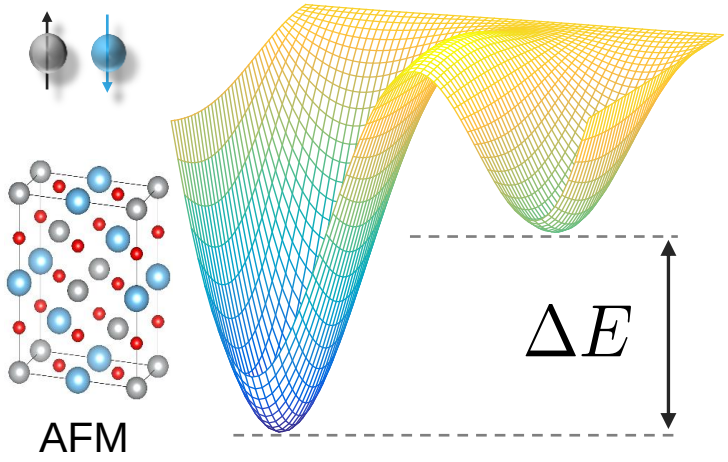
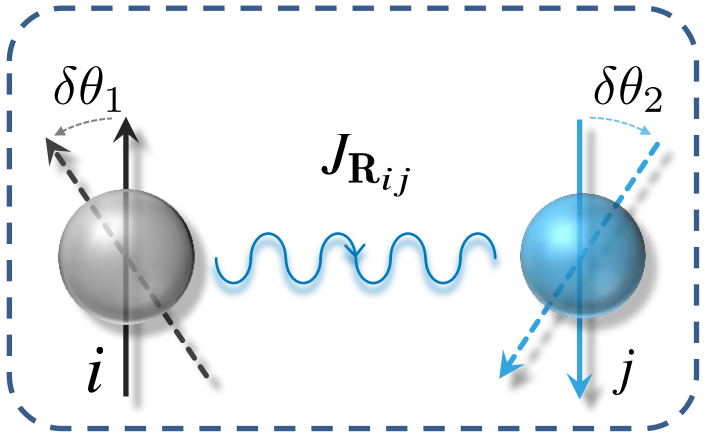
Calculating model parameters: The case of Heisenberg J_{ex}

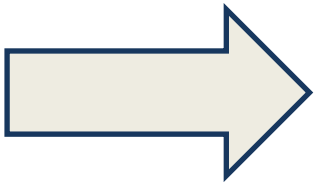




Myung Joon Han (KAIST-Physics, mj.han@kaist.ac.kr)

First-principles Approach to SCES

- ✓ **Strongly correlated electron materials & many outstanding problems (e.g., high-temperature superconductivity)**
- ✓ **'Solving' those problem often means more than just to describe the 'correct' electronic structure.**
- ✓ **Many different experimental and theoretical methods & techniques (traditionally this has not been a main field of research for first-principles calculations.)**



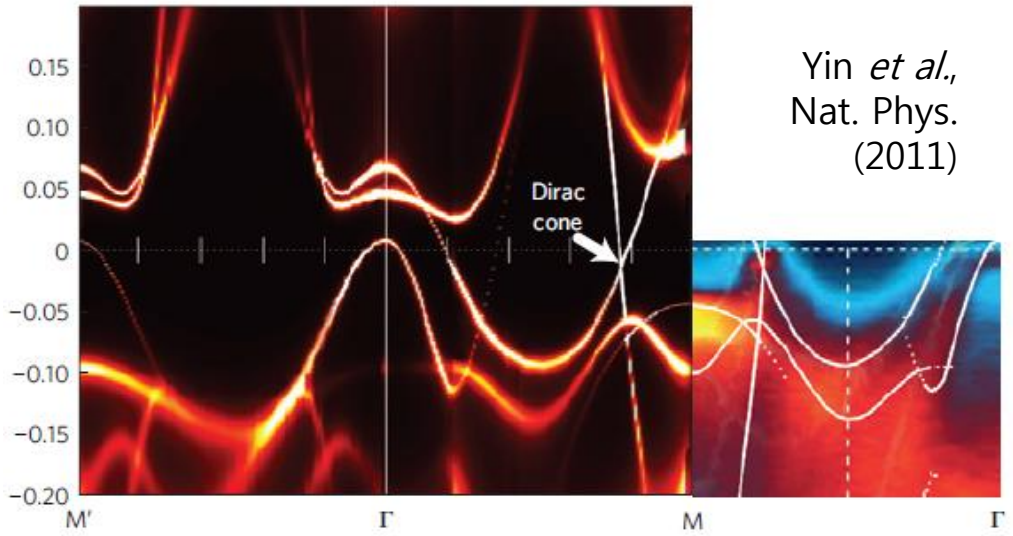
Constructing the bridges

Having/providing the unique facets

First-principles Approach (1)

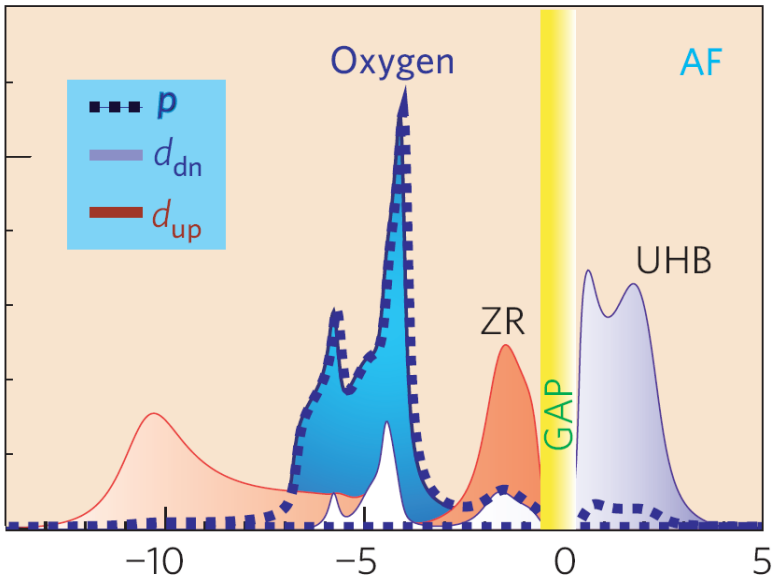
Calculating ***the correct/realistic electronic structure***

