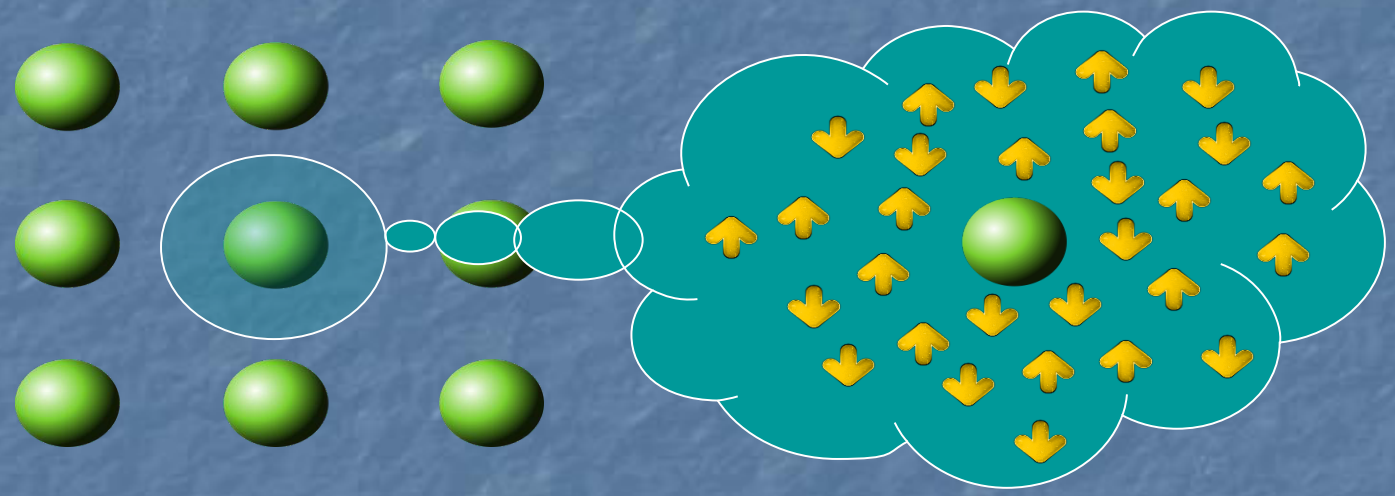
Dynamical mean field theory

$$H = H_{LDA} + \sum_R \sum_{\xi_1\xi_2\xi_3\xi_4} U_{\xi_1\xi_2\xi_3\xi_4} c^\dagger_{R\xi_1} c^\dagger_{R\xi_2} c_{R\xi_3} c_{R\xi_4}$$

The Hubbard model is mapped into an Anderson Impurity Model



FICTITIOUS SYSTEM REPRODUCING THE DYNAMICS

The mapping is made with the condition of preserving the local Green's function and is exact in the limit of infinite nearest neighbors

Exact Diagonalization Solver

The finite size problem can be solved exactly with a direct construction of all the accessible many-body states.

N=5 electrons in K=10 orbitals:

$$
\begin{aligned}
|\Psi_1^5\rangle &= |1111100000\rangle, \\
|\Psi_2^5\rangle &= |1111010000\rangle, \\
&\vdots \\
|\Psi_M^5\rangle &= |0000011111\rangle.
\end{aligned}
$$

M corresponds to $\binom{K}{N}$

Too large for standard computational resources!

Block diagonalization $\longrightarrow$ up to 30 bath states!

Exact Diagonalization Solver

The finite size problem can be solved exactly with a direct construction of all the accessible many-body states.

N=5 electrons in K=10 orbitals:

Once the many-body states have been determined, the one-particle Green's function can be obtained through the Lehmann representation

$$G^{\mathrm{ED}}(i\omega)_{\xi_1\xi_2} = \frac{1}{Z}\sum_{\nu\mu}\frac{\langle\mu|\hat{c}_{\xi_1}|\nu\rangle\langle\nu|\hat{c}^{\dagger}_{\xi_1}|\mu\rangle}{i\omega + E_\mu - E_\nu}\left(e^{-\beta E_\mu} + e^{-\beta E_\nu}\right)$$

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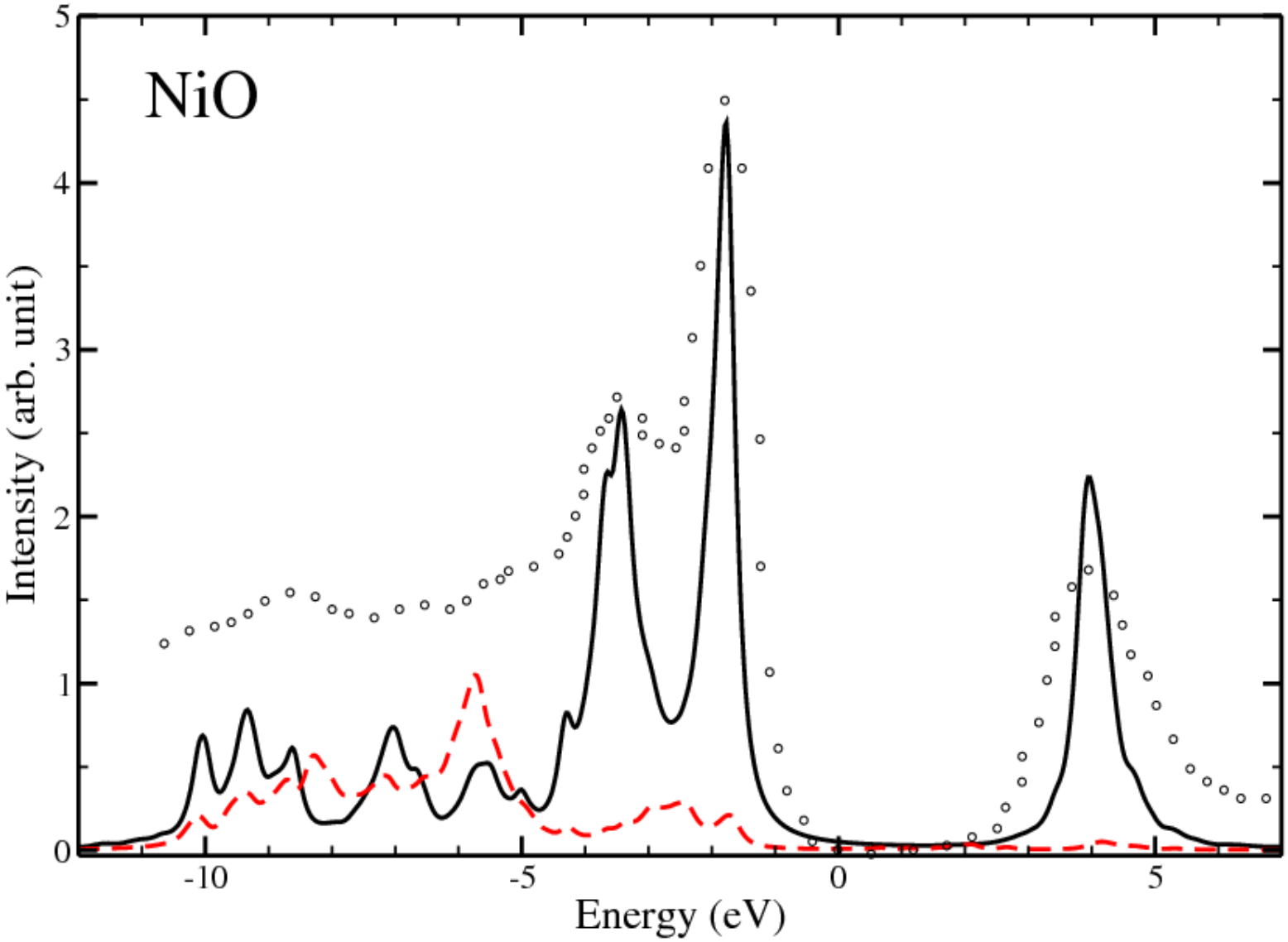
NiO – ED



