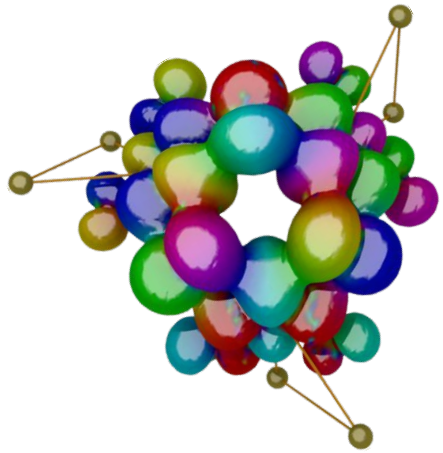
$Na_3Ir_3O_8$

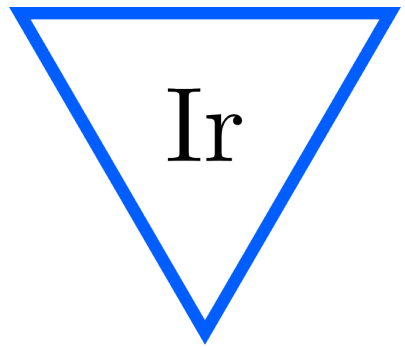
– a metal by spin-orbit interaction –

Marc Höppner
Solid State Spectroscopy
MPI for Solid State Research

Vancouver
2015/10/23



Why Iridates?



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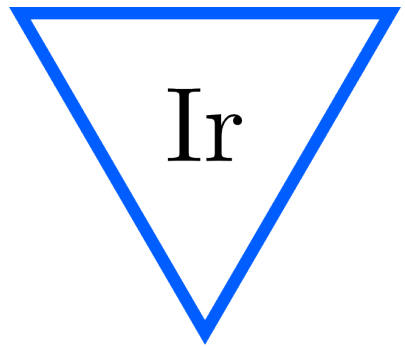
lattice



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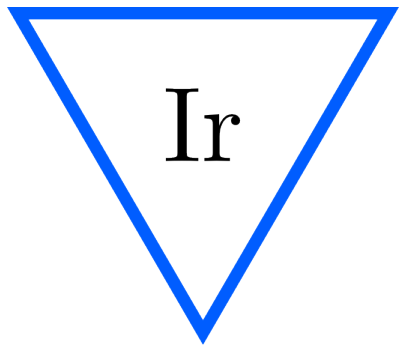
spin-orbit
interaction (soi)



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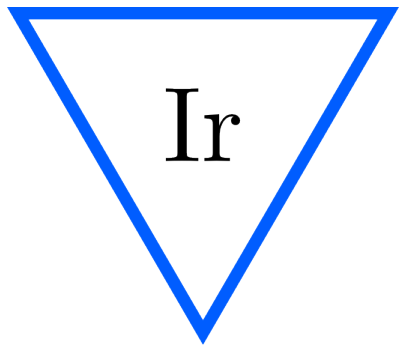

many-body interactions

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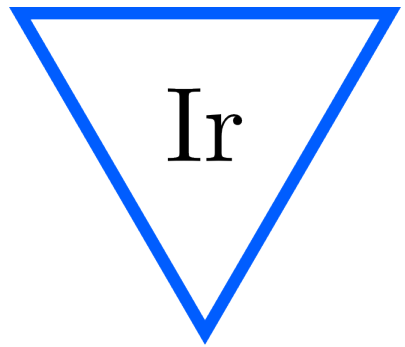

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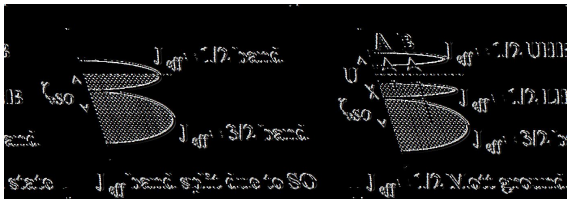
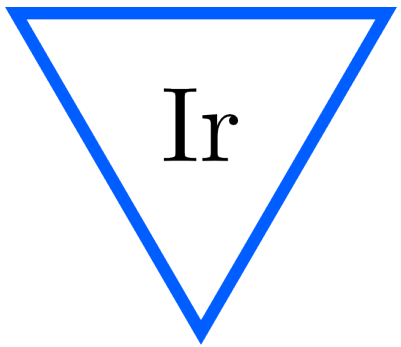


BJ Kim et al. PRL **101**, 076402 (2008)



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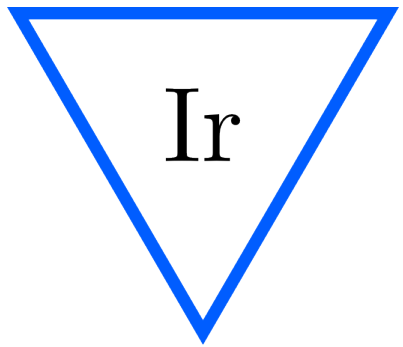

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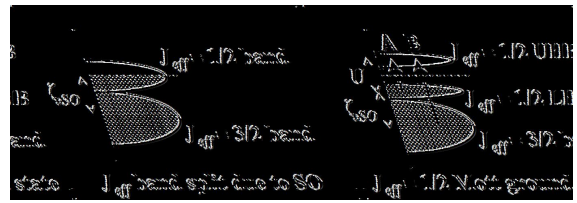

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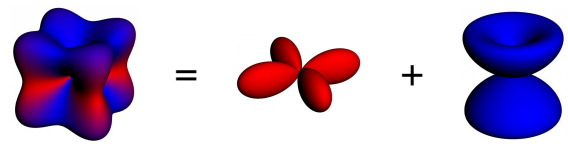

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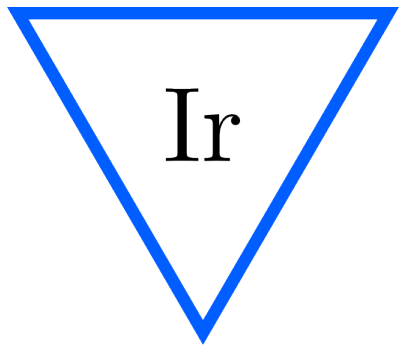

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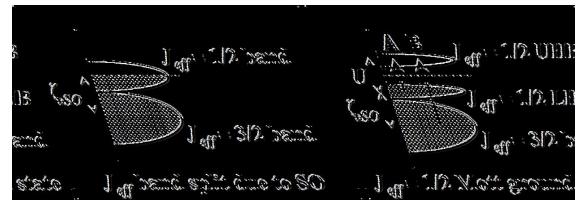

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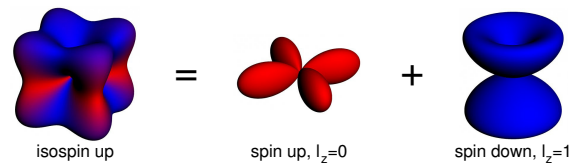

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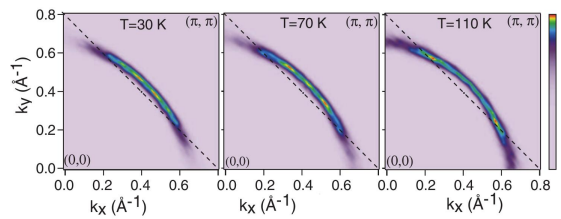

YK Kim et al. Science **345**, 187-190 (2014)

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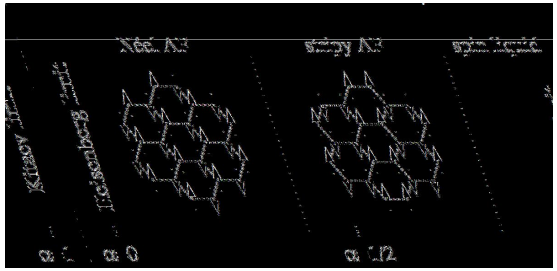

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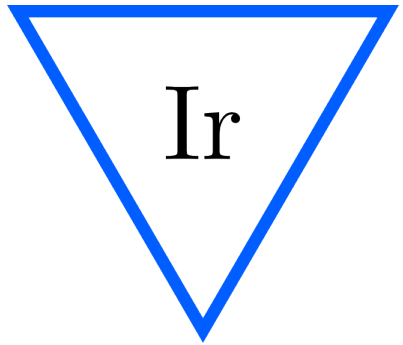

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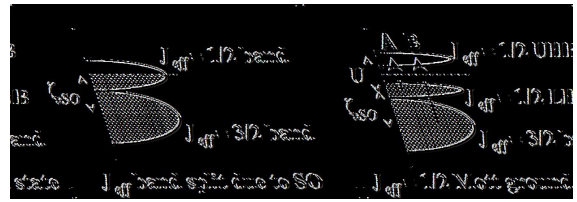

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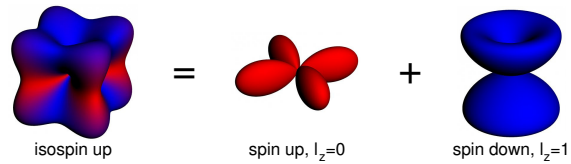

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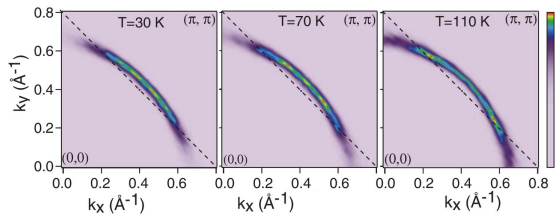

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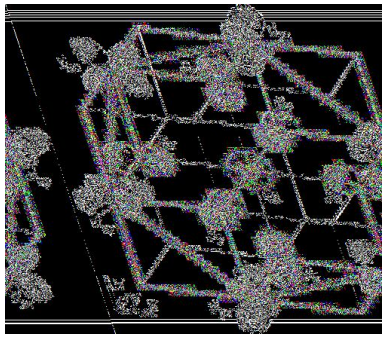
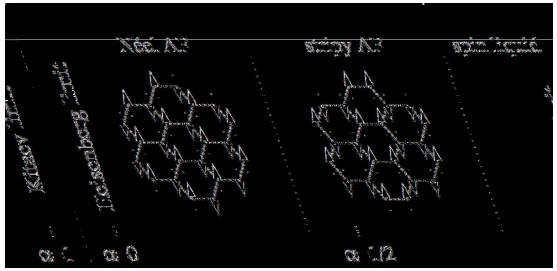


I. I. Mazin et al. PRL **109**, 197201 (2012)



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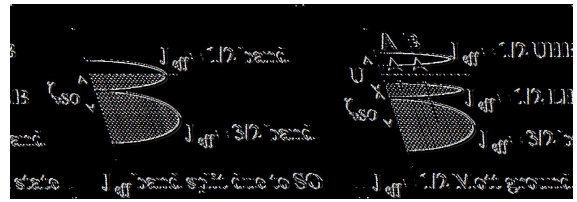

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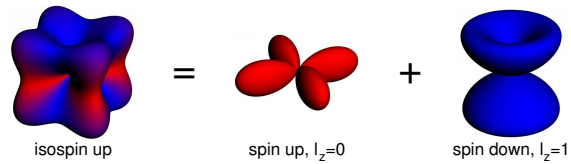

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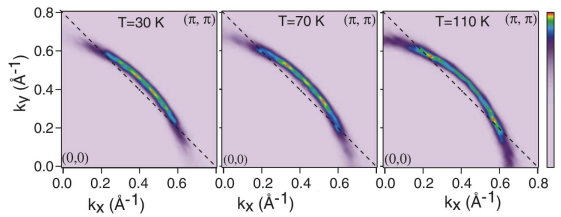

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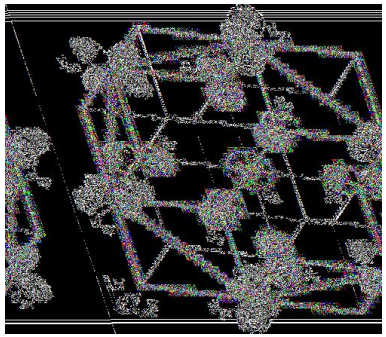

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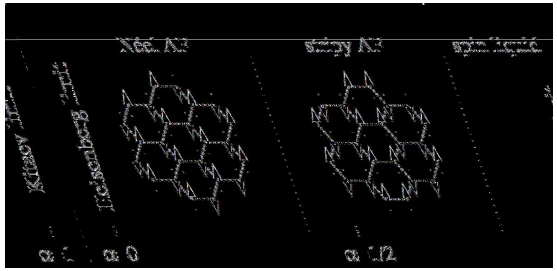

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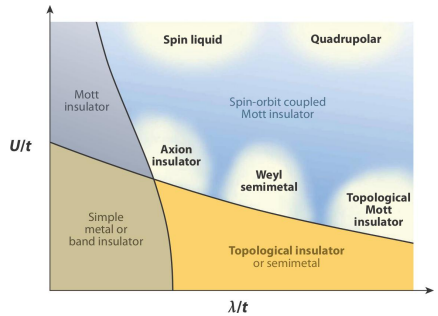

W. Witczak-Krempa et al. Annu. Rev. CMP **5**, 57-82 (2014)

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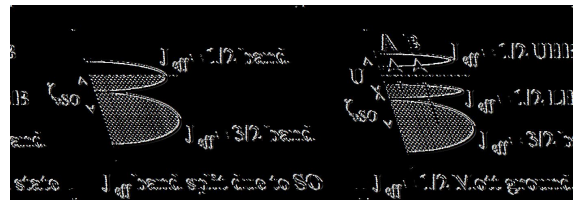

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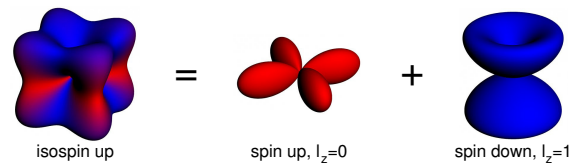

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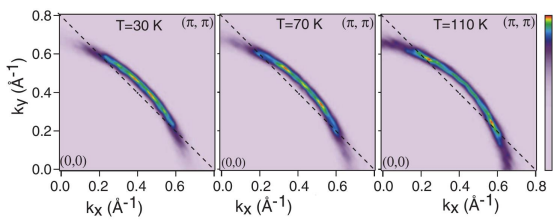

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$Na_3Ir_3O_8$

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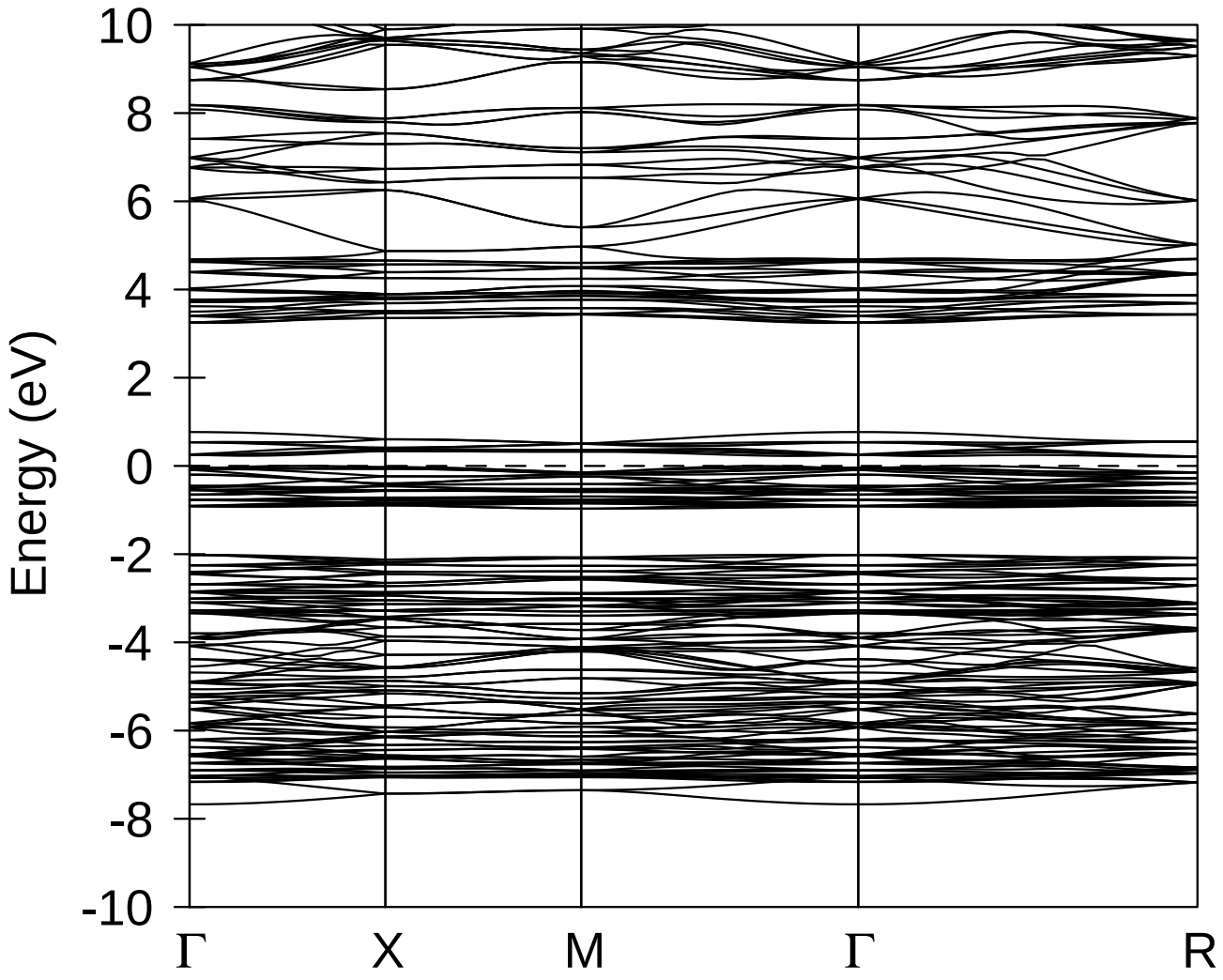
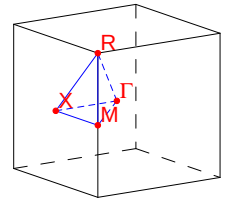
Why isn't $Na_3Ir_3O_8$ a regular metal?

spaghetti . . .