- **Conventional approximations (e.g., LDA and GGA) are known to fail for the case of correlated electron systems.**
- **LDA+U, +DMFT (dynamical mean-field theory), GW, etc.**



Yin *et al.*, Nat. Phys. (2011)

Weber et al., Nature Phys. (2010)



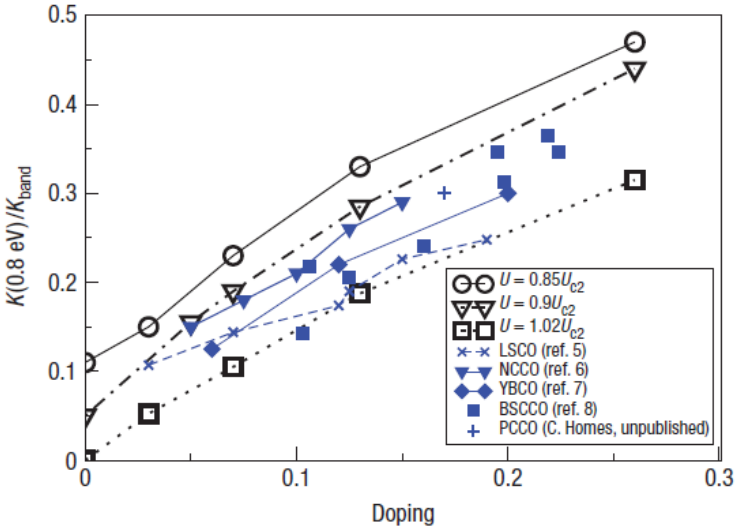
First-principles Approach (2)

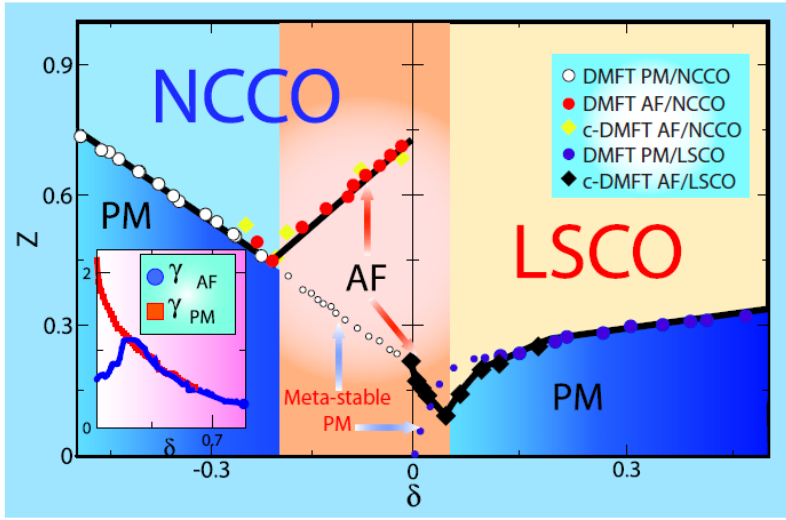
Direct estimation of key quantity or parameter

LETTERS
PUBLISHED ONLINE: 27 JUNE 2010 | DOI: 10.1038/NPHYS1706
nature physics

Strength of correlations in electron- and hole-doped cuprates

Cédric Weber*, Kristjan Haule and Gabriel Kotliar





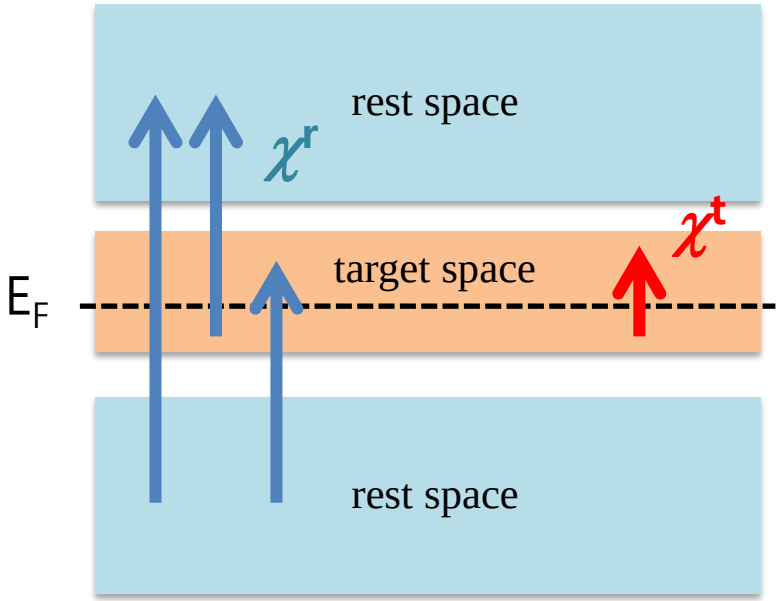
LETTERS

Optical conductivity and the correlation strength of high-temperature copper-oxide superconductors