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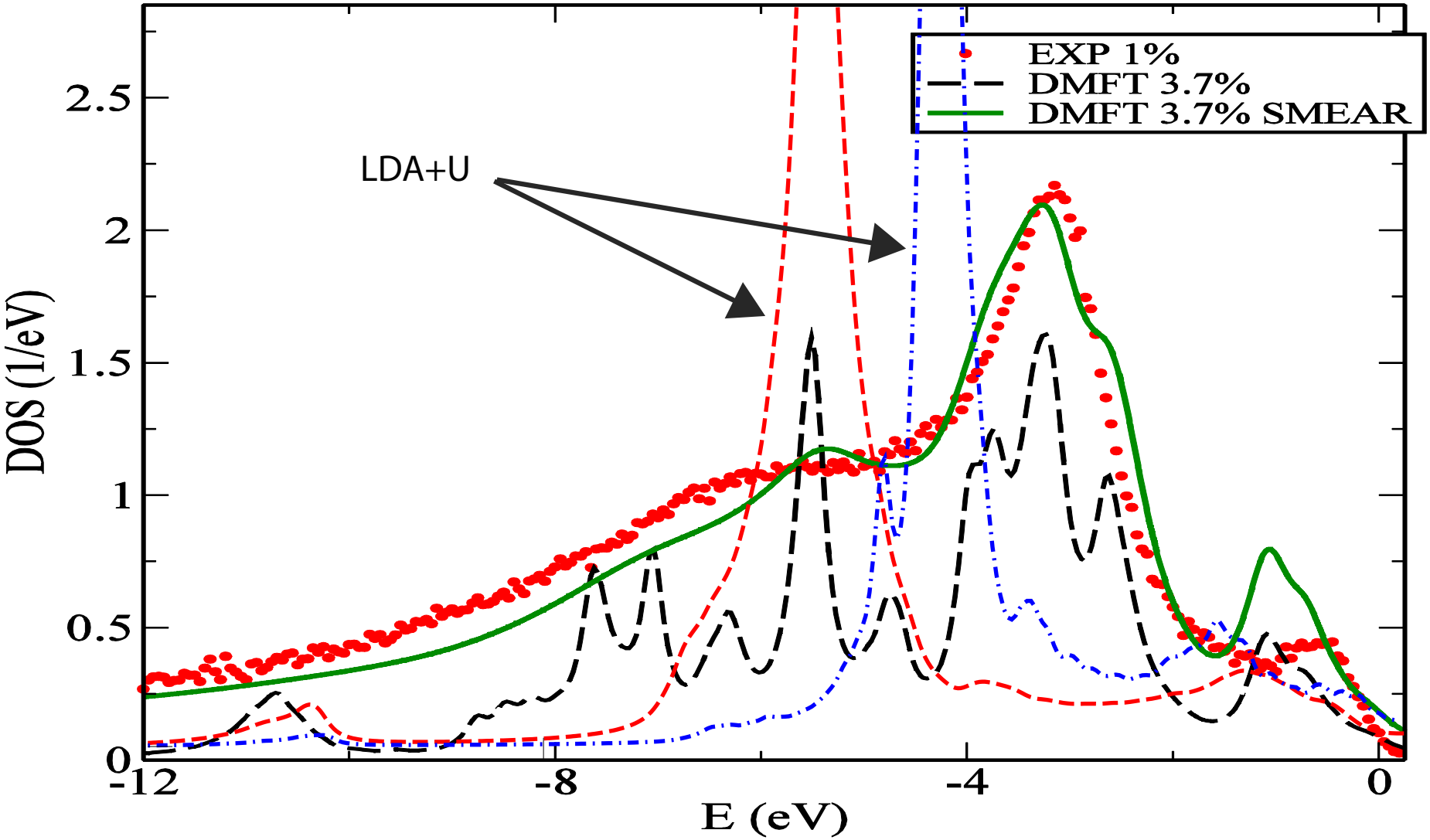
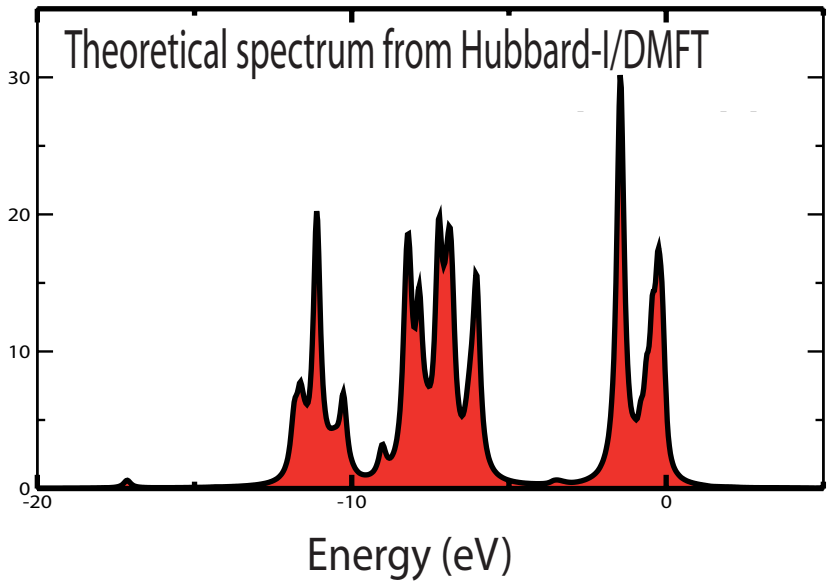
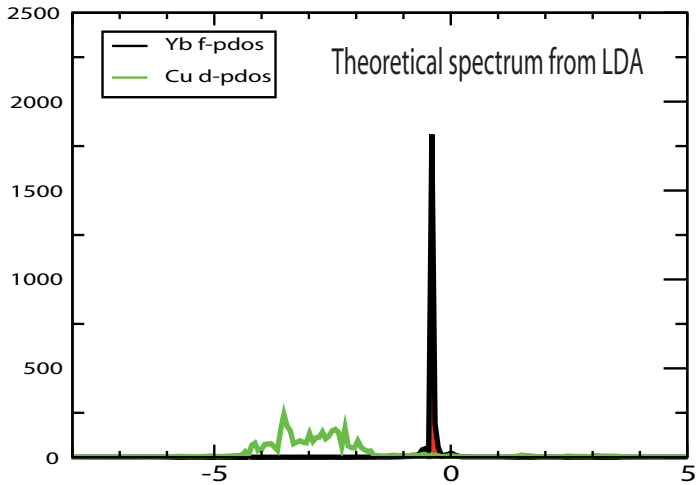
Valence band of Mn-doped GaAs