BZ

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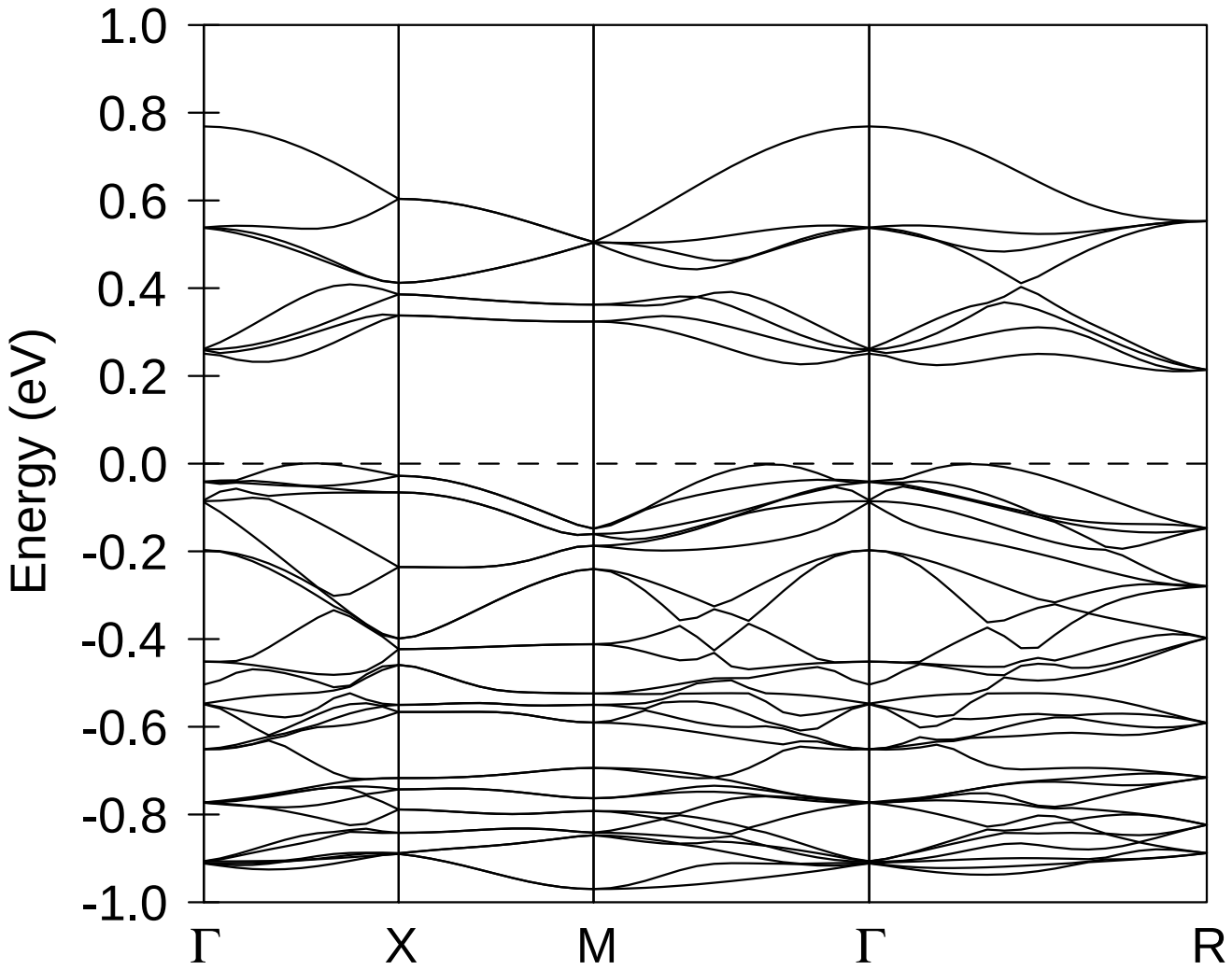

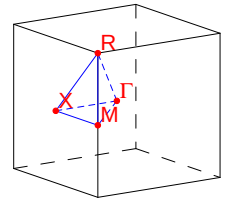

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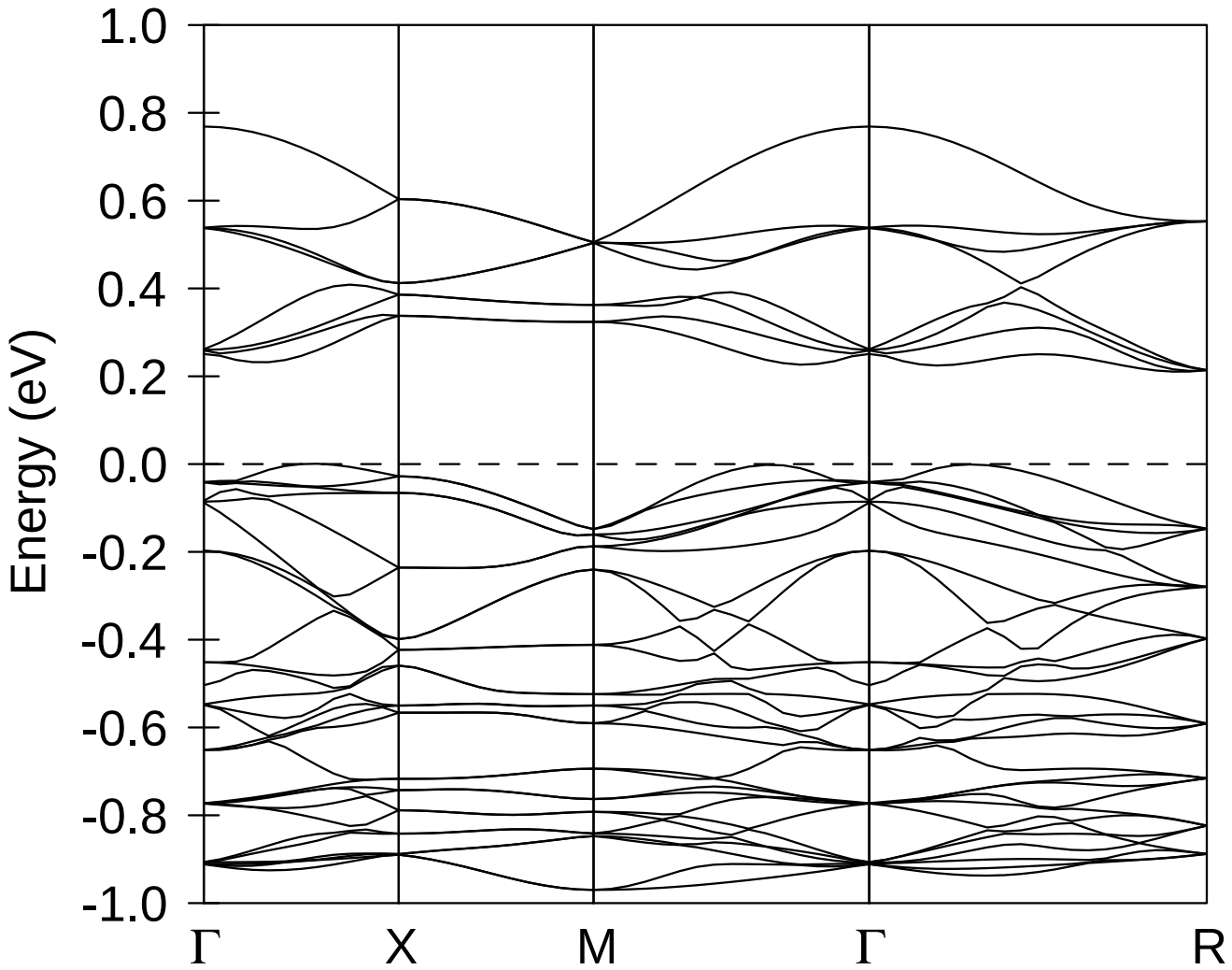
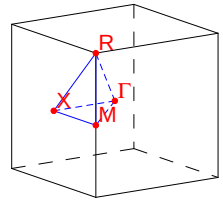
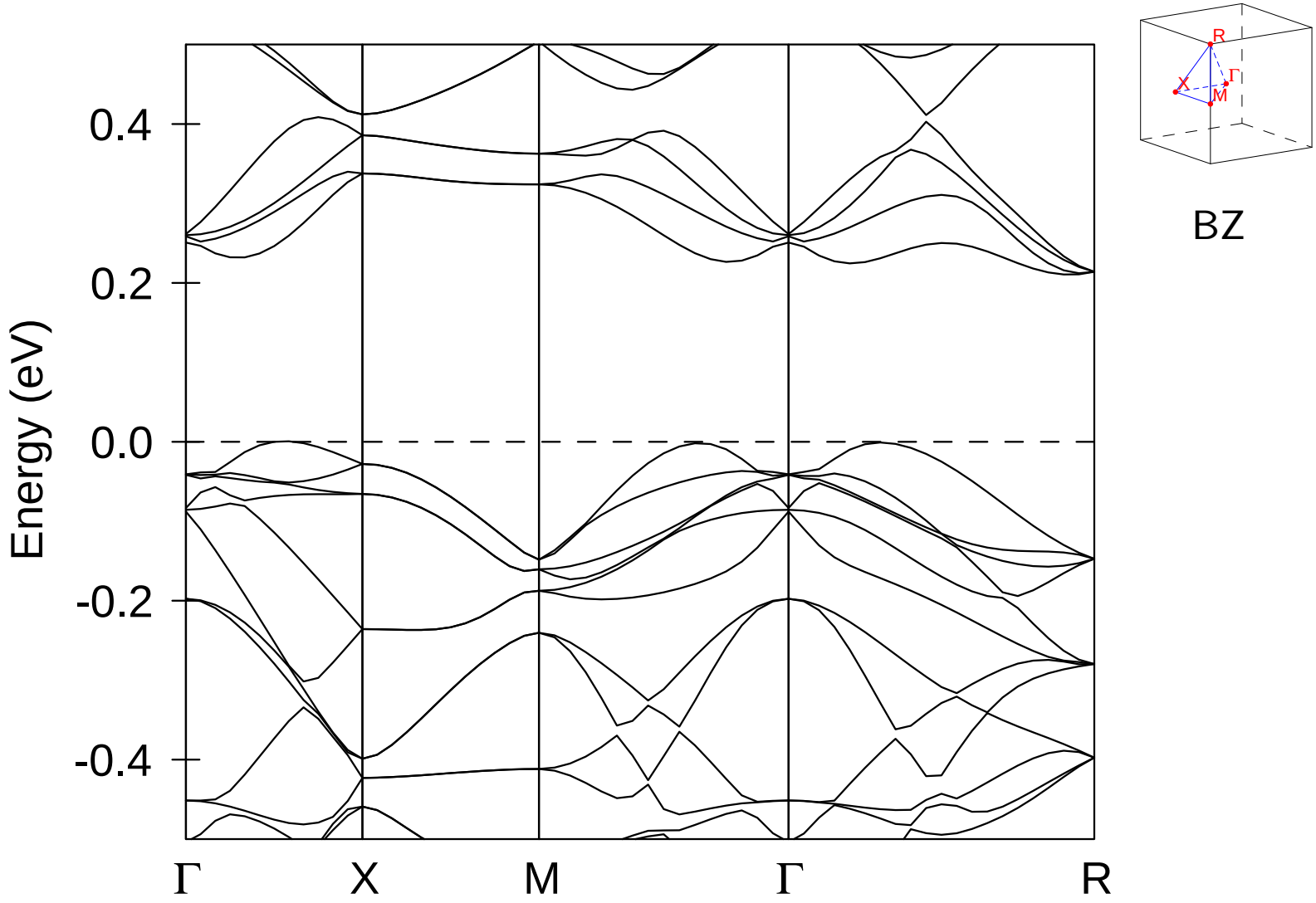




BZ

$\rightarrow$ $Na_3Ir_3O_8$ is a band insulator in DFT?

spaghetti . . .



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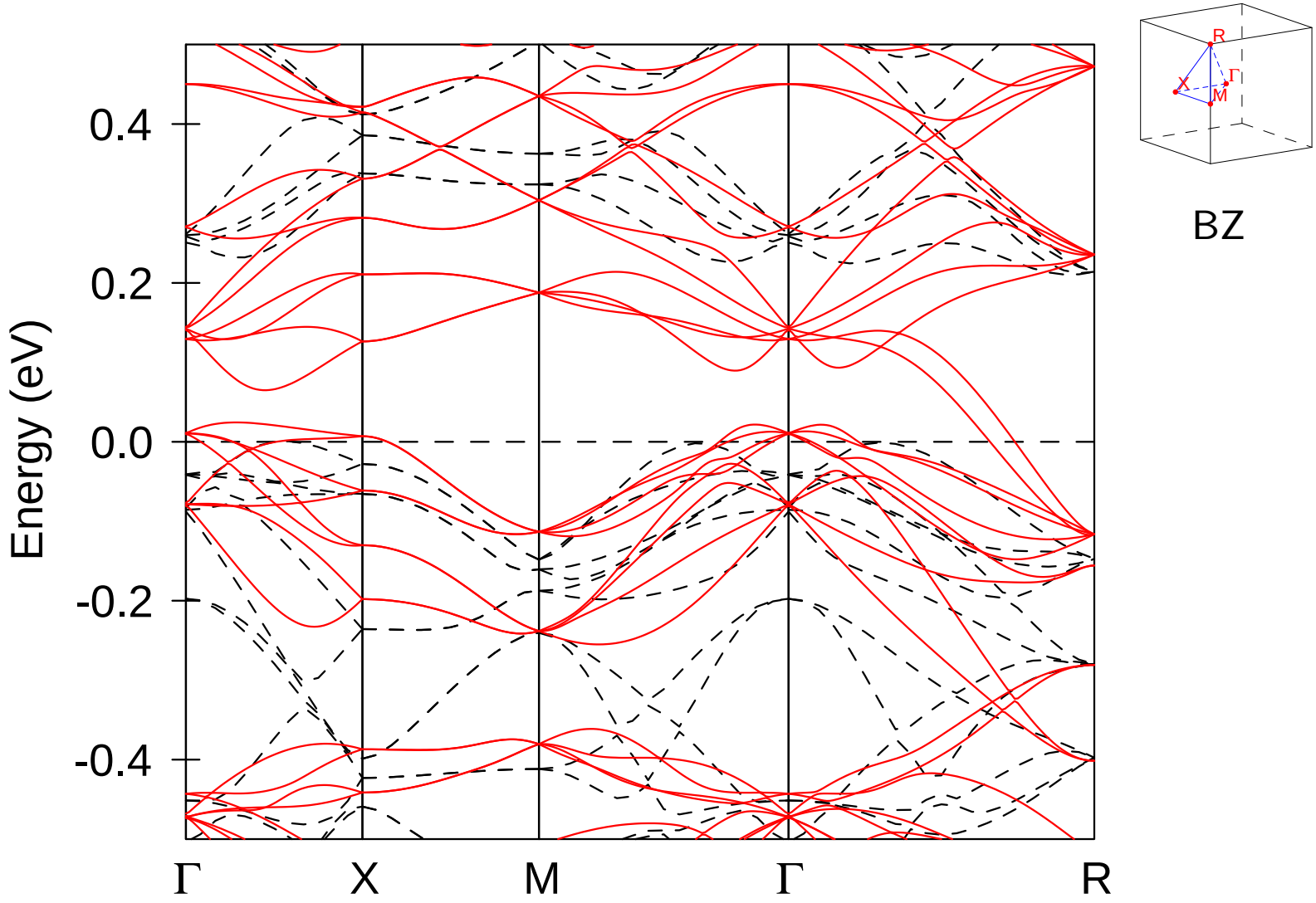