ARMIN COMANAC[1], LUCA DE' MEDICI[2], MASSIMO CAPONE[3,4] AND A. J. MILLIS[1]*

First-principles Approach (2) – cont'd

$\chi^t = \chi - \chi^r$



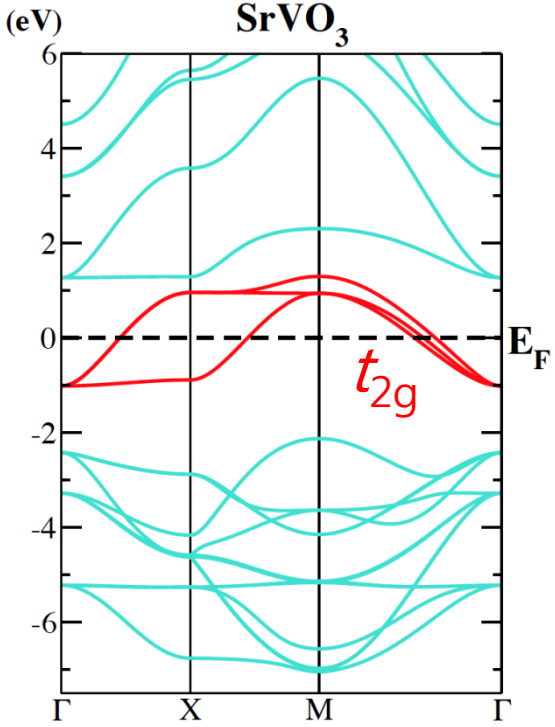


Figure from L. Vaugier's thesis

From Dyson's equation for W in RPA, $W = v + v\chi_0 W$

fully screened Coulomb, W

$$W = [1 - v\chi_0]^{-1}v = [1 - v\chi_0{}^r - v\chi_0{}^t]^{-1}v$$
$$= [\{1 - (1 - v\chi_0{}^r)^{-1}v\chi_0{}^t\}(1 - v\chi_0{}^r)]^{-1}v$$
$$= [1 - W^r\chi_0{}^t]^{-1}W^r$$

partially screened Coulomb, W^r

First-principles Approach (2) – cont'd

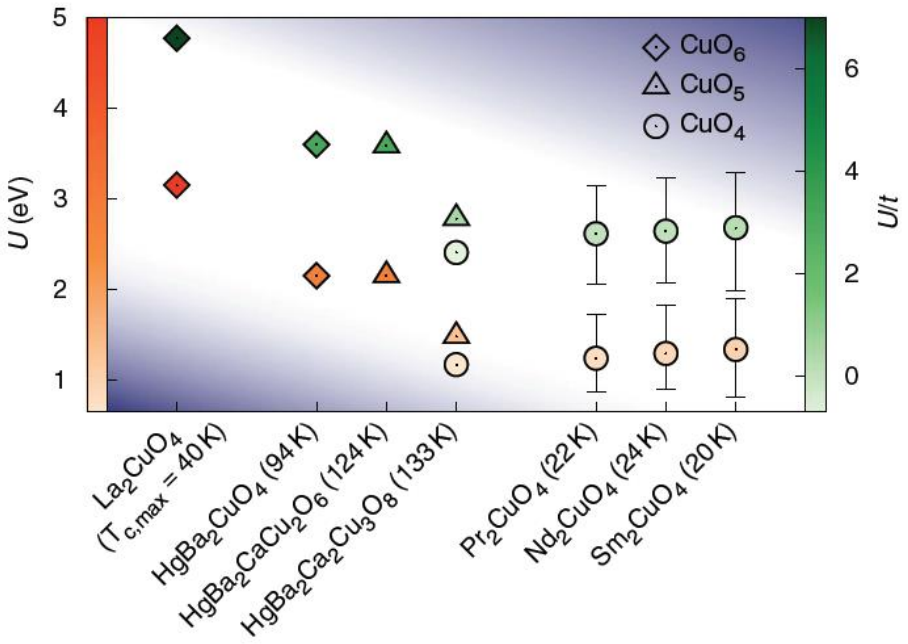
SCIENTIFIC REPORTS

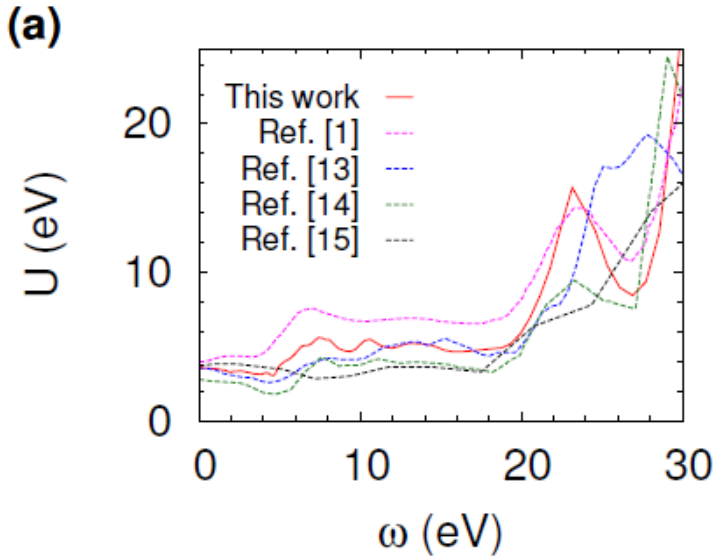
OPEN

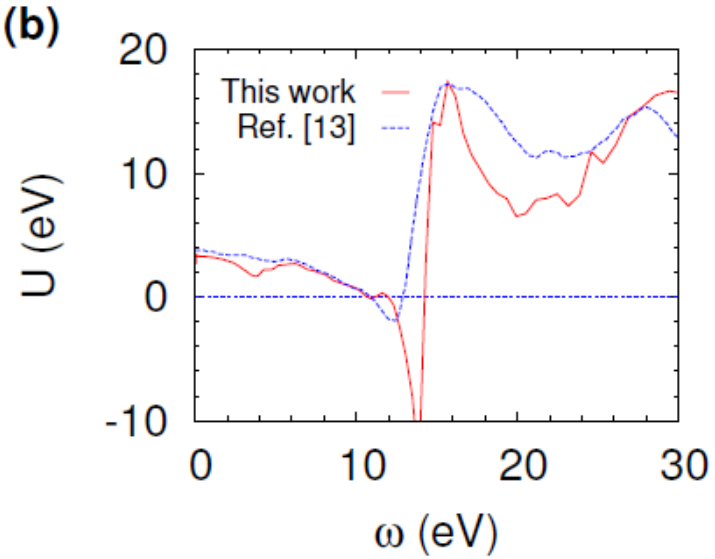
Received: 28 May 2016
Accepted: 26 August 2016
Published: 16 September 2016