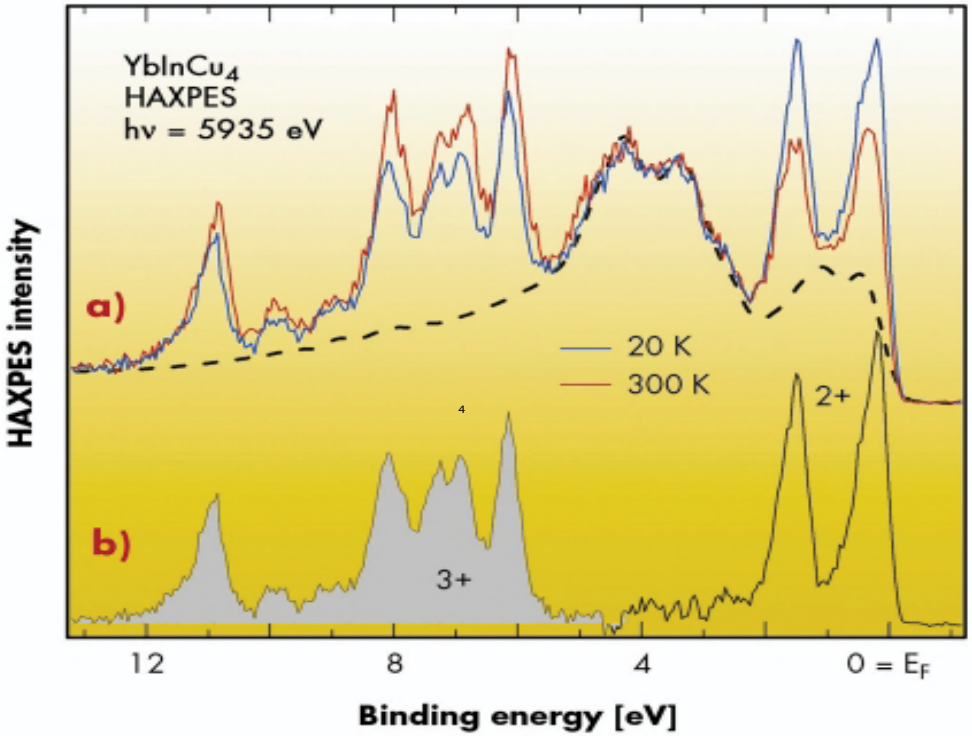


Electronic structure of mixed valent materials-$YbInCu_4$





Experimental XPS spectrum



PHYSICAL REVIEW B 79, 165104 (2009)

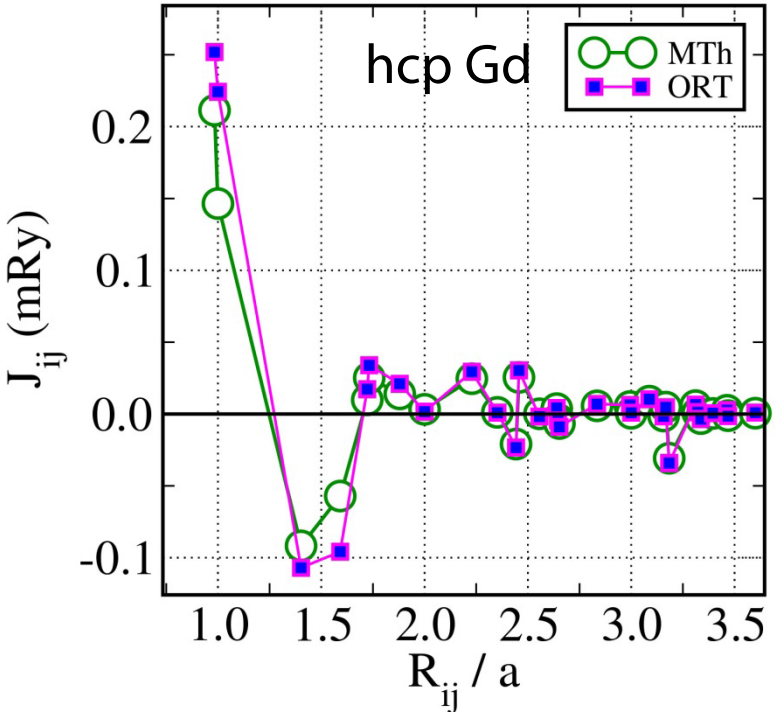
New correlated compounds

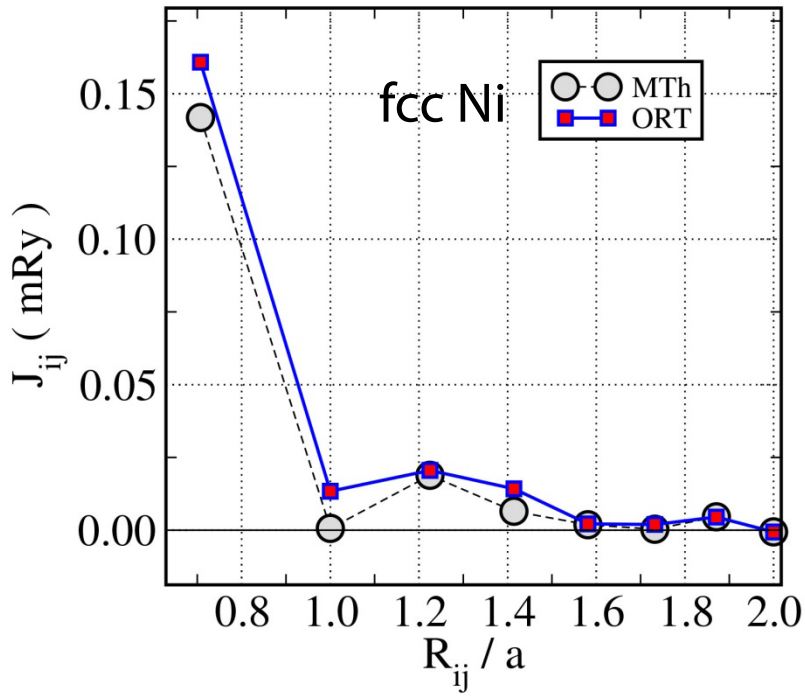
U >> W	4f shell of RE, 5f shell of Ac
U ~ W	URu2Si2, UPt3, ?
U << W	bcc Fe, fcc Ni, steel, alpha-U....