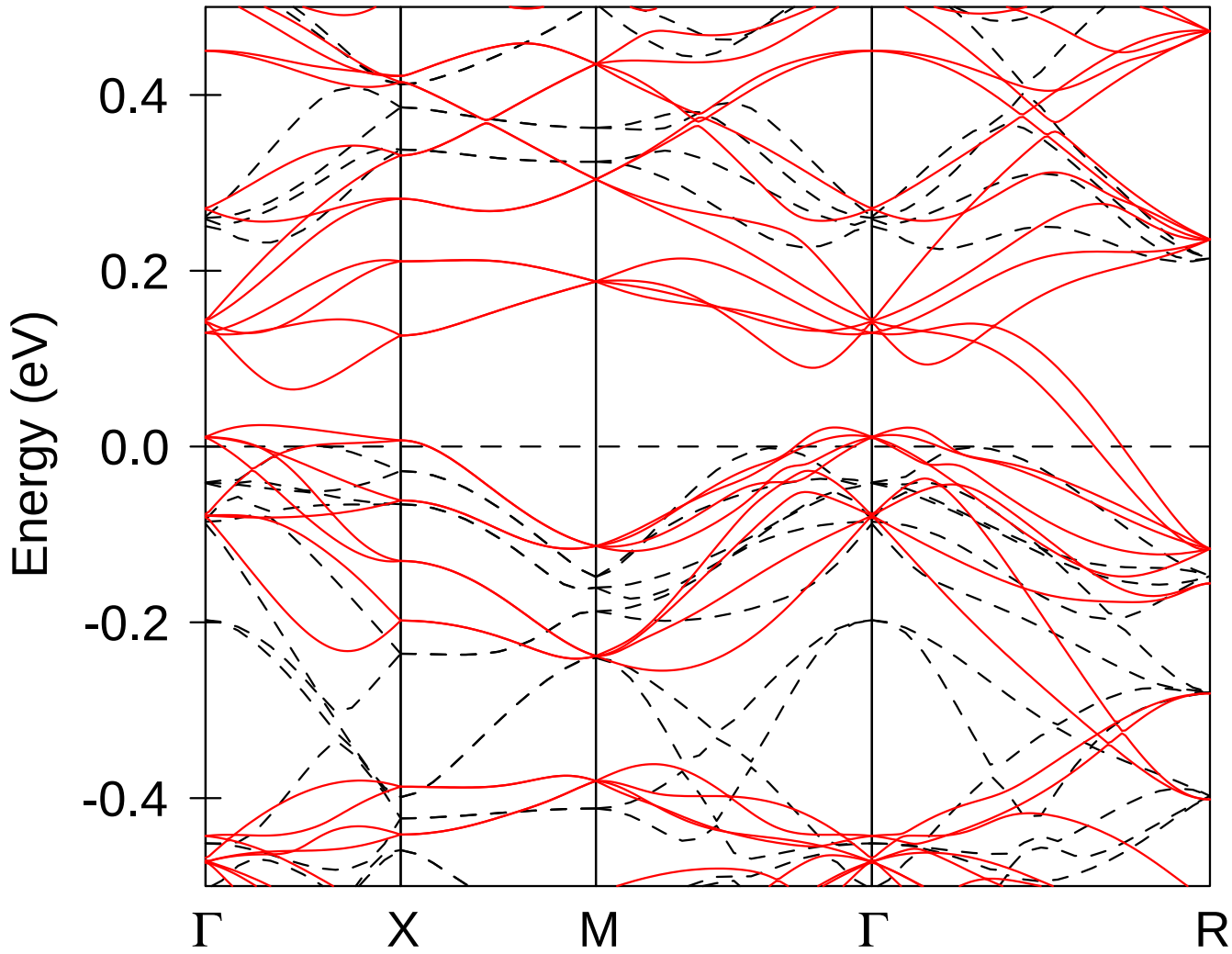

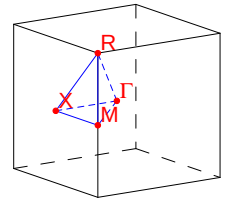

BZ

→ SOI closes the gap and drives $\mathrm{Na_3Ir_3O_8}$ into a bad-metal regime

Ⓐ Why is $\mathrm{Na_3Ir_3O_8}$ a band insulator in plain DFT?

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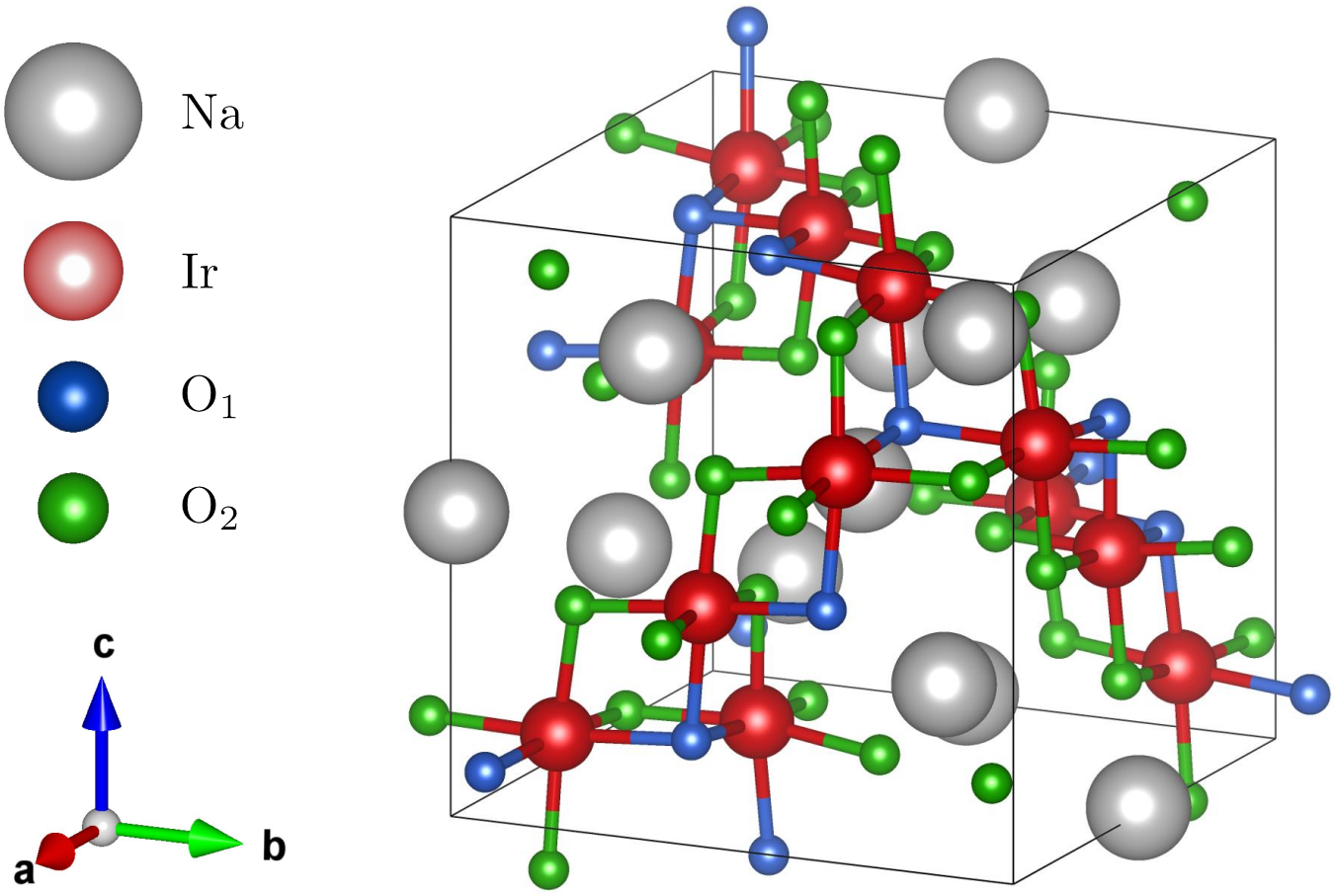
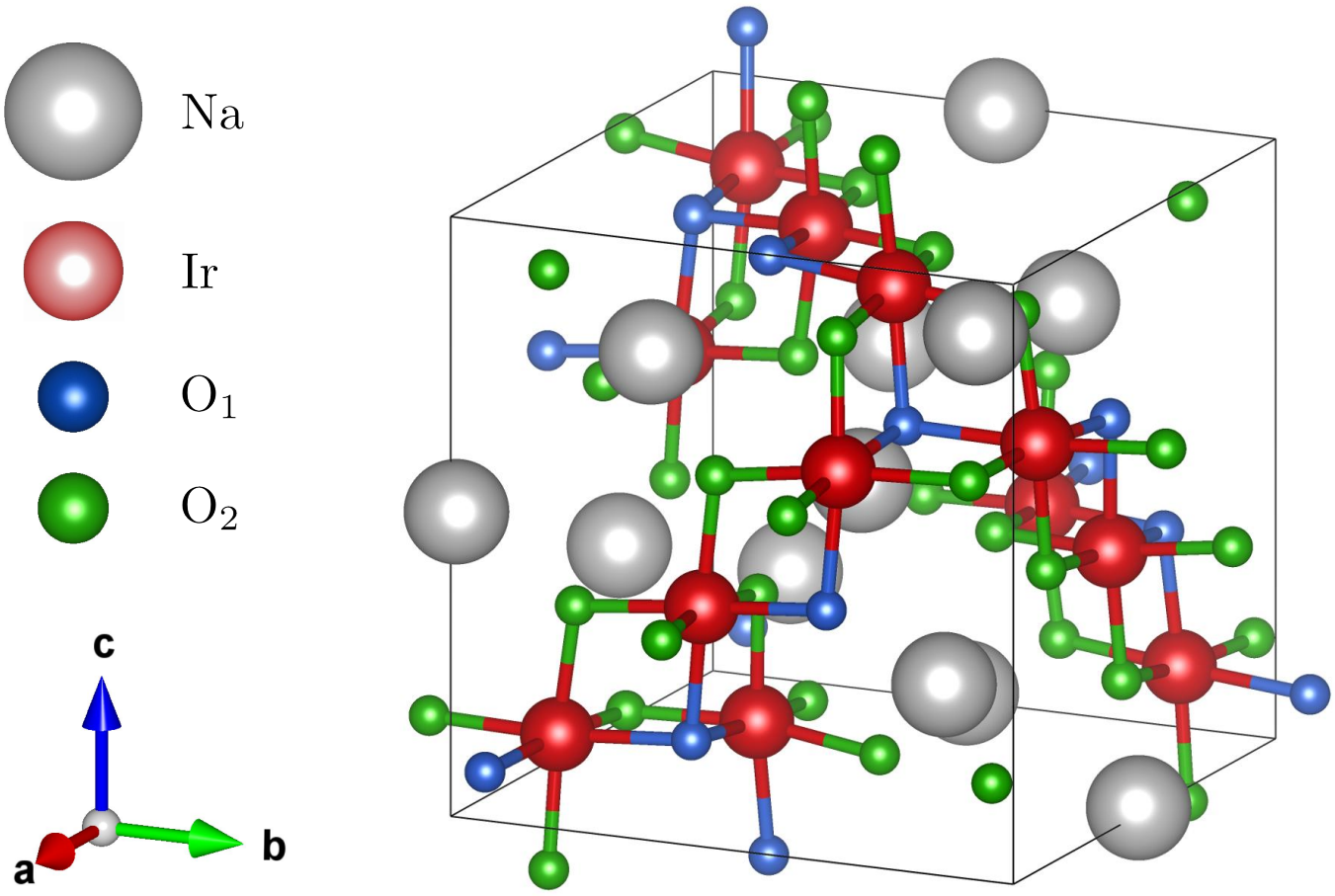
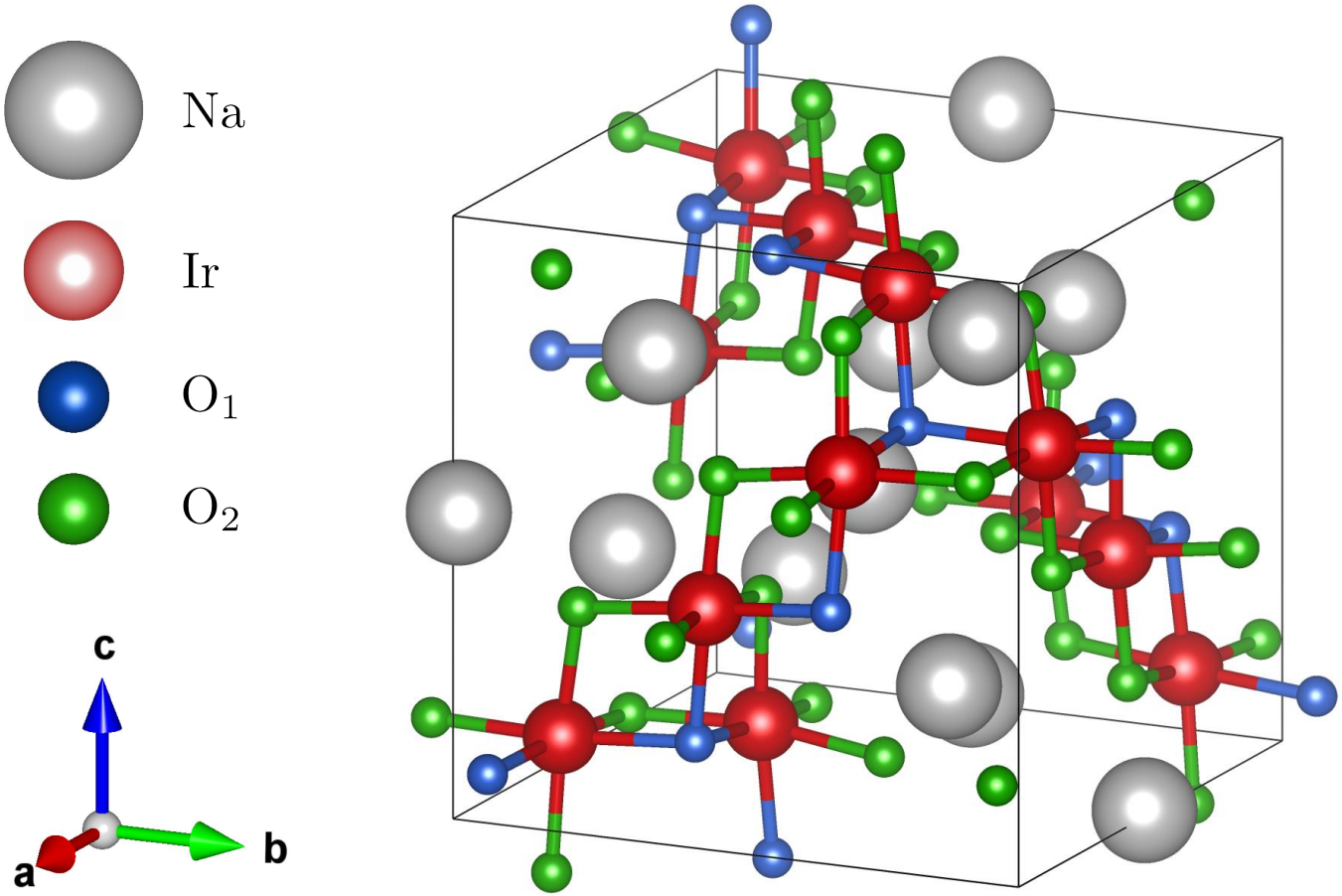
Ⓑ Why does the spin-orbit interaction drive the band insulator into a semi-metal?