Direct theoretical evidence for weaker correlations in electron-doped and Hg-based hole-doped cuprates

Seung Woo Jang[1], Hirofumi Sakakibara[2,3], Hiori Kino[4], Takao Kotani[2], Kazuhiko Kuroki[5] & Myung Joon Han[1,6]







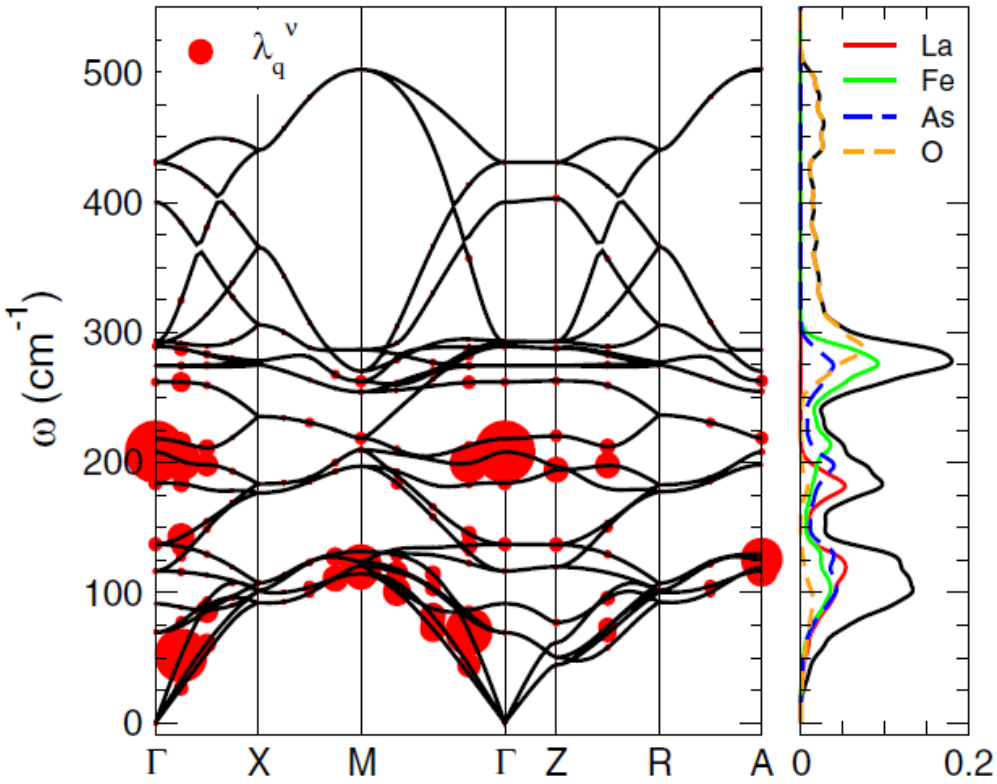
Calculation by S. W. Jang

First-principles Approach (3)

Calculating new concept and/or quantity?!

- ✓ Effective charge
- ✓ Charge transfer energy
- ✓ Chern number

Boeri et al., PRL (2008)



Heisenberg Exchange Parameter

$$H = -J_{12}\, S_1 \cdot S_2$$

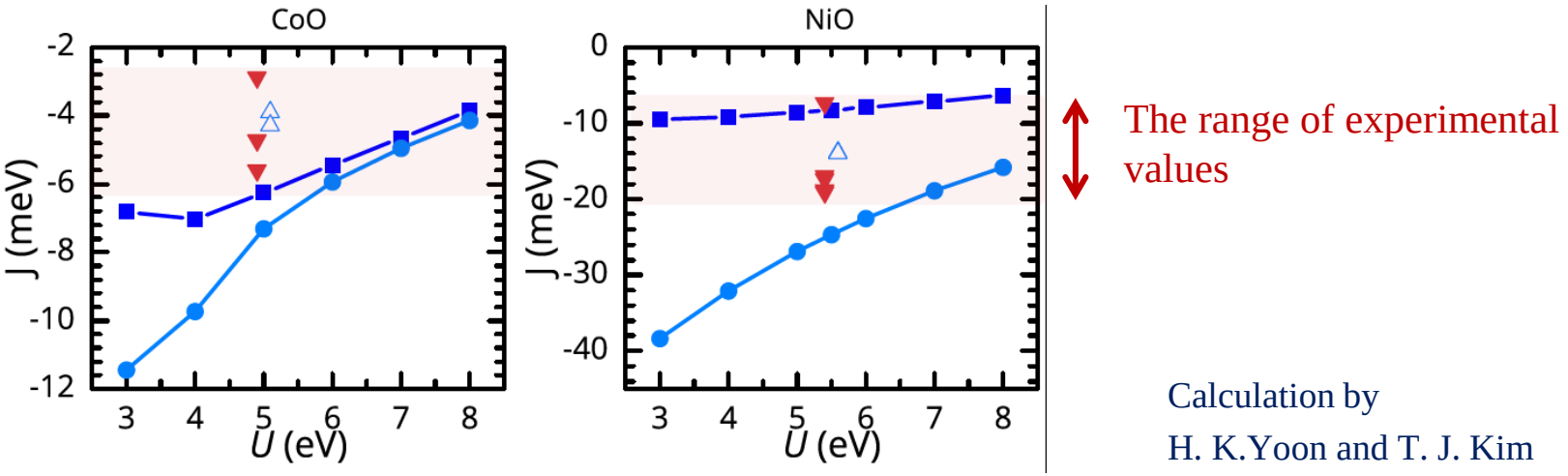
- ✓ **The sign and the strength of two-spin interaction represented by a constant J_{12}**