Heisenberg Hamiltonian

$$\mathcal{H}_{iex} = -\frac{1}{2}\sum_{i\neq j} J_{ij}\mathbf{m}_i \cdot \mathbf{m}_j$$

$$\bar{J}_{ij}^{Q,Q'} = \frac{1}{4\pi}\,\mathrm{Im}\int_C \mathrm{tr}_L\left[\delta_i^M(z)\,\bar{g}_{ij}^{Q,Q'\uparrow}(z)\,\delta_j^{Q'}(z)\,\bar{g}_{ji}^{Q',Q\downarrow}(z)\right]\mathrm{d}z\,.$$





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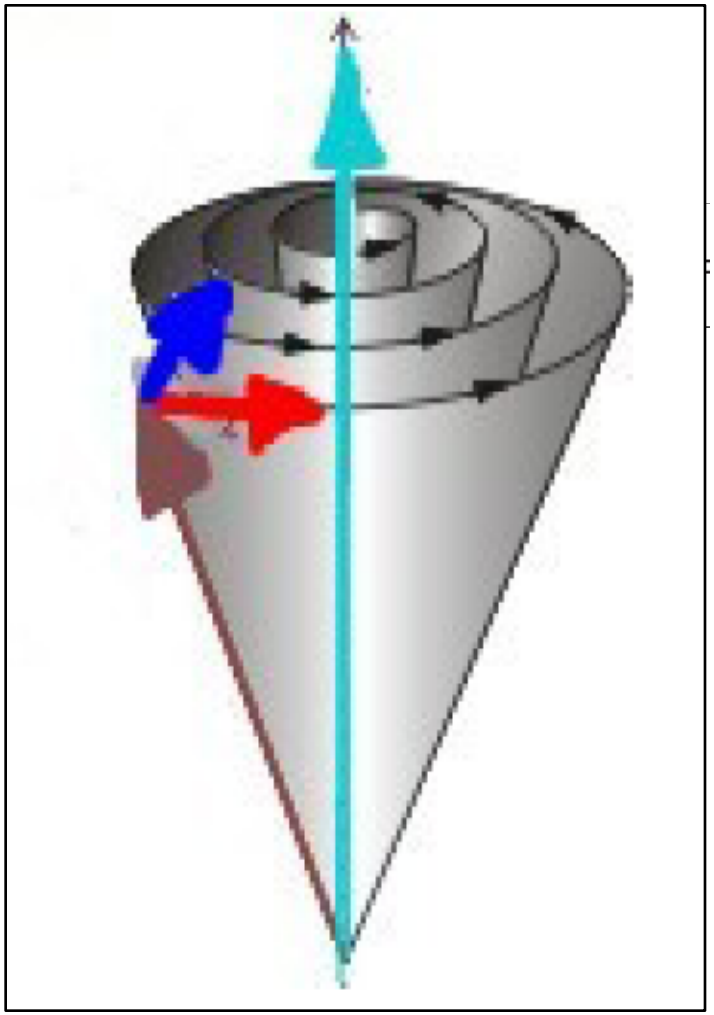
Atomistic Landau-Lifshitz equation



$$\frac{d\mathbf{m_i}}{dt} = -\gamma \mathbf{m_i} \times \mathbf{B_i} - \gamma \frac{\alpha}{m_i}[\mathbf{m_i} \times [\mathbf{m_i} \times \mathbf{B_i}]]$$

Precession Damping

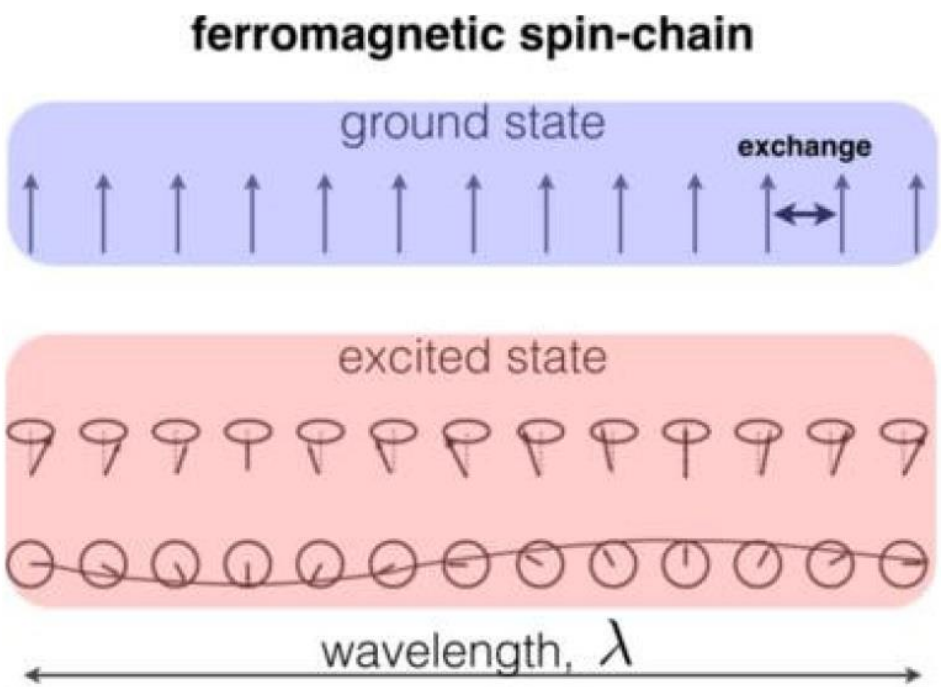
Energy dissipation

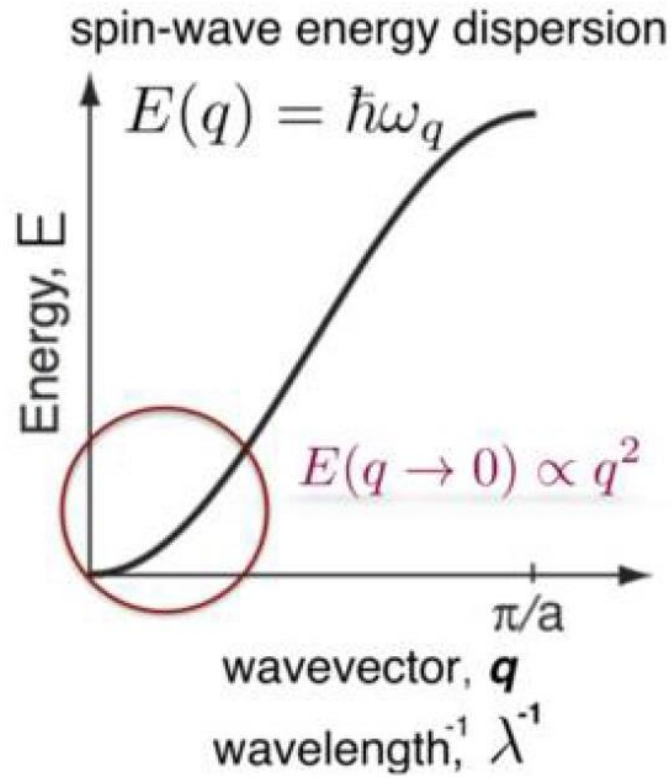
$$\frac{dE}{dt} = \frac{dE}{d\mathbf{m}} \cdot \frac{d\mathbf{m}}{dt} = \mathbf{B} \cdot \frac{d\mathbf{m}}{dt}$$