Na
Ir
O_1
O_2
c
b
a



- first-order: O-octahedron around Ir atoms



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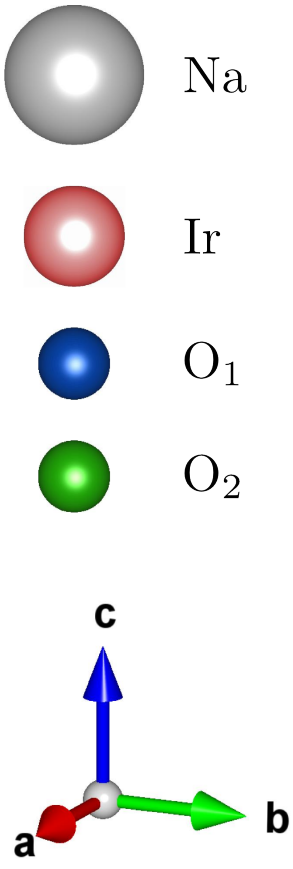

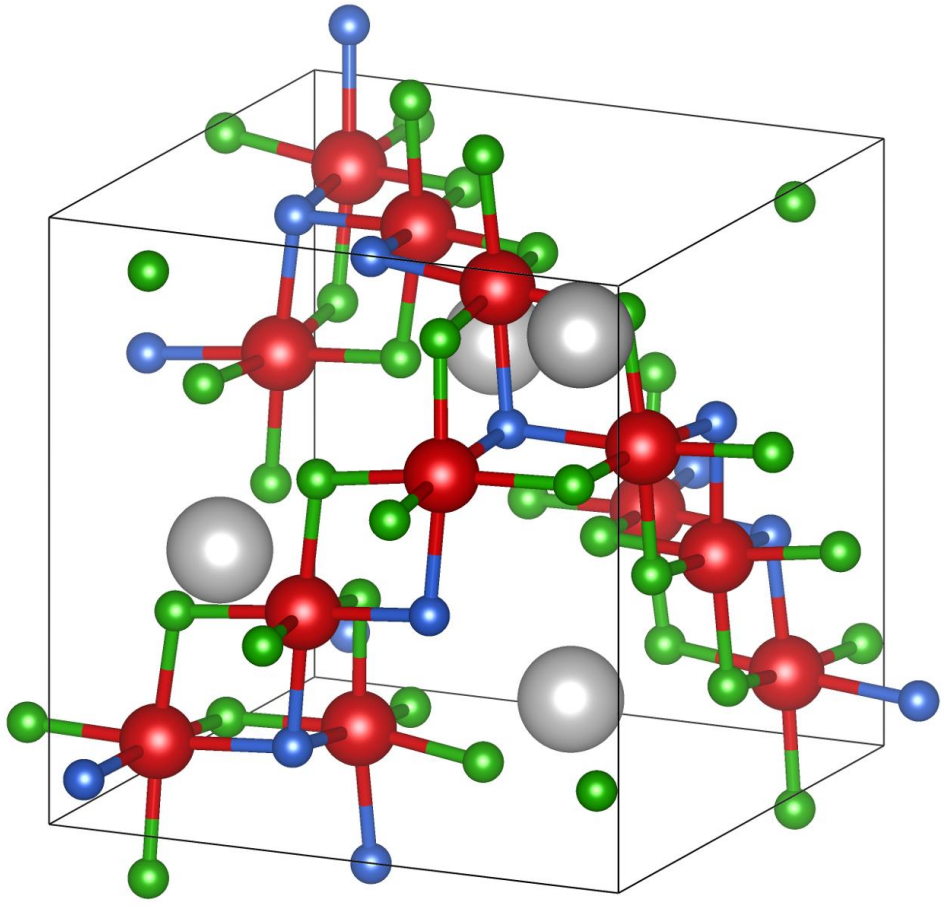

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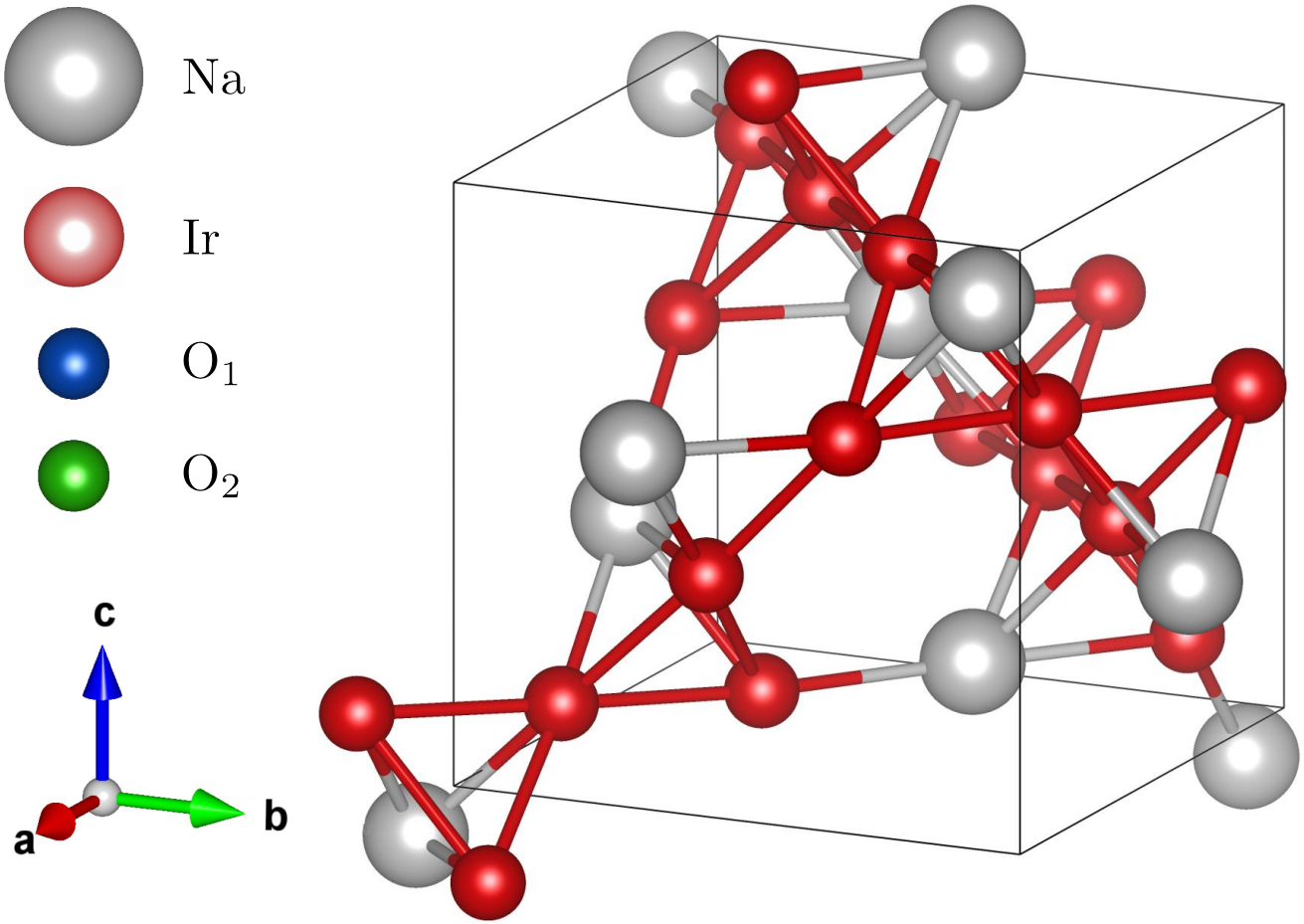
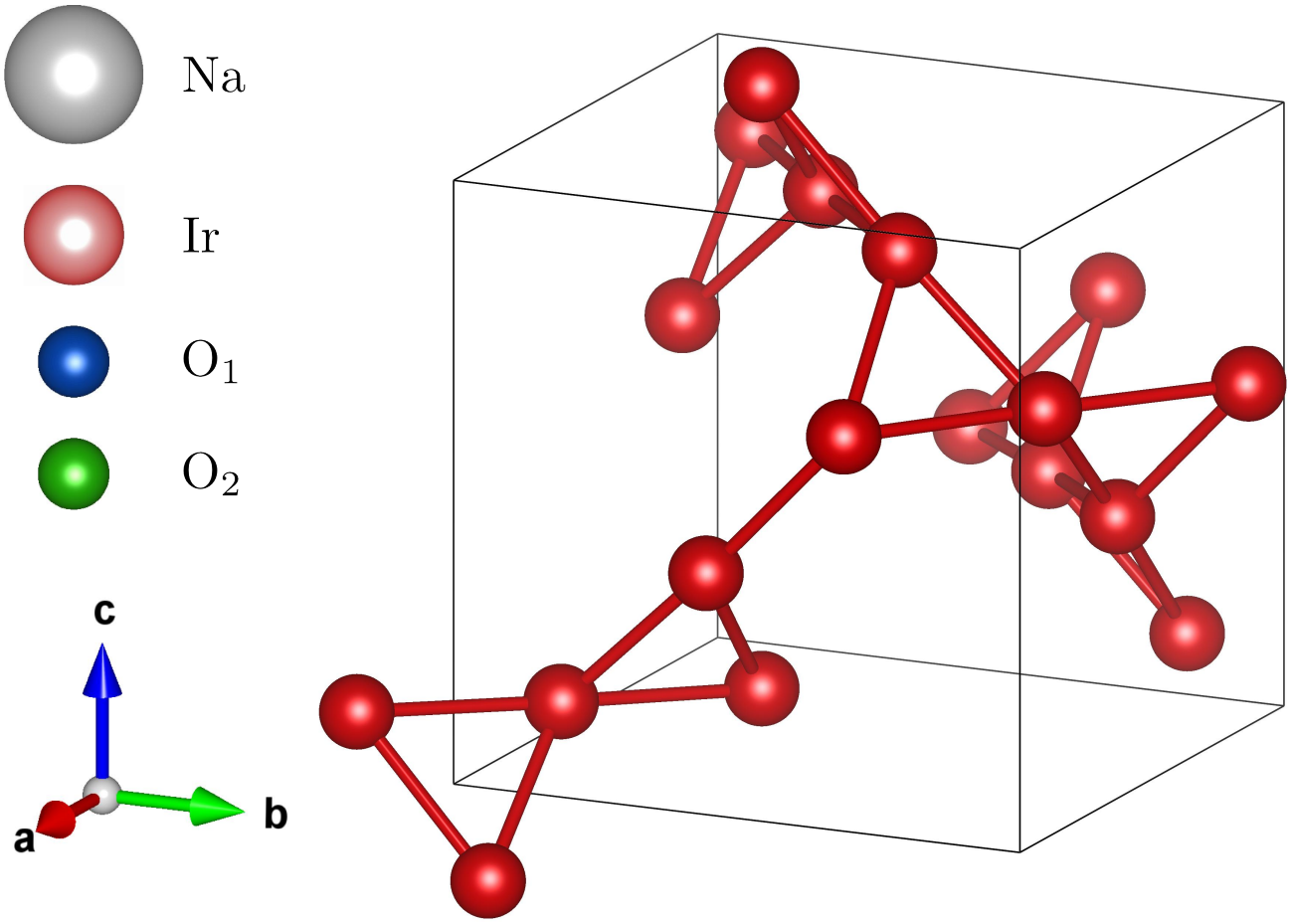


- first-order: O-octahedron around Ir atoms
- edge-sharing octahedra



- pseudo kagome lattice in 3D $\Rightarrow$ hyper-kagome

We have:

- $N_{\text{basis}} = 12 \text{ sites} \times 5 \text{ orbitals} \times 2 \text{ spins} = 120$

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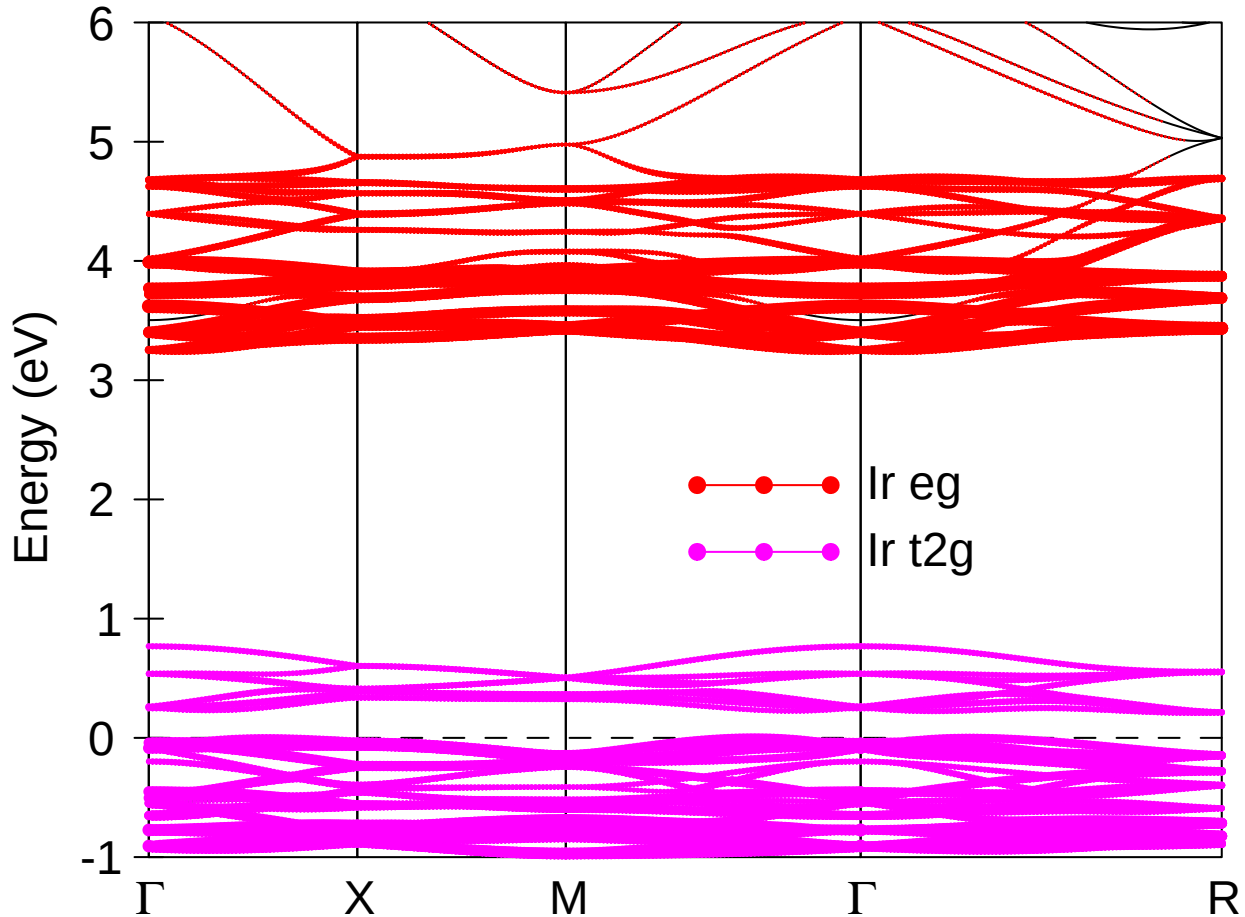

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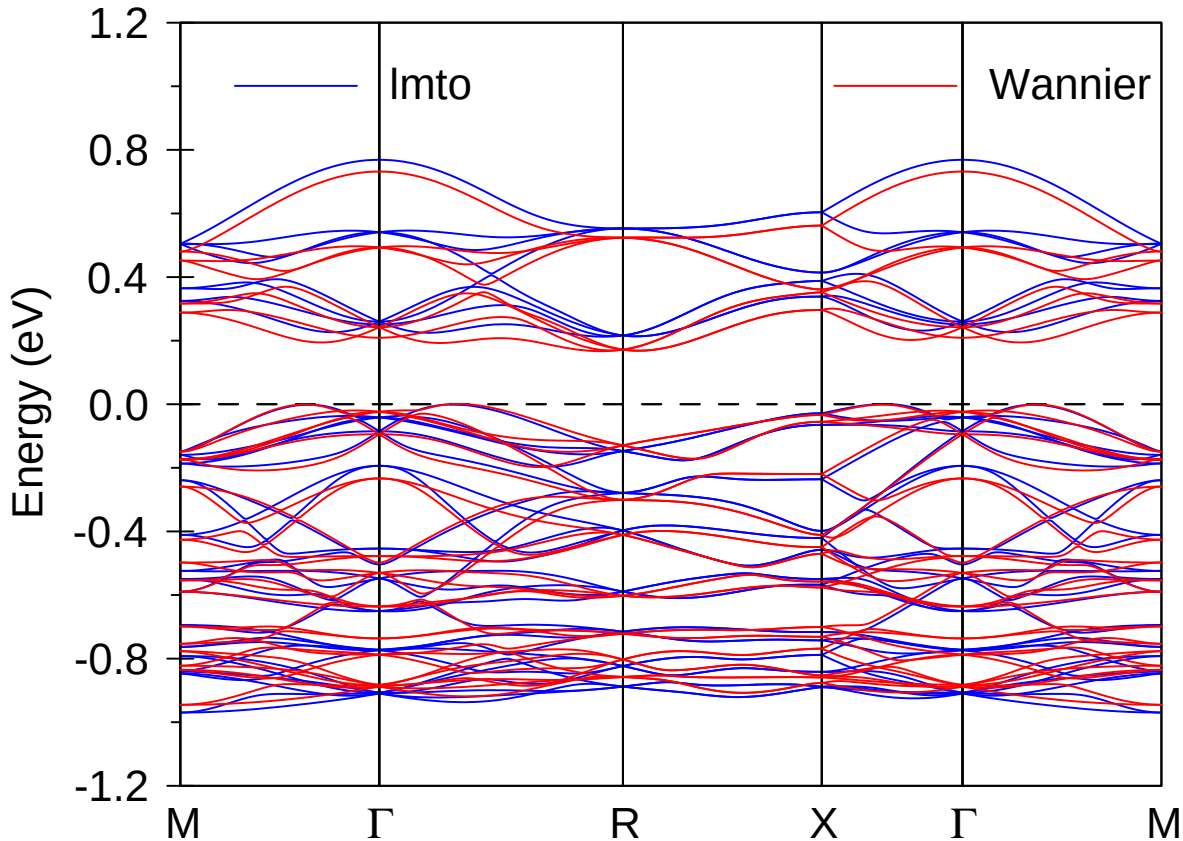
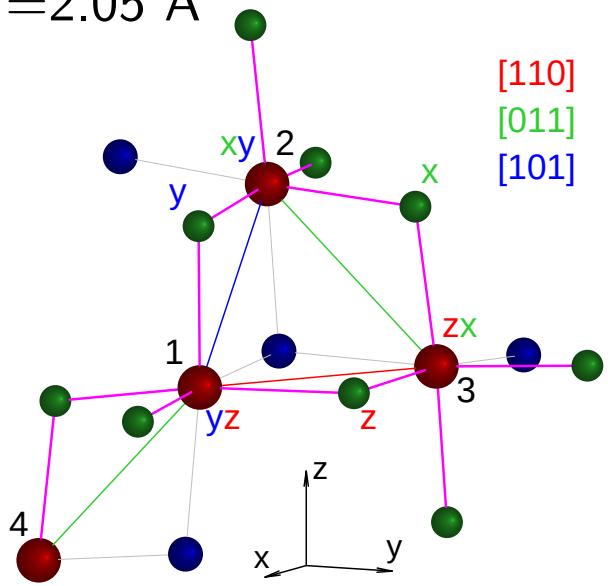


model

- there are two bonds: $d_{\mathrm{IrO_2}}$=1.98 Å and $d_{\mathrm{IrO_1}}$=2.05 Å