- ✓ **(With the minus sign in front of it,) the positive and negative J_{12} corresponds to the parallel (ferro-) and antiparallel (antiferro) spin alignment, respectively.**

Determining J

- ✓ **Not always straightforward to determine it from experiments (sample quality, fitting, …etc)**
- ✓ **Model-based theories often just assume Js.**

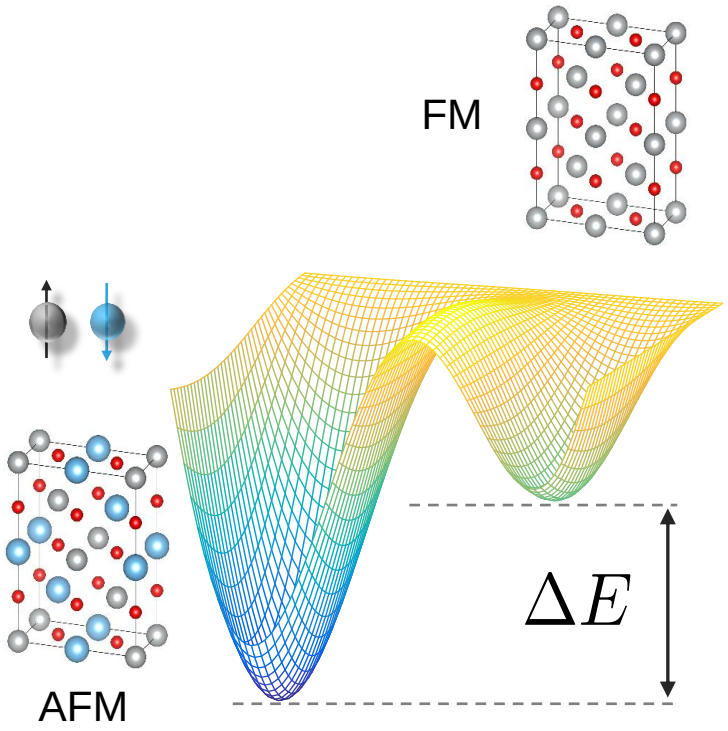
- ✓ **Independent method or way to estimate J**
- ✓ **Extract some more (hopefully unique) information**



Calculation by
H. K.Yoon and T. J. Kim

Calculating J from Total Energies

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\,\vec{S}_i \cdot \vec{S}_j \quad \Rightarrow \quad E = -\frac{1}{2} J_{ij}\,S_i\,S_j$$



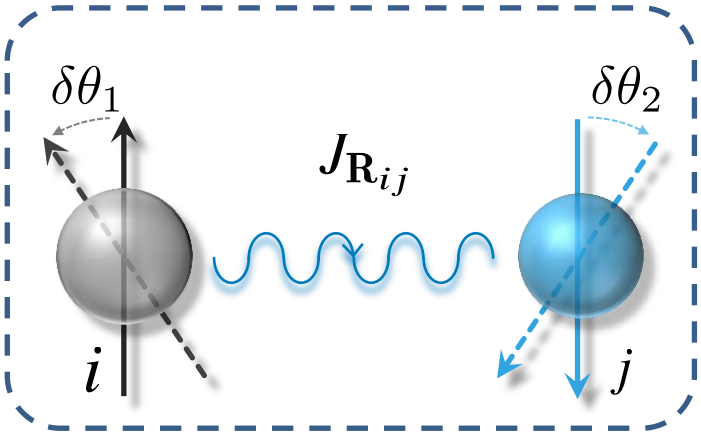
Metastable spin structure (not the ground state) can usually be stabilized (from the self-consistent) by choosing the desired spin orientation as the input.

→ Total energies corresponding to different spin orders can be estimated and compared.

Calculating J as a Response Function

$$J^{\alpha\beta}(\mathbf{R}_{ij}) = \sum_{\mathbf{q}} J^{\alpha,\beta}_{\mathbf{R}_{ij}}(\mathbf{q}) e^{-i\mathbf{R}_{ij}\mathbf{q}}$$

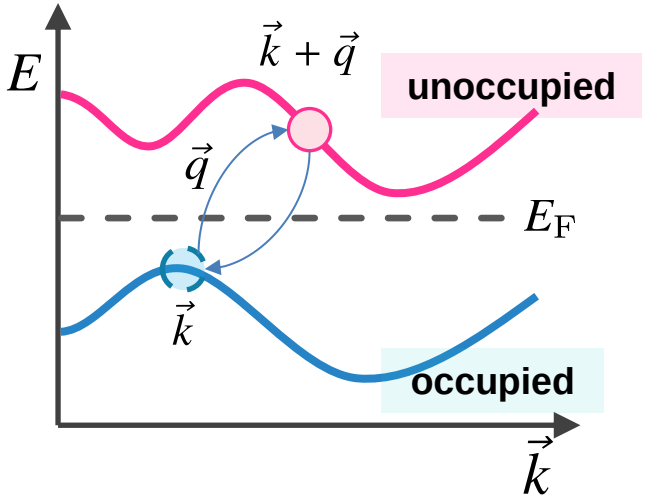
$$J^{\forall \text{orbitals}}_{\mathbf{R}_{ij}}(\mathbf{q}) = \sum_{\alpha,\beta} J^{\alpha,\beta}_{\mathbf{R}_{ij}}(\mathbf{q})$$



$$J^{\alpha,\beta}_{\mathbf{R}_{ij}}(\vec{q}) = \sum_{n,n'} \sum_{k} \frac{f_{\uparrow n,k} - f_{\downarrow n',k+q}}{\epsilon_{\downarrow n,k} - \epsilon_{\uparrow n',k+q} - i\eta} M(n\alpha, n'\beta)$$

$$M(n\alpha, n'\beta) = \langle \psi_{\uparrow\mathbf{k},\alpha} | V_i | \psi_{\downarrow\mathbf{k}+\mathbf{q},\beta} \rangle \times \langle \psi_{\downarrow\mathbf{k}+\mathbf{q},\beta} | V_j | \psi_{\uparrow\mathbf{k},\alpha} \rangle$$