$$\mathbf{B} \cdot \frac{d\mathbf{m}}{dt} \propto 0 + \alpha$$

$$\frac{dE}{dt} \longleftrightarrow \alpha$$

Magnetic excitations





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Surface magnons

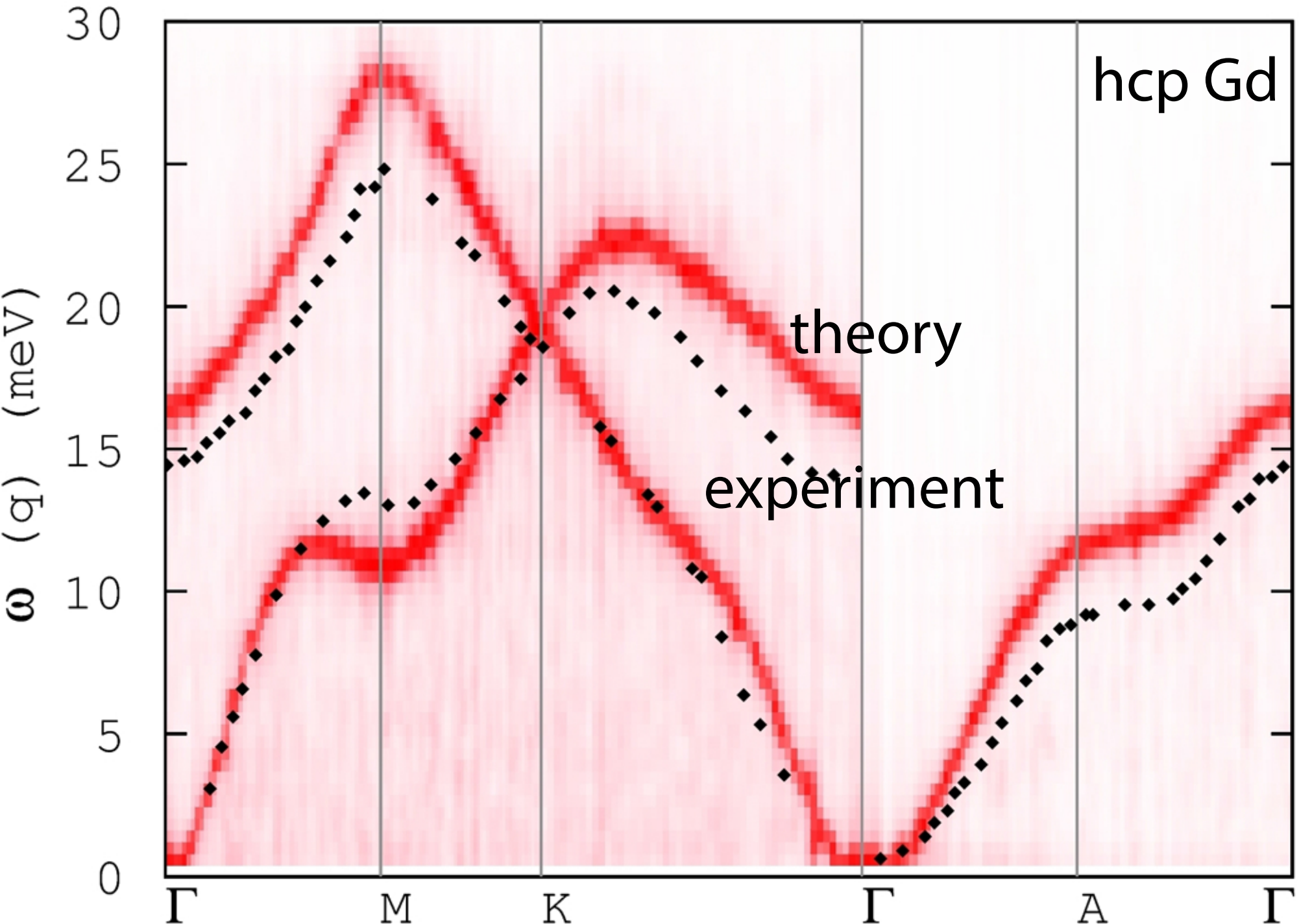
From the time-dependence of the atomic moments, calculate the spin-correlation function

$$C^k(\mathbf{r}-\mathbf{r'},t) =< m^k_{\mathbf{r}}(t)m^k_{\mathbf{r'}}(0) > - < m^k_{\mathbf{r}}(t) >< m^k_{\mathbf{r'}}(0) >,$$

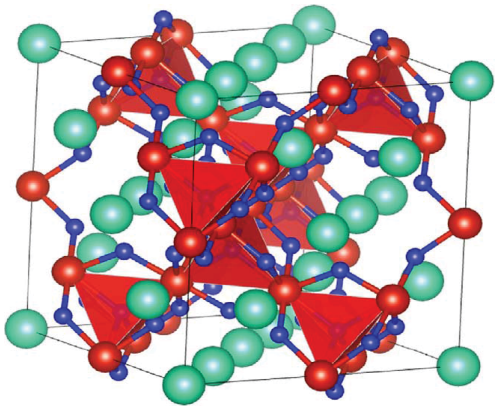
where k=x, y and z-component of atomic moment

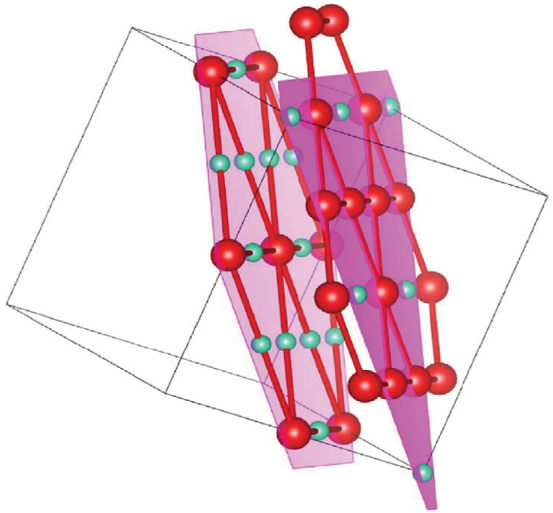
Spatial and temporal Fourier transform gives the dynamical structure factor

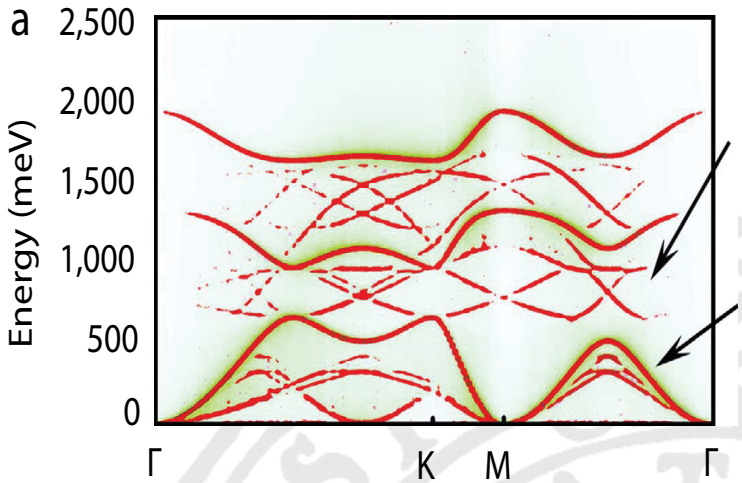
$$S^k(\mathbf{q},\omega) = \frac{1}{\sqrt{2\pi}N}\sum_{\mathbf{r},\mathbf{r'}} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r'})}\int_{-\infty}^{\infty} e^{i\omega t}C^k(\mathbf{r}-\mathbf{r'},t)dt$$