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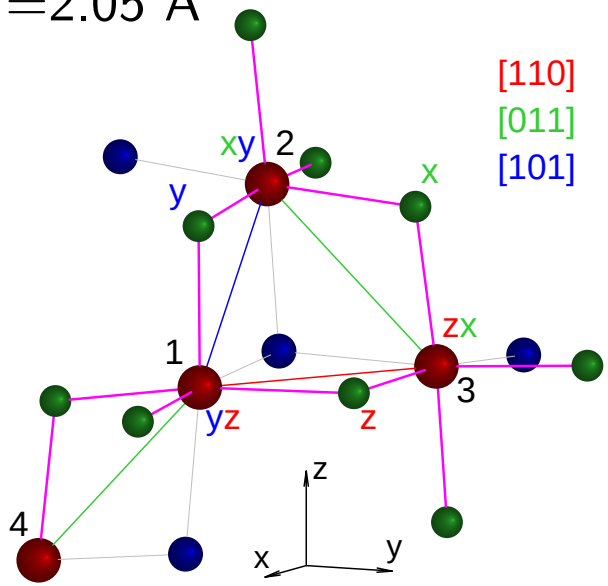

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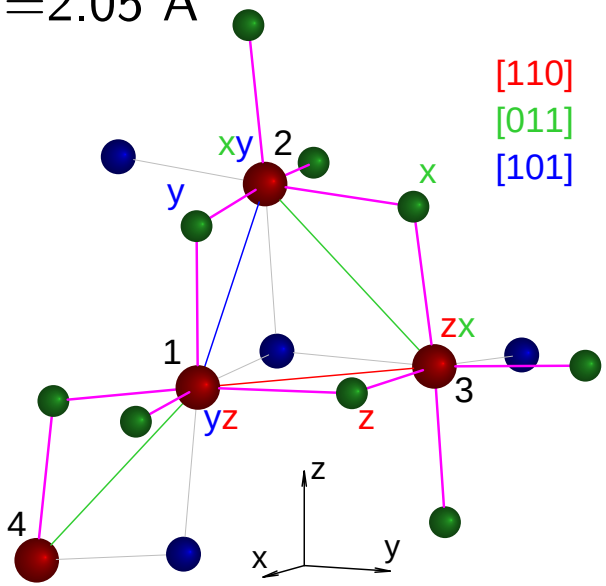
- **k**-integrated occupation matrix:

$$\begin{pmatrix} d_{zx} & d_{yz} & d_{xy} & \\ +1.324 & -0.595 & -0.596 & d_{zx} \\ -0.595 & +1.324 & -0.597 & d_{yz} \\ -0.596 & -0.597 & +1.325 & d_{xy} \end{pmatrix}$$



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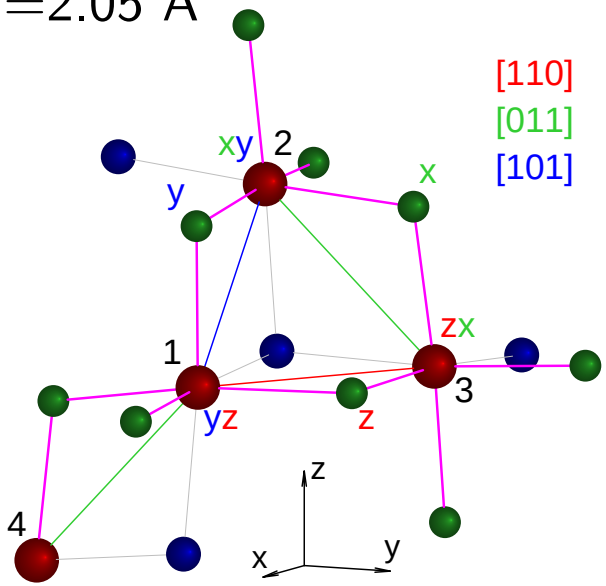

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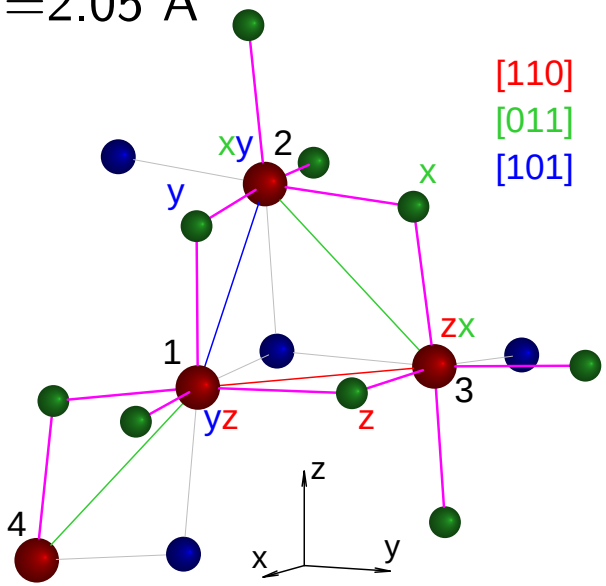

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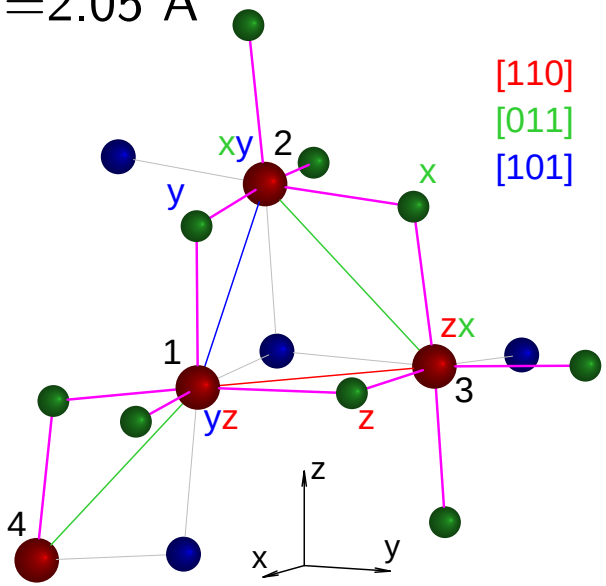

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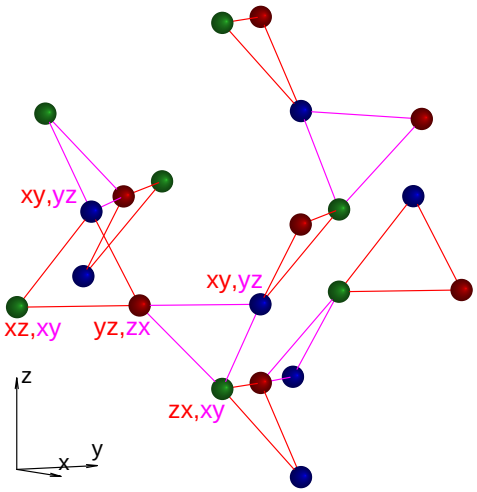


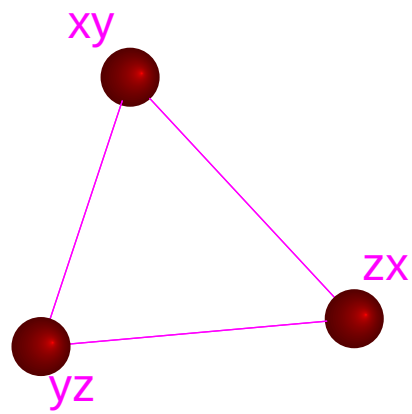
$\Downarrow$

The hyper-kagome lattice splits into triangles

a single triangle

2× bonding MO: $\varepsilon_{bn} = -t'$, $n = 1, 2$

$$\phi_{bn} = \frac{1}{\sqrt{3}} \left(d_{xy} + e^{i2\pi n/3} d_{yz} + e^{i4\pi n/3} d_{zx} \right)$$



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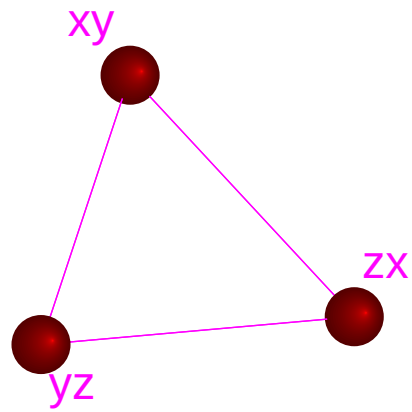

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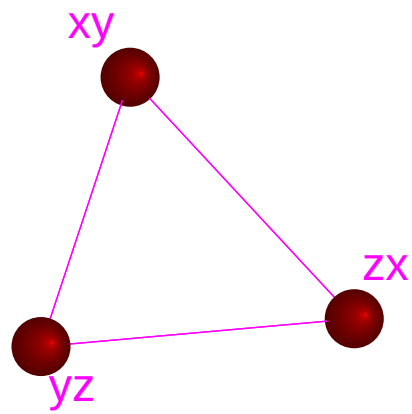

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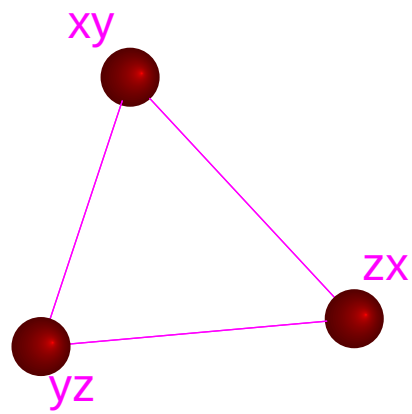

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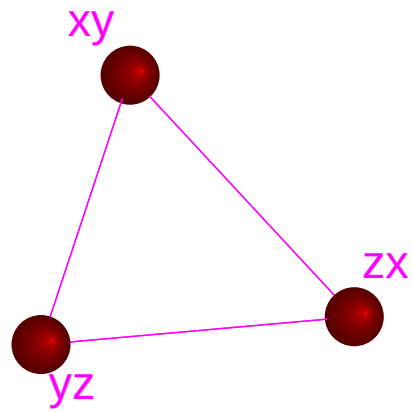

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$+$

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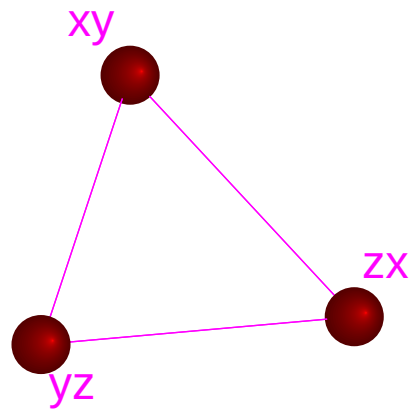

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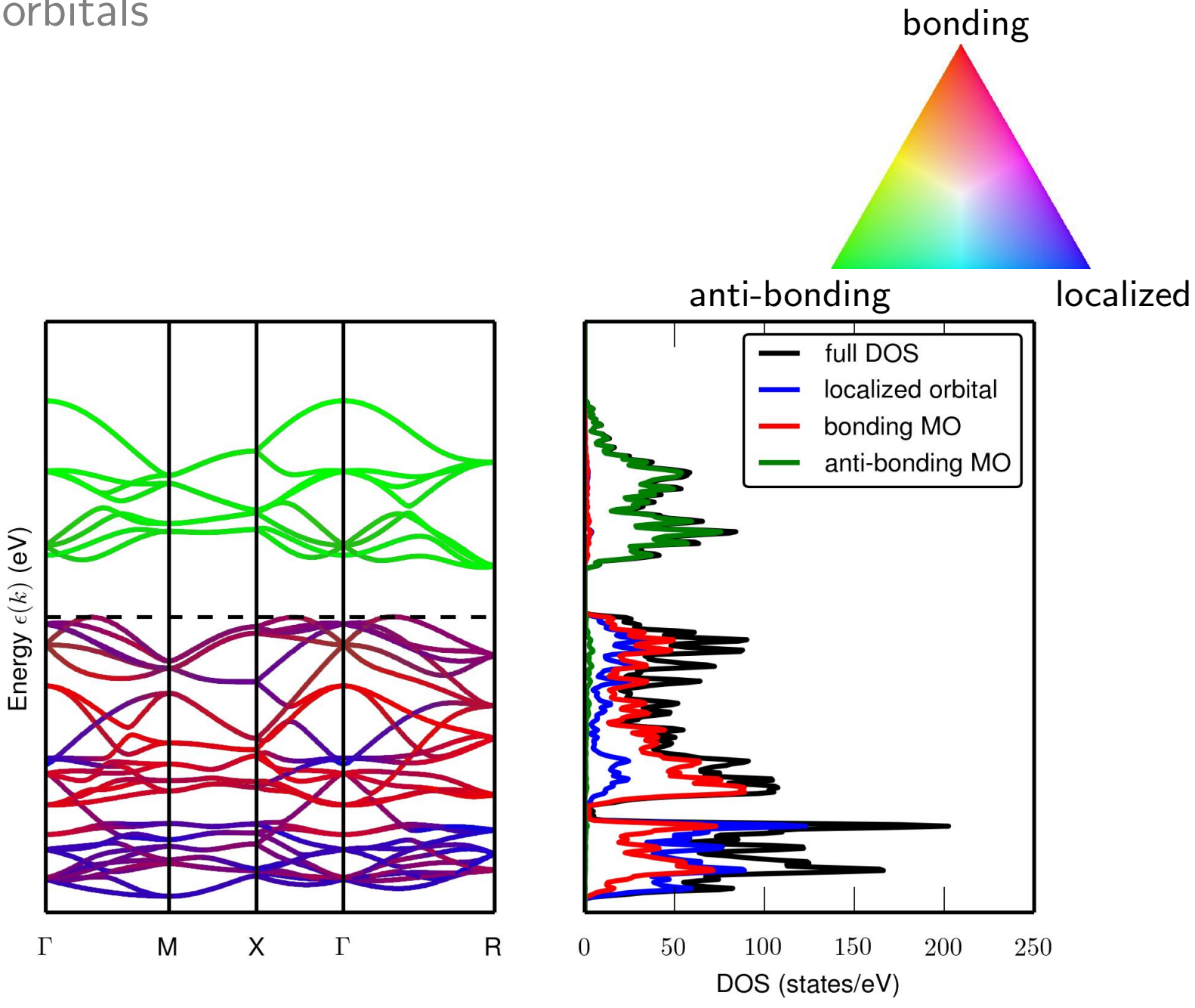
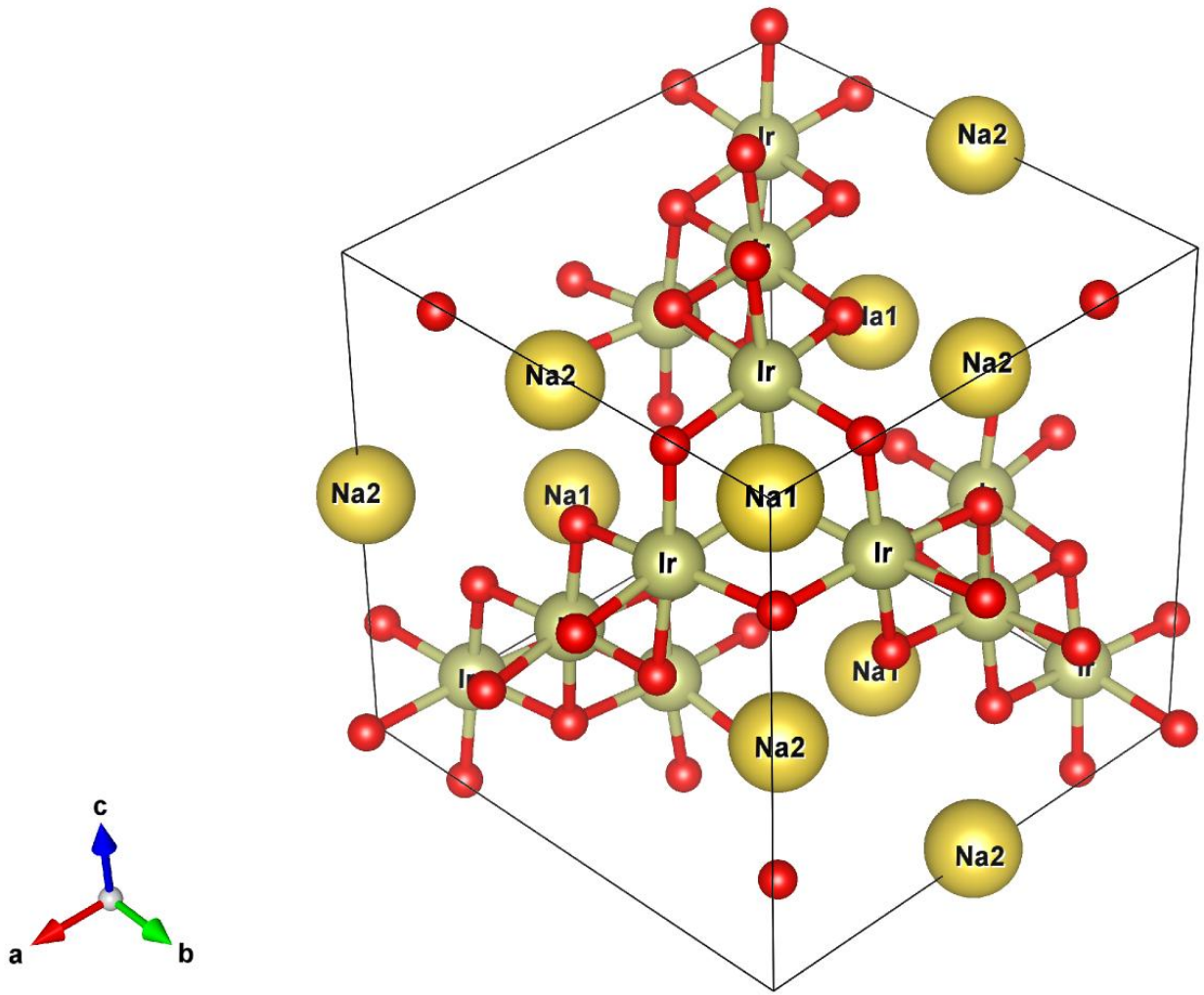
Without SOI $\mathrm{Na_3Ir_3O_8}$ would be insulating due to the formation of quasi-molecular orbitals on $\mathrm{Ir_3}$ triangles