Orbital index : α, β
Two spin site : $\mathbf{R}_i = \mathbf{R} + \mathbf{r}$ and $\mathbf{R}_j = \mathbf{R}' + \mathbf{r}'$
$\mathbf{R}_{ij} = \mathbf{R}_j - \mathbf{R}_i$



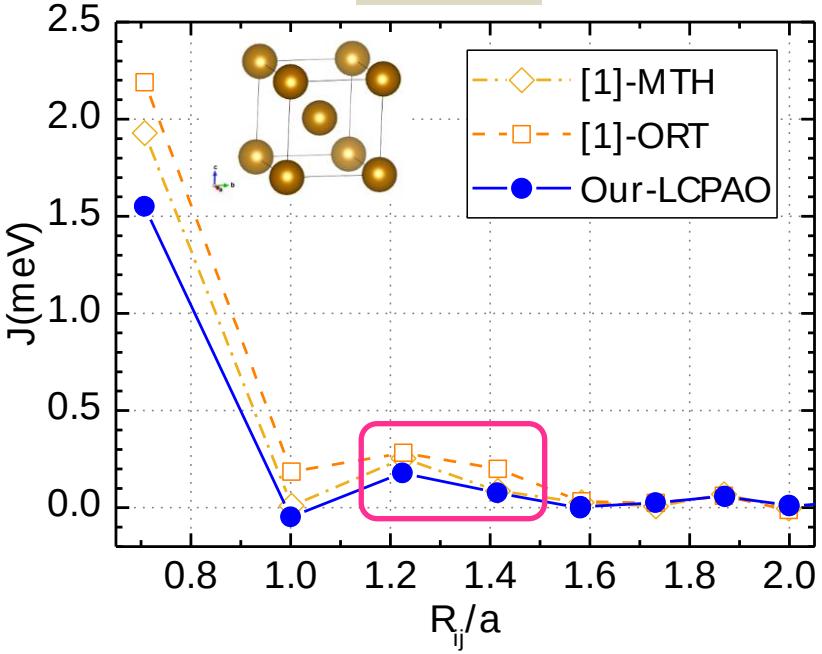
CF: Neutron scattering measurement

Liechtenstein et al. PRL (2009)
MJH et al. PRB (2004)

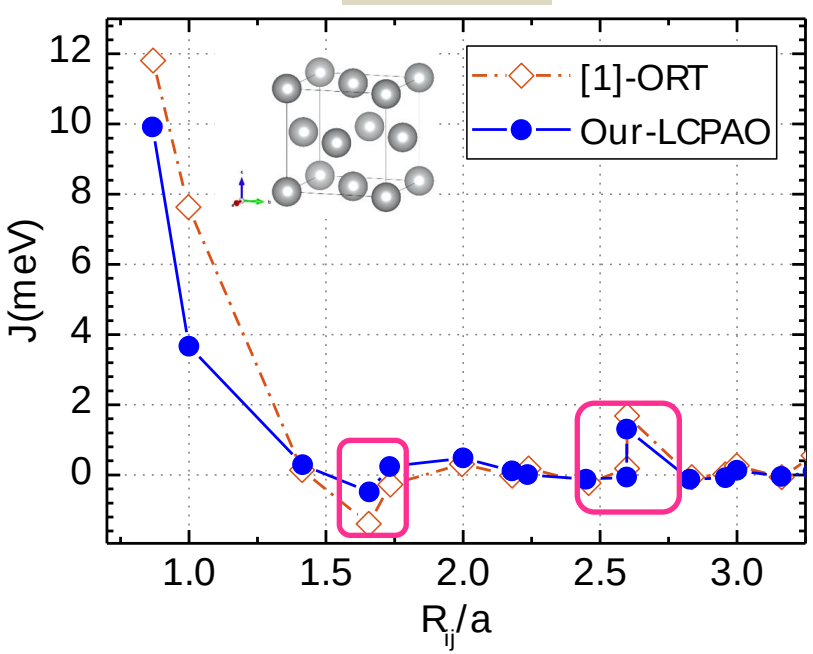
Advantage

- ✓ **No need to perform the multiple large-supercell calculations**
- ✓ **Being able to describe the long range behavior**
- ✓ **More similar with neutron scattering**

fcc Ni



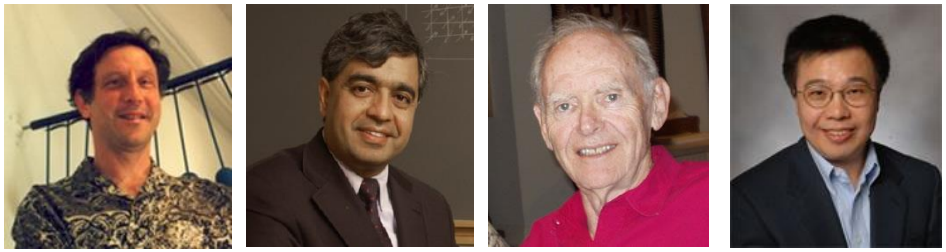
bcc Fe



[1] Kvashnin et al., Phys. Rev. B **91**, 125133 (2015)