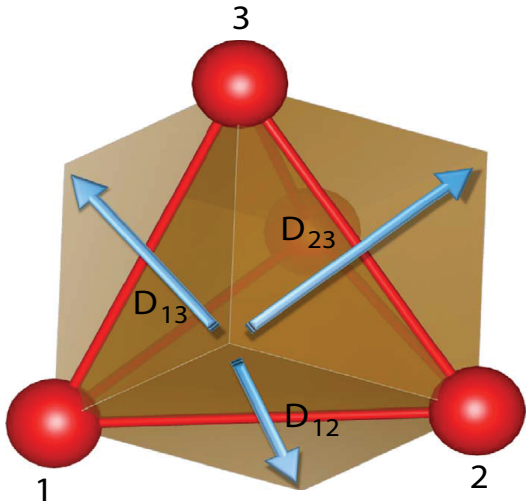

hcp Gd
theory
experiment
ω (q) (meV)
30
25
20
15
10
5
0
Γ
M
K
Γ
A
Γ

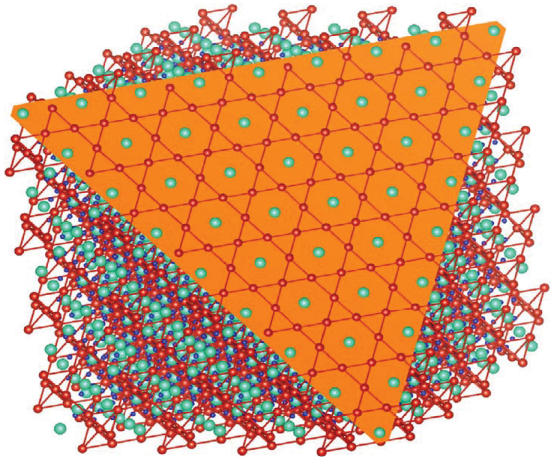
Topological excitations in the Kagome lattice











Lu V O

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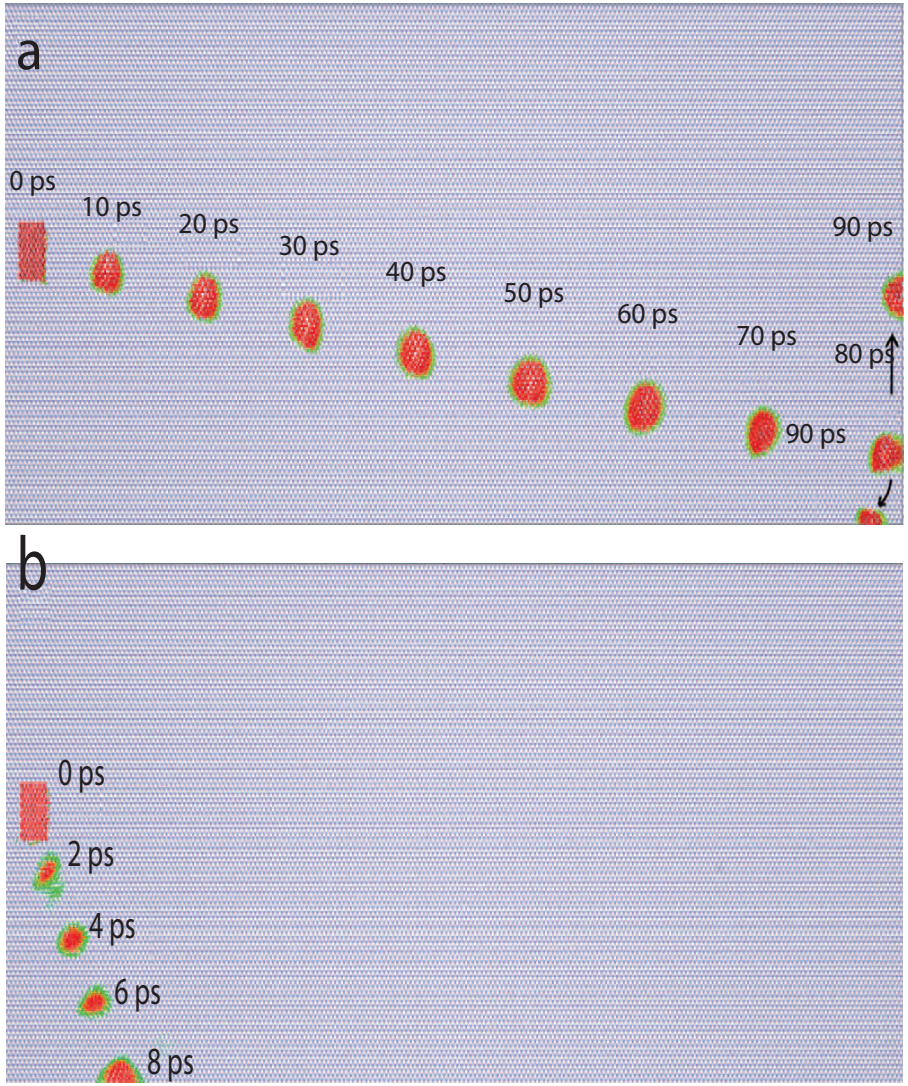
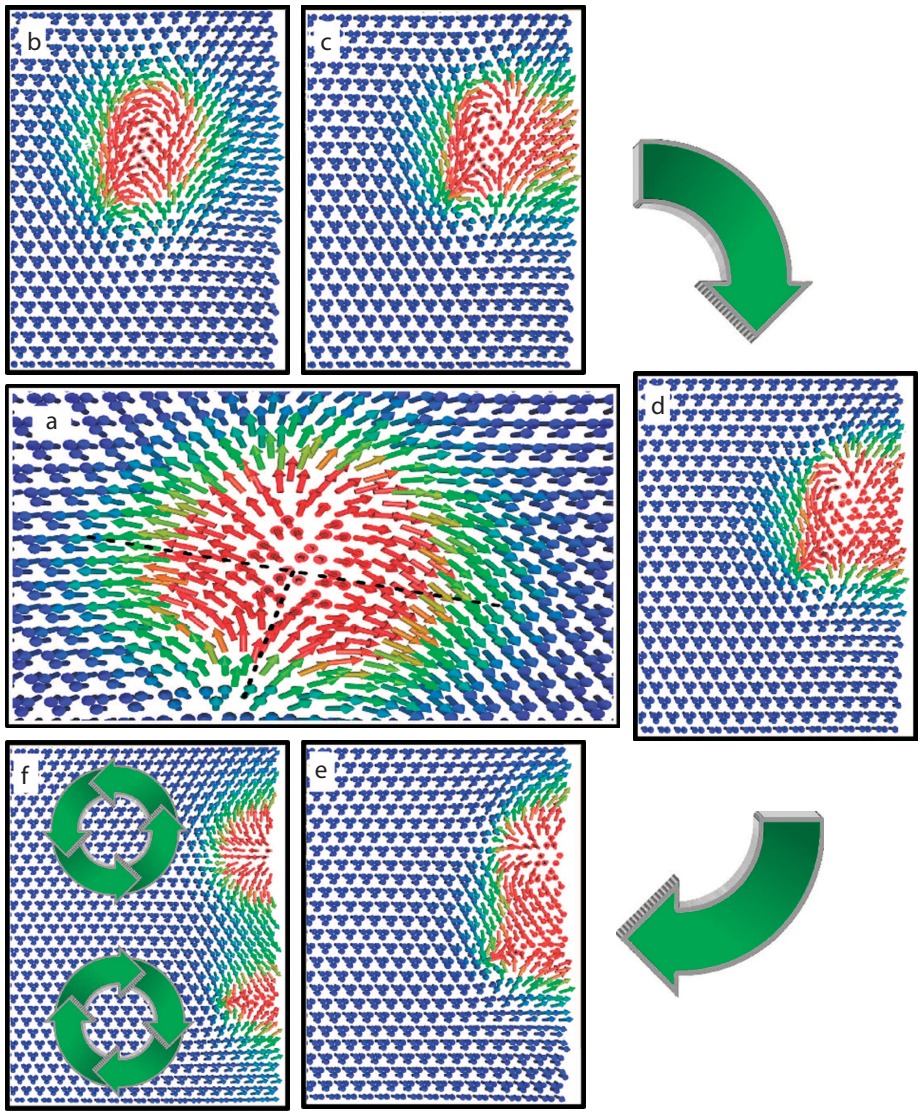
Topological excitations in the Kagome lattice