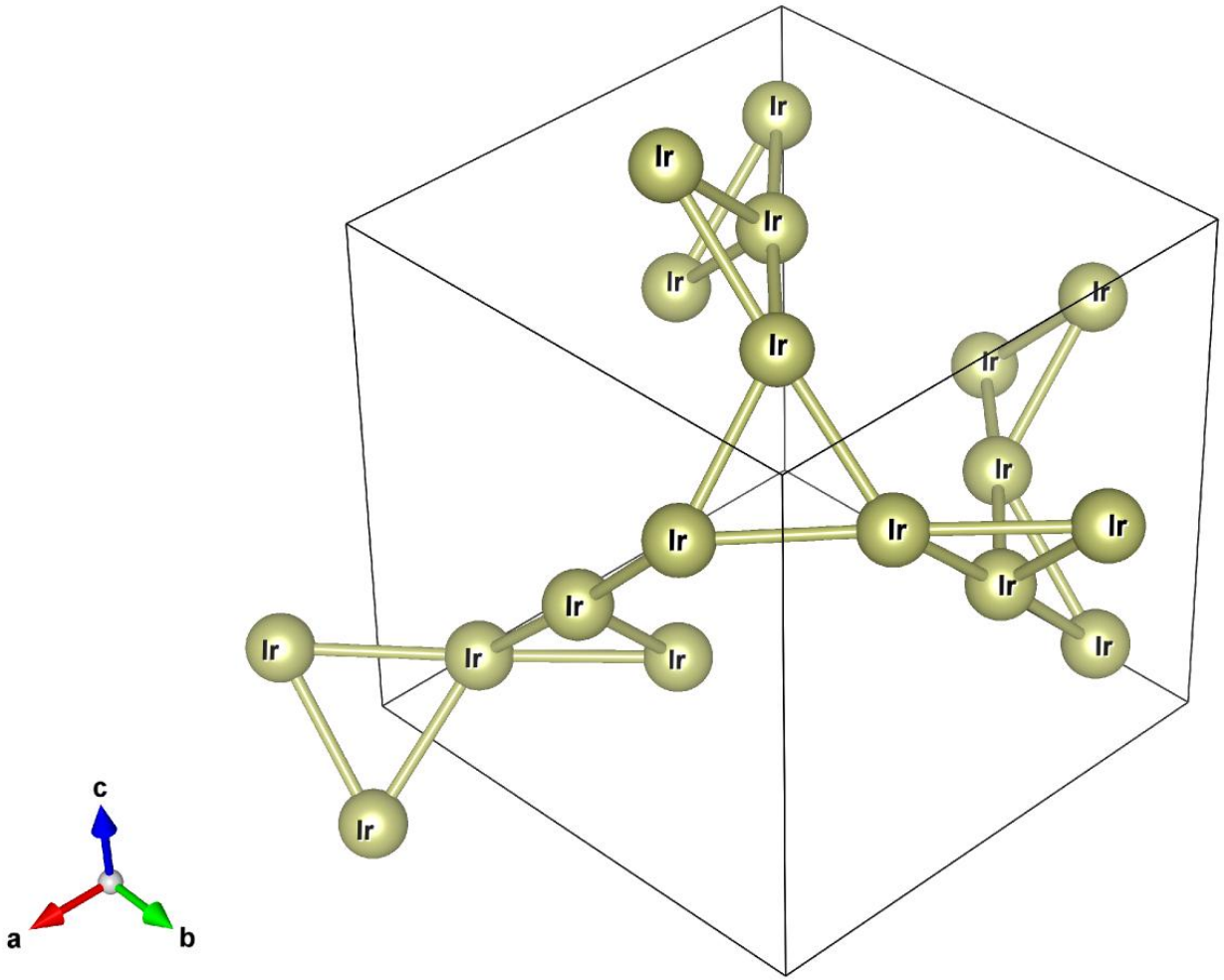
molecular orbitals



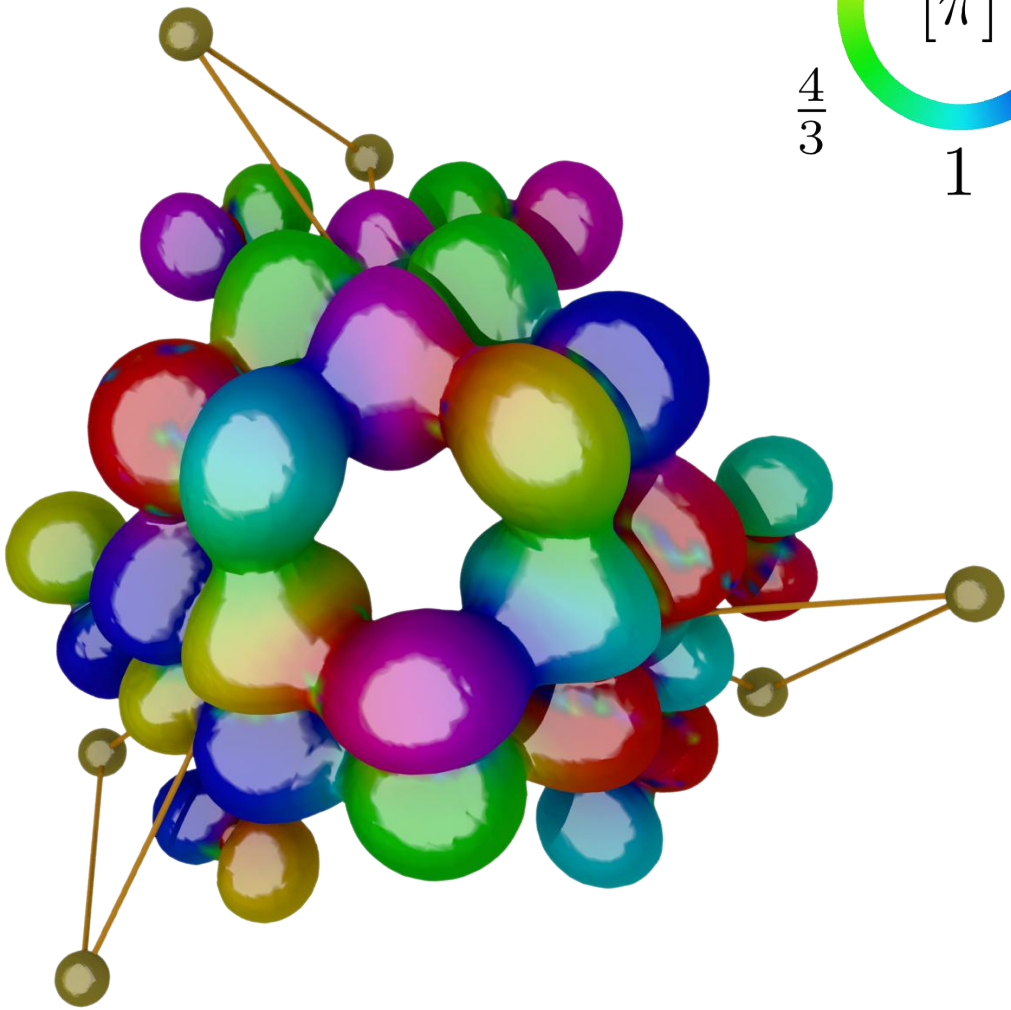
molecular orbitals



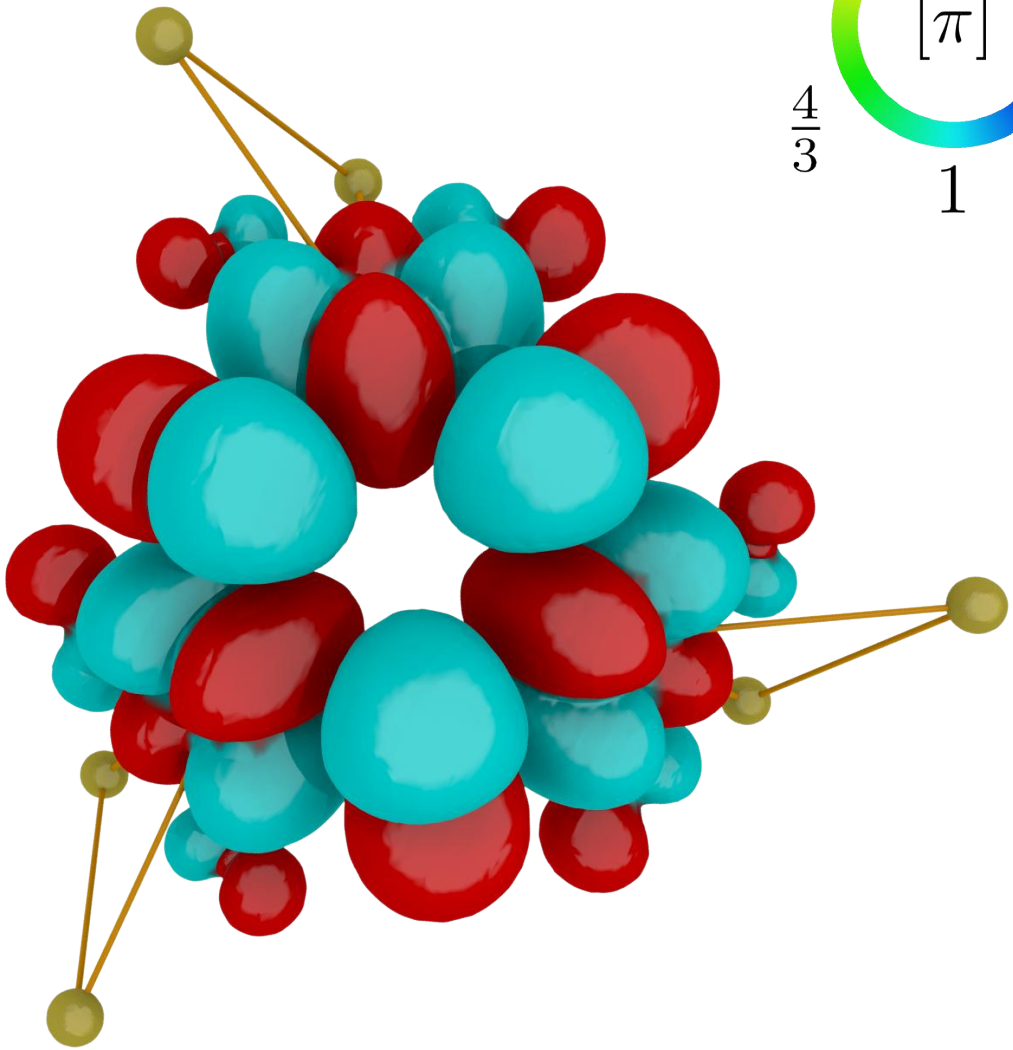
molecular orbitals



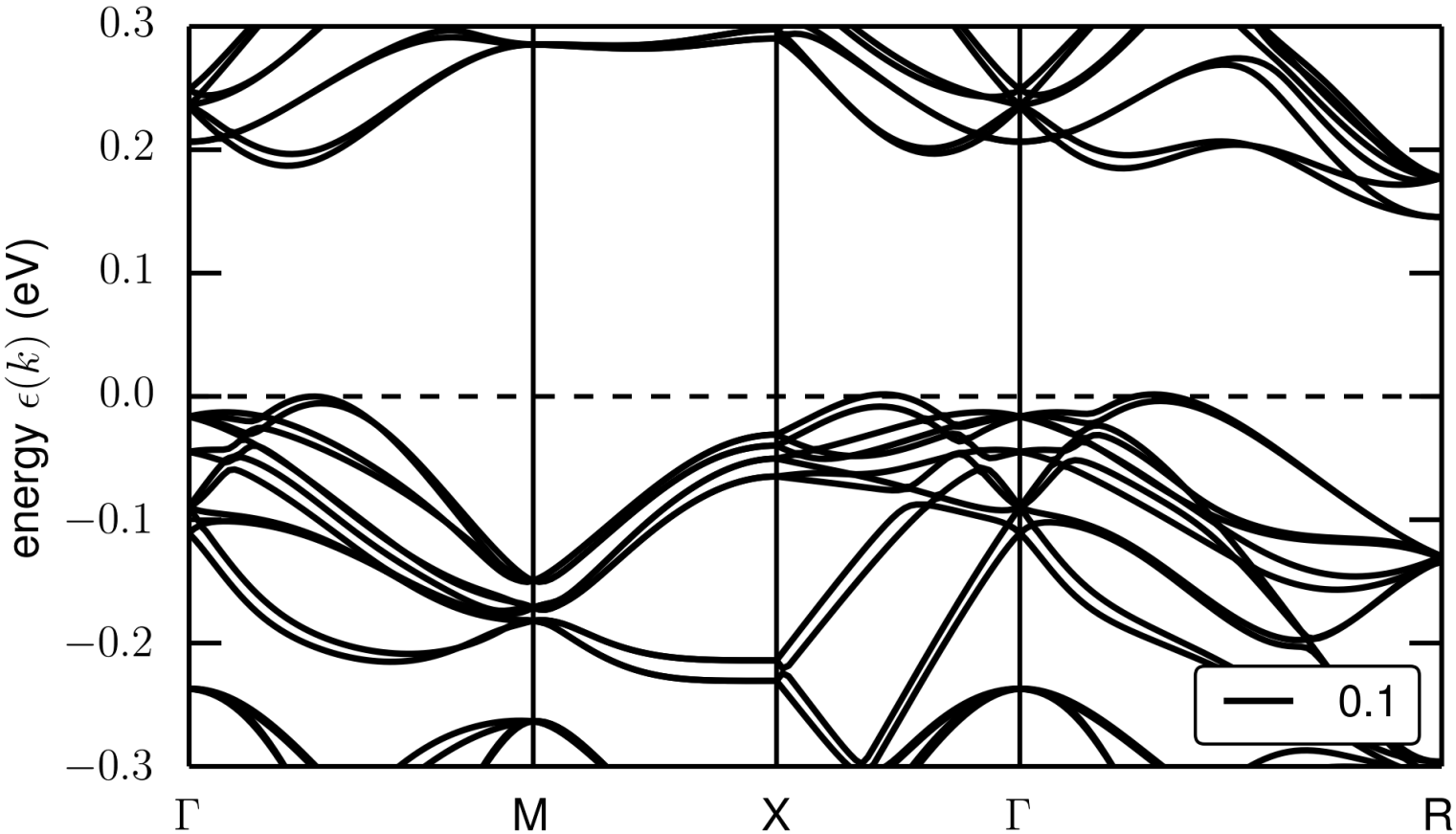
bonding
molecular orbital