Example 1: Fe-pnictides Superconductors

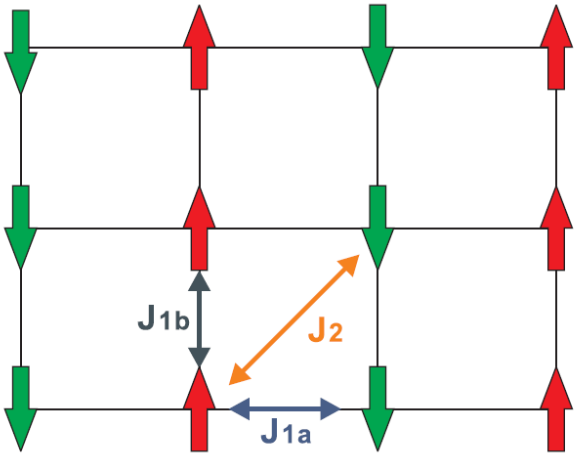
Frustration and quantum criticality?



Si and Abrahams, PRL (2008)
Fang et al., PRB (2008)
Xu et al., PRB (2008)

TABLE I. Calculated Fe moments (in μ_B) and in-plane exchange interactions (in meV), using experimental z(As).

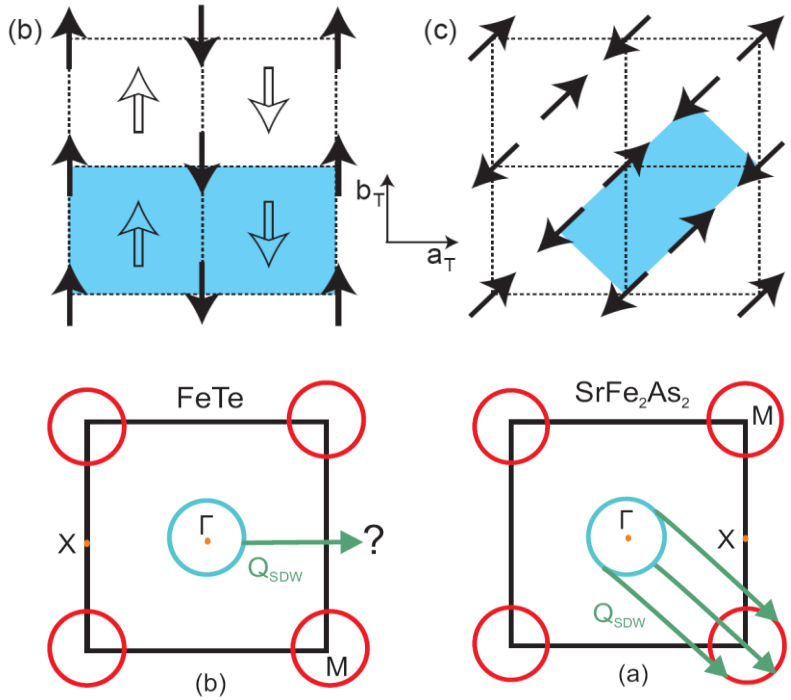
System	Moment	J_{1a}	J_2	J_{1b}	$J_{1a}/2J_2$	$J_{1a}+2J_2$
LaFeAsO	1.69	47.4	22.4	−6.9	1.06	92.2
CeFeAsO	1.79	31.6	15.4	2.0	1.03	62.4
PrFeAsO	1.76	57.2	18.2	3.4	1.57	93.6
NdFeAsO	1.49	42.1	15.2	−1.7	1.38	72.5
$CaFe_2As_2$	1.51	36.6	19.4	−2.8	0.95	75.4
$SrFe_2As_2$	1.69	42.0	16.0	2.6	1.31	74.0
$BaFe_2As_2$	1.68	43.0	14.3	−3.1	1.51	71.5
KFe_2As_2	1.58	42.5	15.0	−2.9	1.42	72.5
LiFeAs	1.69	43.4	22.9	−2.5	0.95	89.2



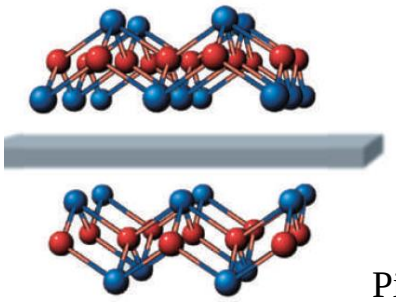
MJH et al., PRL (2009)

Example 2: Superconducting FeTe

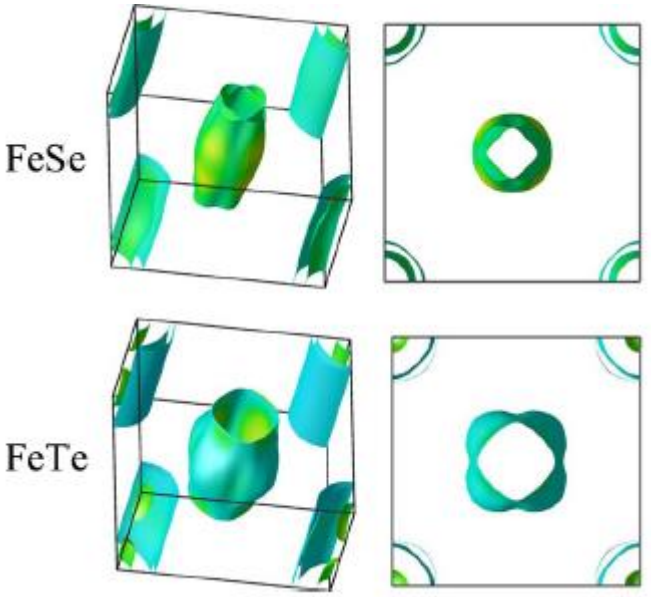
Spin fluctuation theory : Yes or No?