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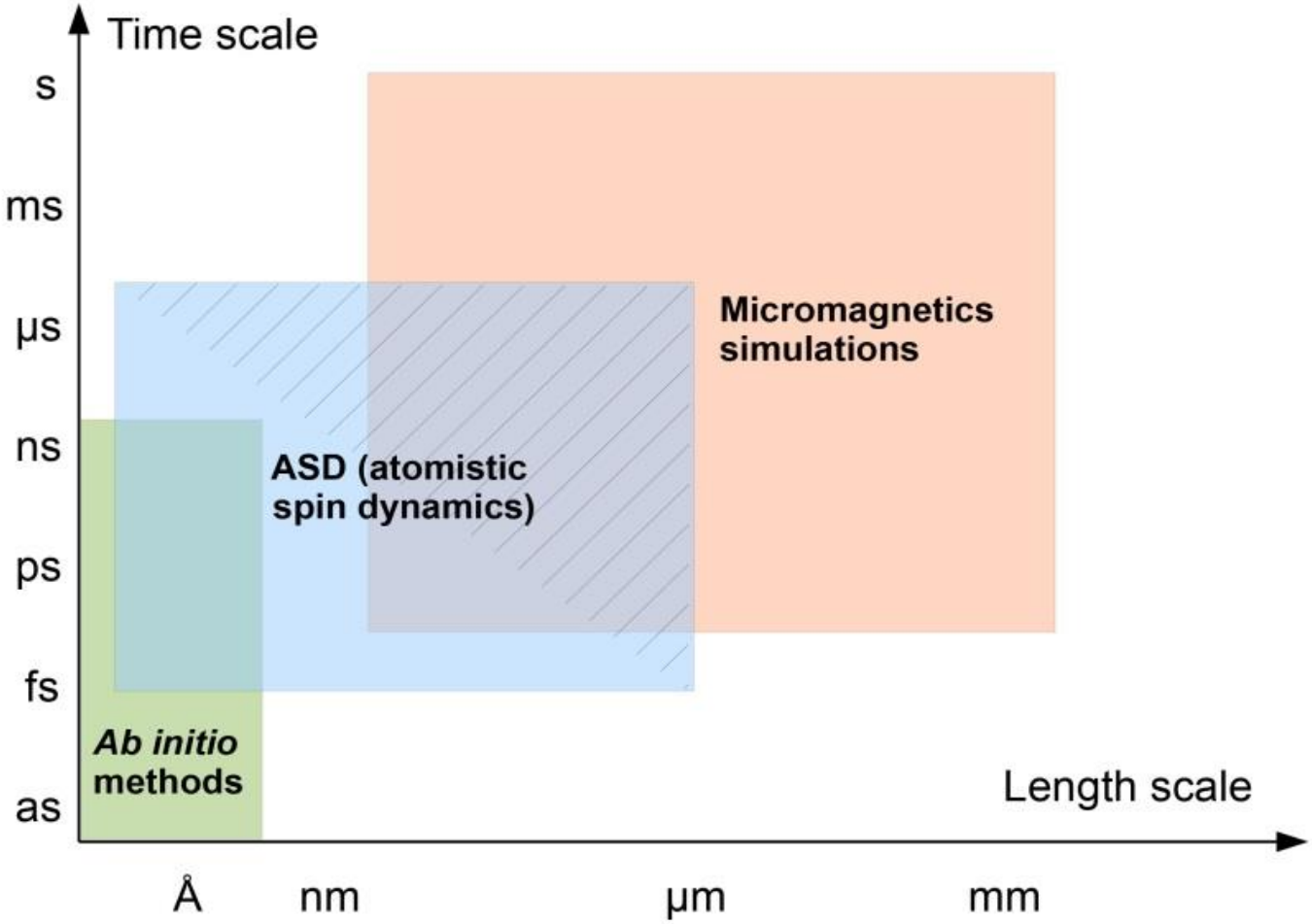
Comp. Mat. Sci. **67**, 282 (2013).

Phys. Rev. B **90**, 165130 (2014)

Nature Commun. **5**, 4815, (2014)