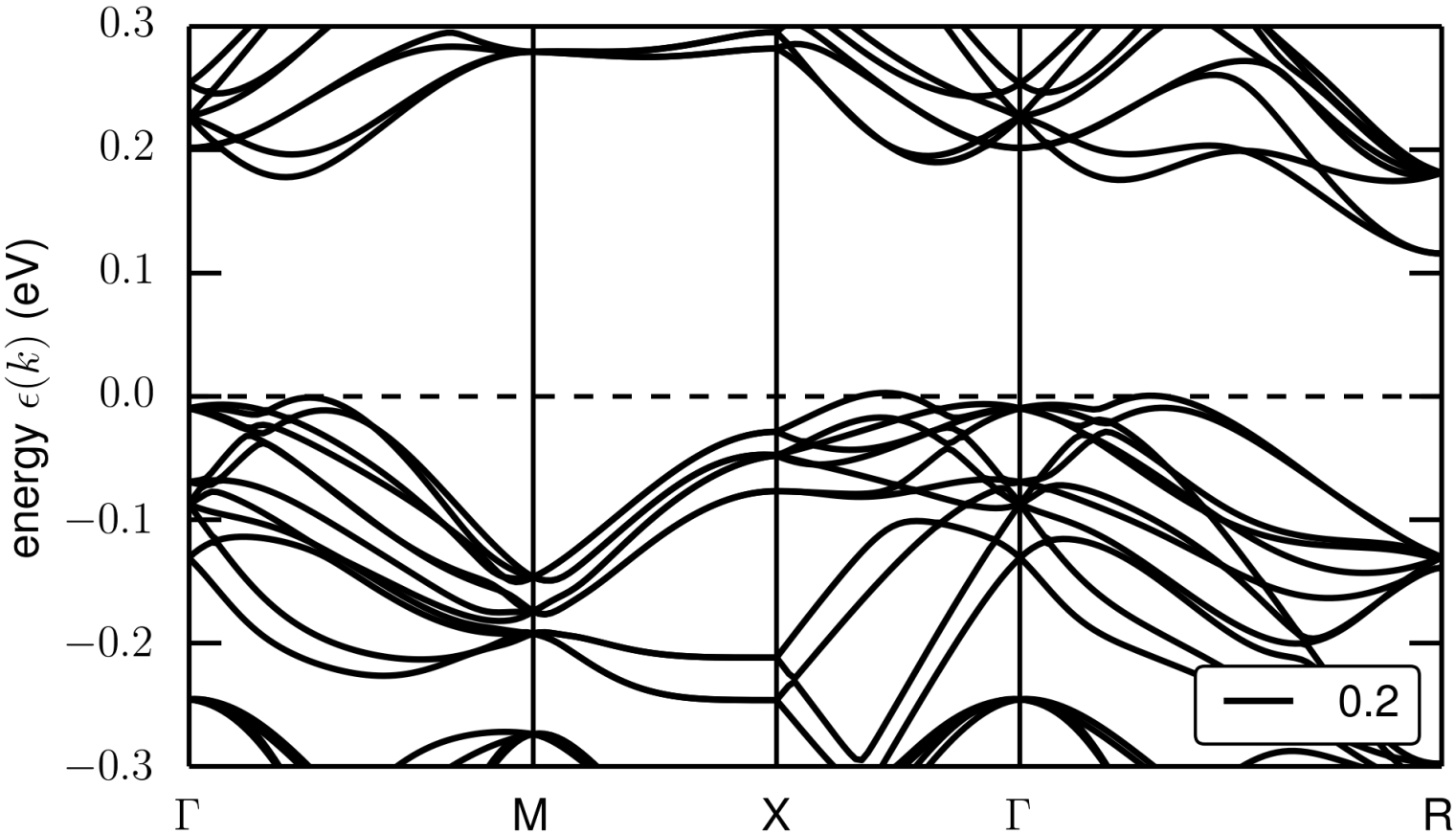
antibonding
molecular orbital



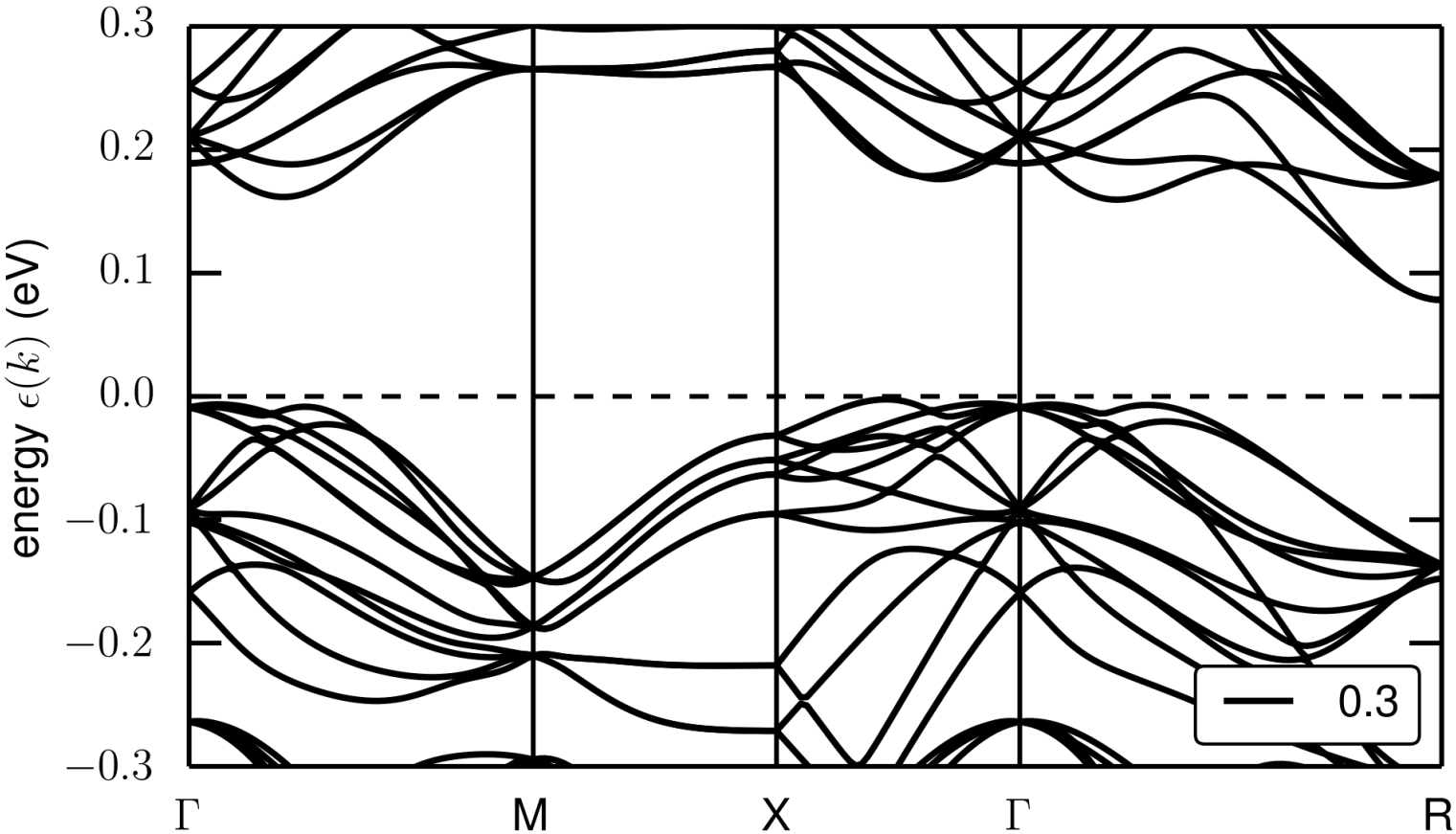
molecular orbitals



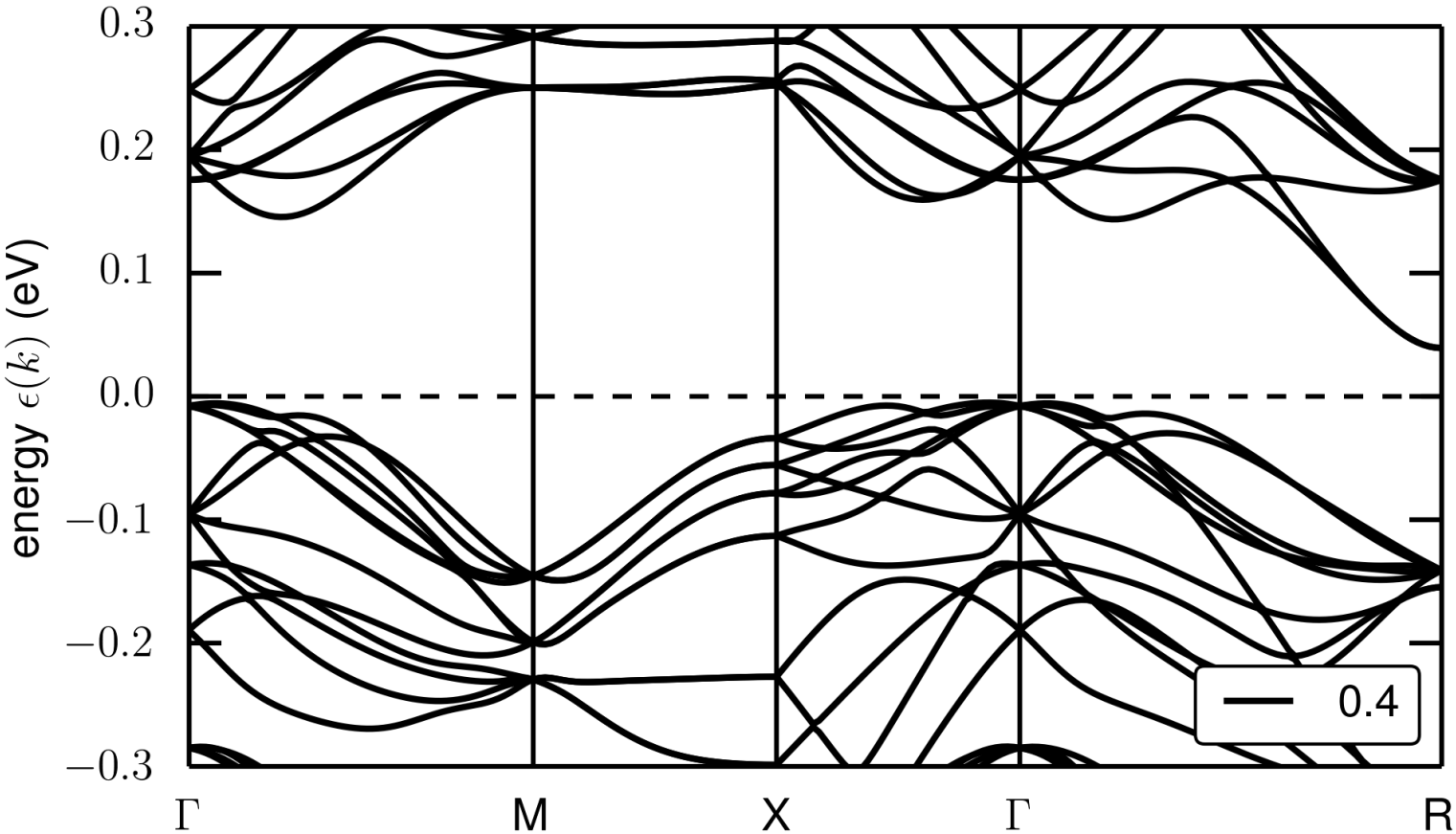
molecular orbitals



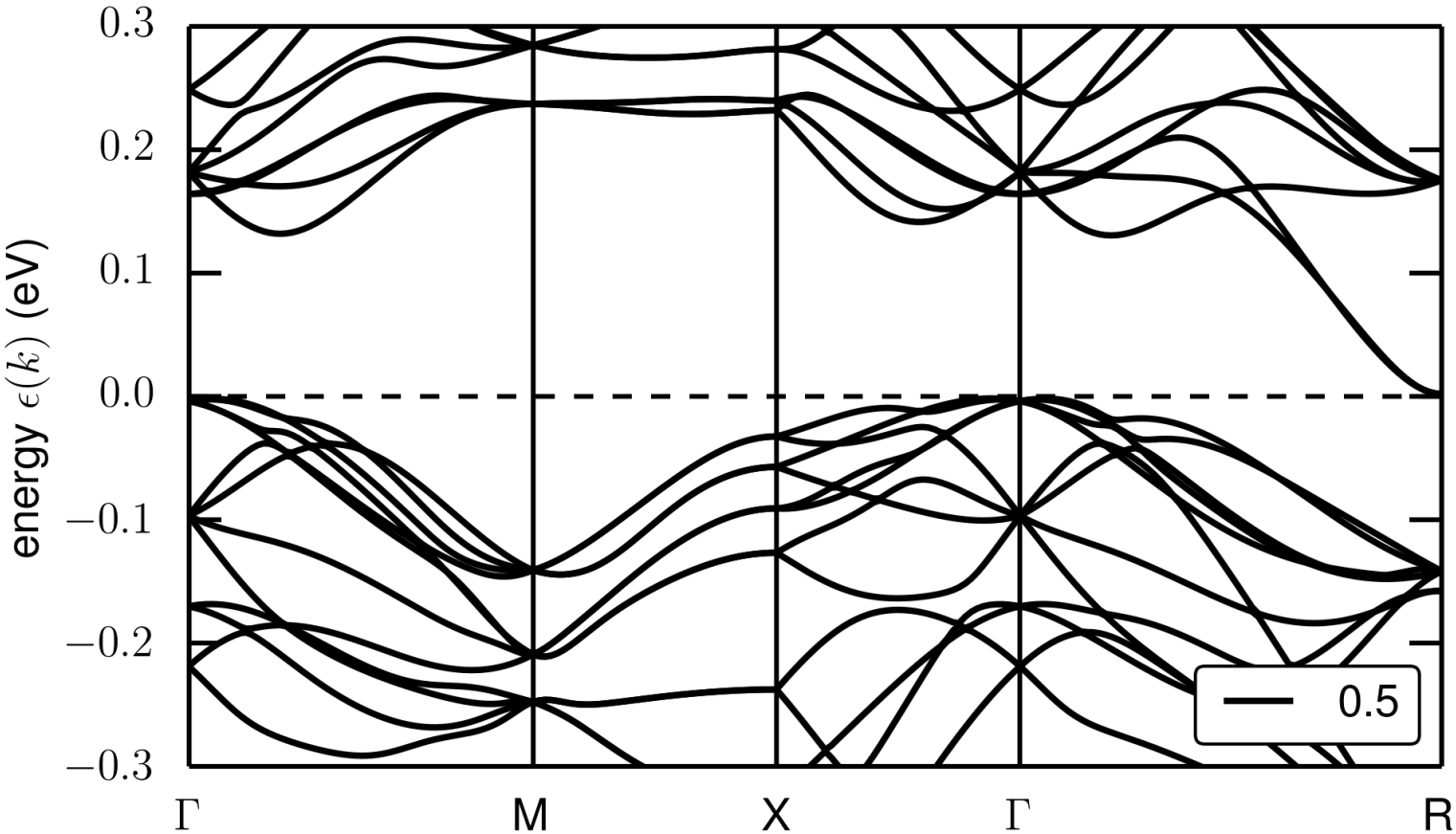
molecular orbitals



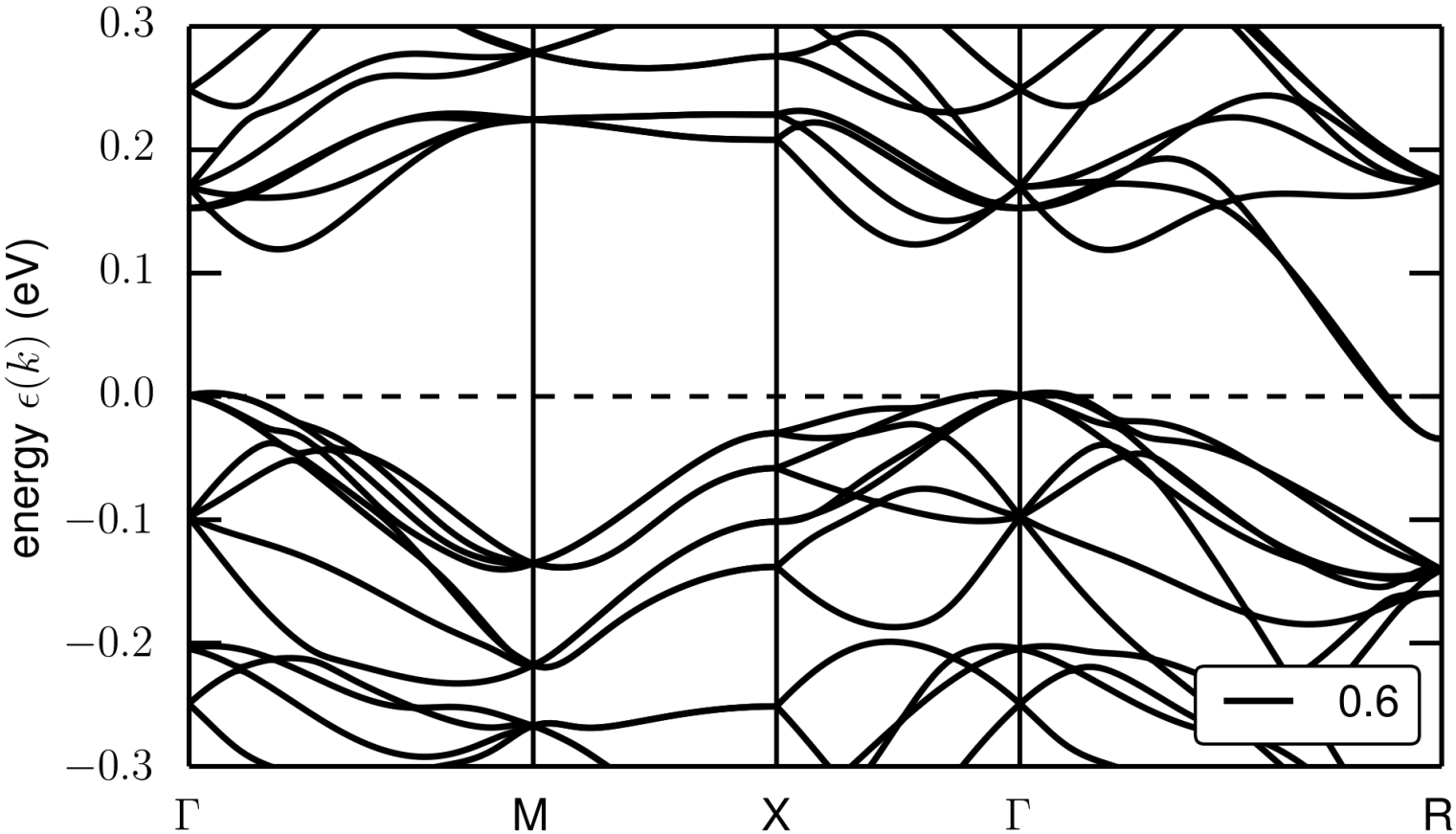