Li et al., PRB (2009)

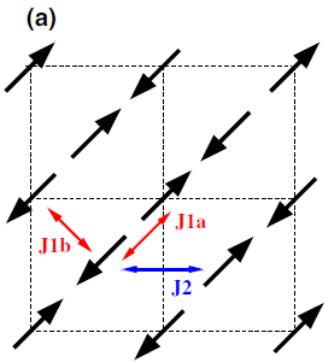


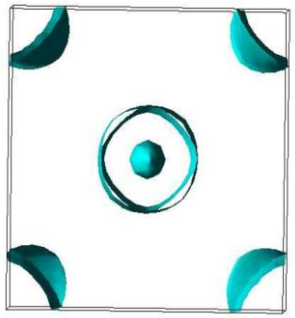
Picture from
Mazin Nature(2010)

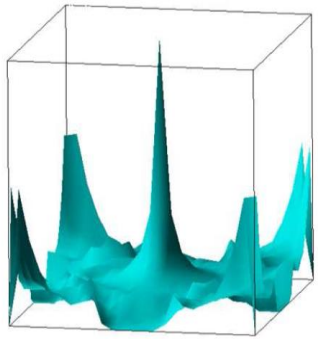


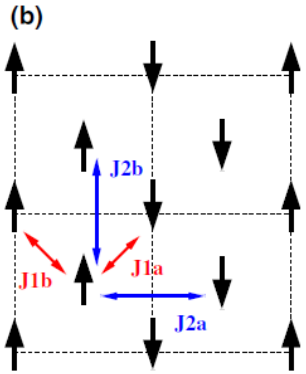
Subedi et al., PRB (2008)

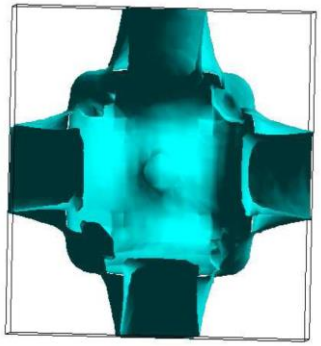
Example 2: FeTe – cont'd

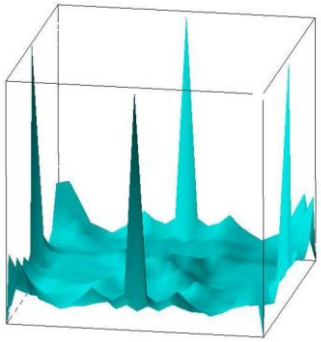


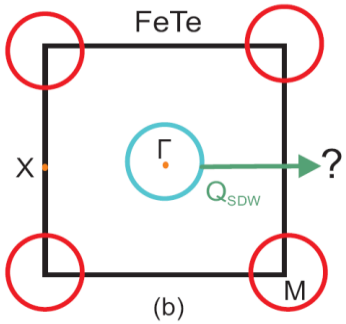












	System	Moment	J_{1a}	J_{1b}	J_{2a}	J_{2b}
Double-stripe	$Fe_{1.068}Te$	2.09 (1.97[b])	−7.6	−26.5	46.5	−34.9
	FeTe	2.16	−4.2	12.9	−6.2	−15.3
Single-stripe	FeTe	2.09	38.6	21.7	5.0	···
	LaFeAsO[a]	1.69 (0.36[c])	47.4	−6.9	22.4	···

Han and Savrasov PRL (2009)
Han and Savrasov PRL (2010)

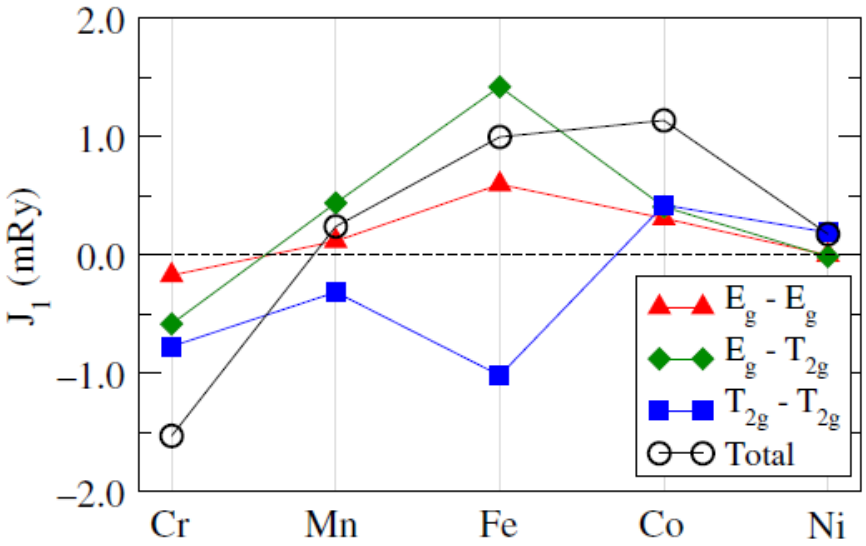
Further Extension

- ✓ **Additional resolution**

Iron
ferromagnet
Tc ~ 1000K

Calculation by Hongki Yoon

J (meV)	D_{xy}	d_{yz}	d_{xz}	$d_{x^2-y^2}$	d_{z^2}
d_{xy}	-0.5	-0.5	-0.5	0.0	1.7
d_{yz}		-0.5	-0.5	1.2	0.4
d_{xz}			-0.5	1.2	0.4
$d_{x^2-y^2}$				2.7	0.0
d_{z^2}					2.7



Kvashnin et al., PRL (2016)

- ✓ **Spin-orbit coupling and other coupling parameters**