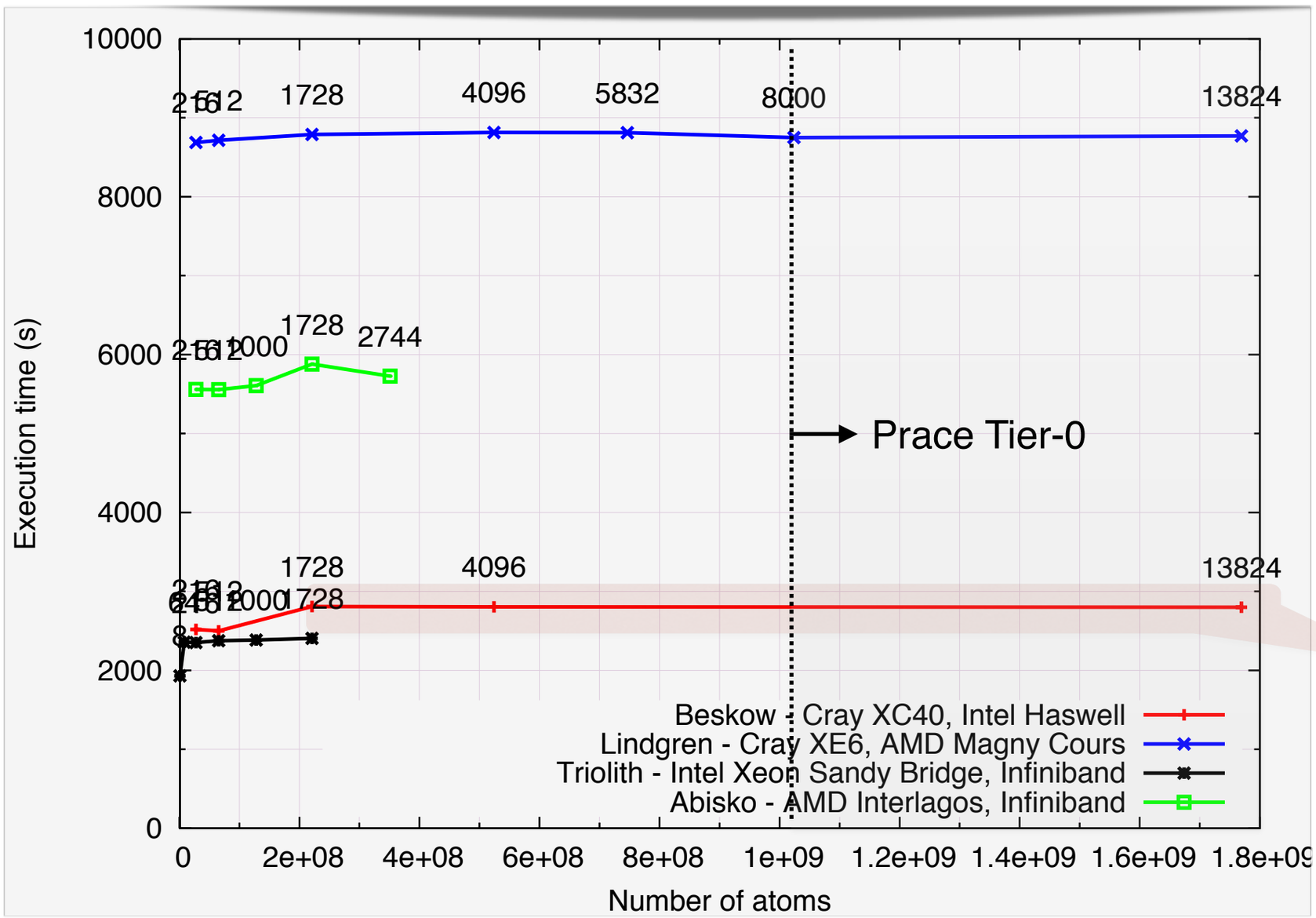
Multiscale simulations



Massive parallel implementation UppASD 4.0

Two levels of parallelization
- Ensemble averaging
- Domain decomposition (similar to Verlet-list approach)
  - "automatic" load balanced
  - all communications are overlapped with computations

Possible to run in hybrid MPI/OpenMP mode (and soon MPI/CUDA)



FeCo-B2
J_{ij} cutoff 3a

Excellent weak scaling

Beskow

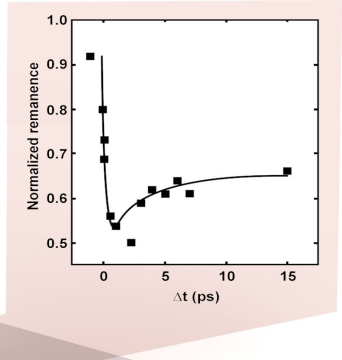
Time scales

UPPSALA UNIVERSITET

Lifetime of magnetic data storage media
http://www.clir.org/pubs/reports/pub54/4life_expectancy.html
http://www.apple.com

Atomistic Spin-Dynamics

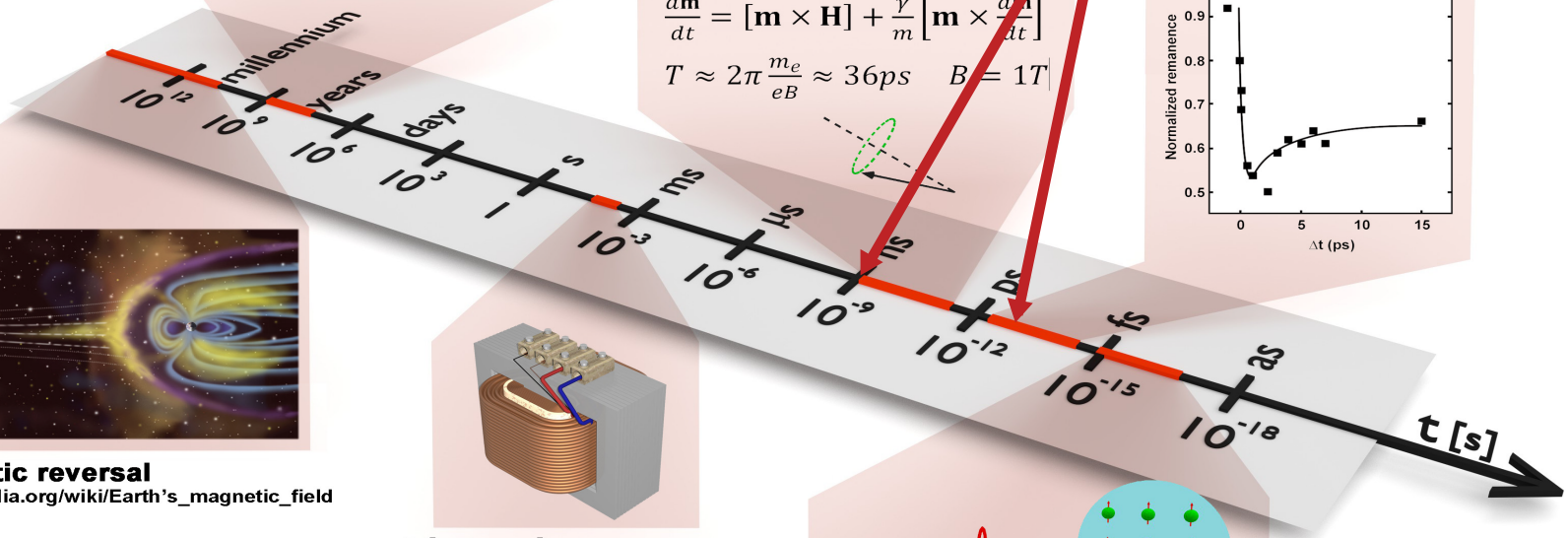
Demagnetization by fs Laser
E Beaurepaire et. al, PRL, 76, 4250 (1996)

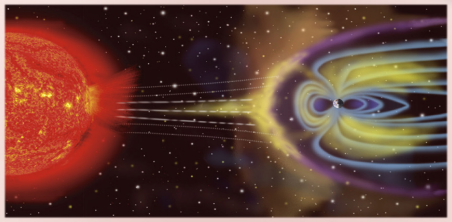


Magnetization precession

$$\frac{d\mathbf{m}}{dt} = [\mathbf{m} \times \mathbf{H}] + \frac{\gamma}{m}\left[\mathbf{m} \times \frac{d\mathbf{H}}{dt}\right]$$

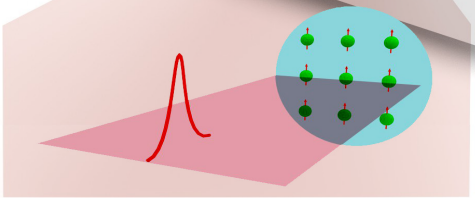
$$T \approx 2\pi \frac{m_e}{eB} \approx 36ps \qquad B = 1T$$





Geomagnetic reversal
http://en.wikipedia.org/wiki/Earth's_magnetic_field

AC Transformer
http://en.wikipedia.org/wiki/Transformer



Coherent interaction between light and magnetization
Bigot et. al, Nat Phy vol 5(7), 515 (2009)