molecular orbitals



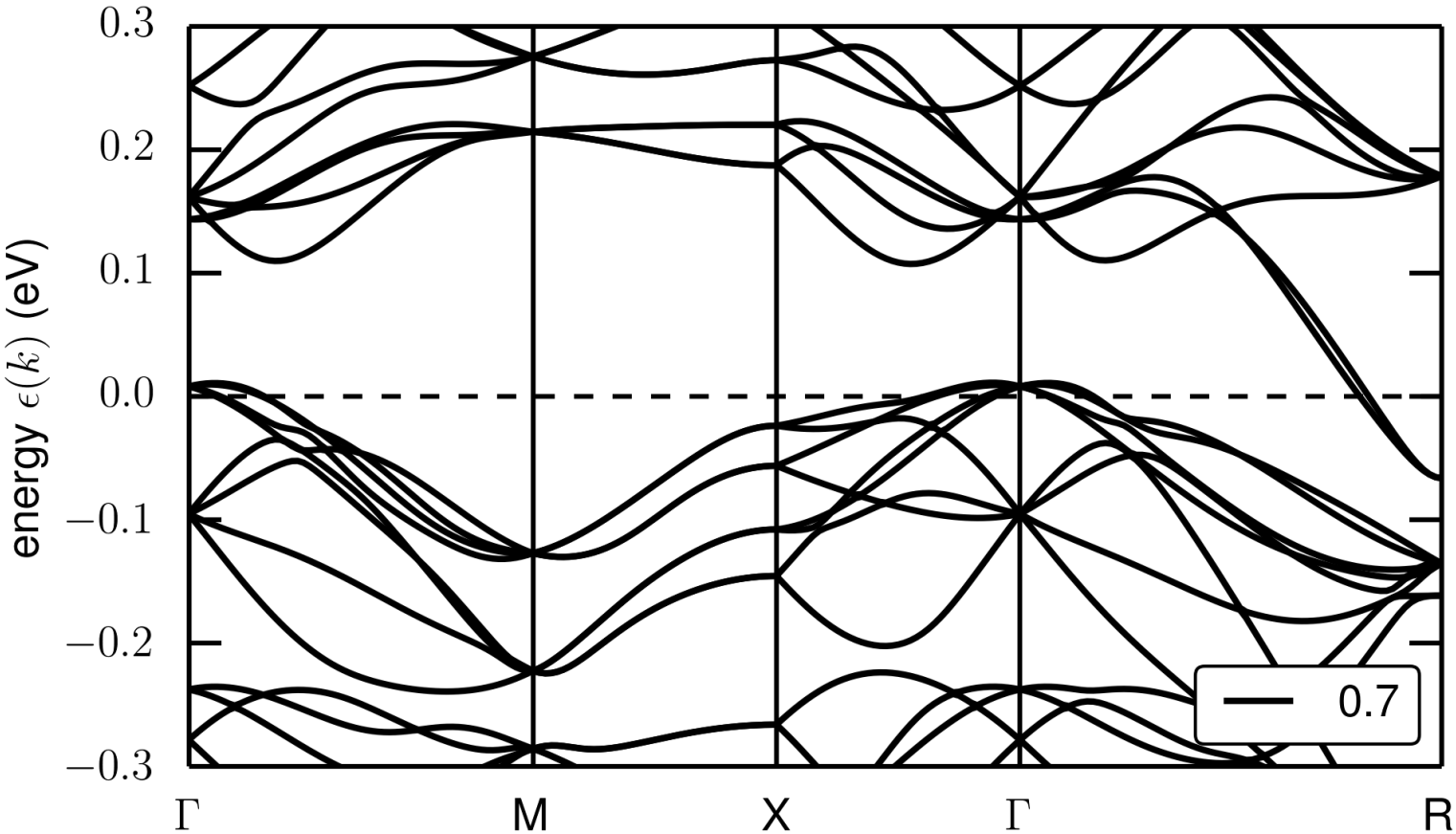
molecular orbitals



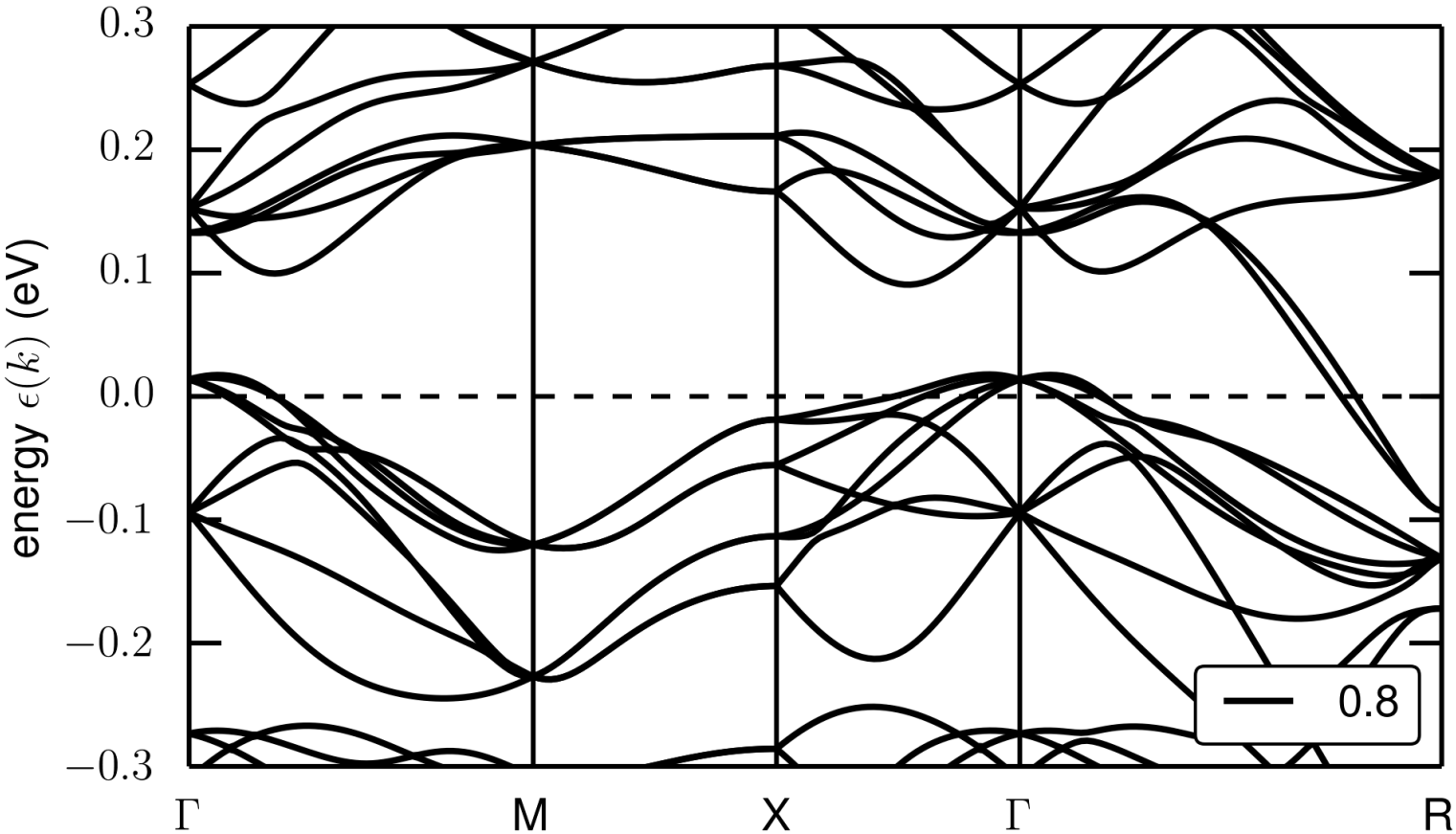
molecular orbitals



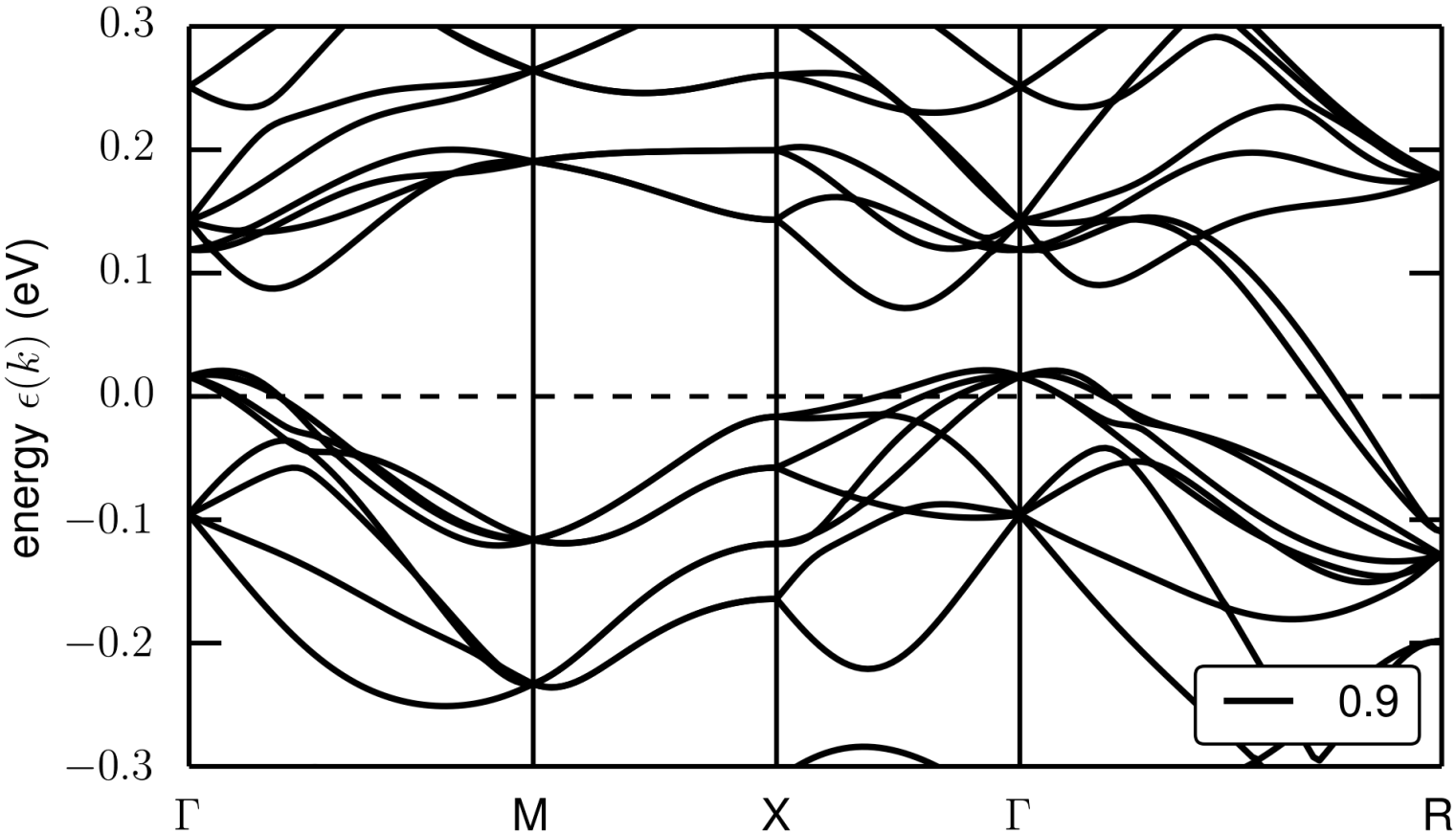
molecular orbitals



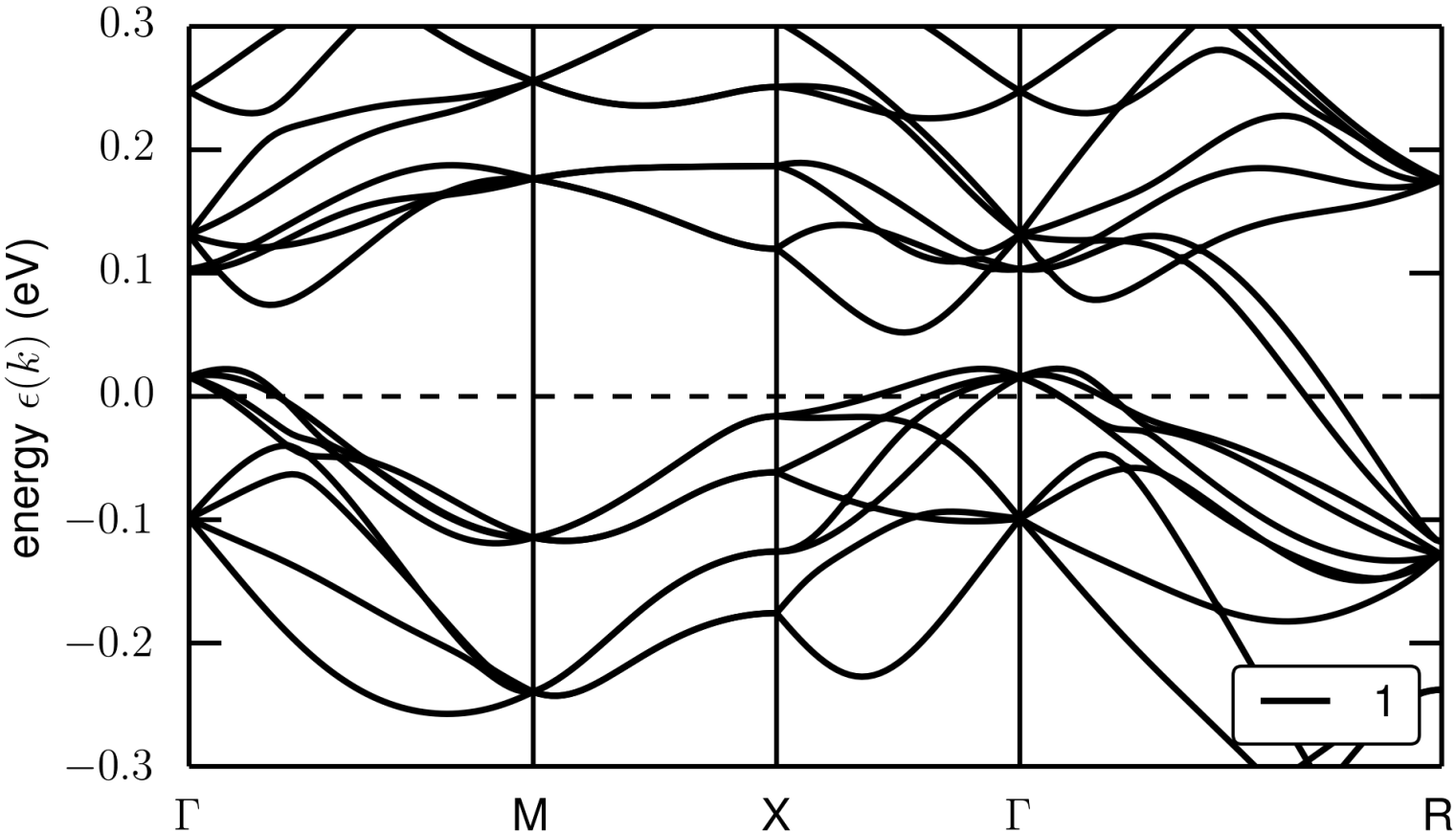
molecular orbitals

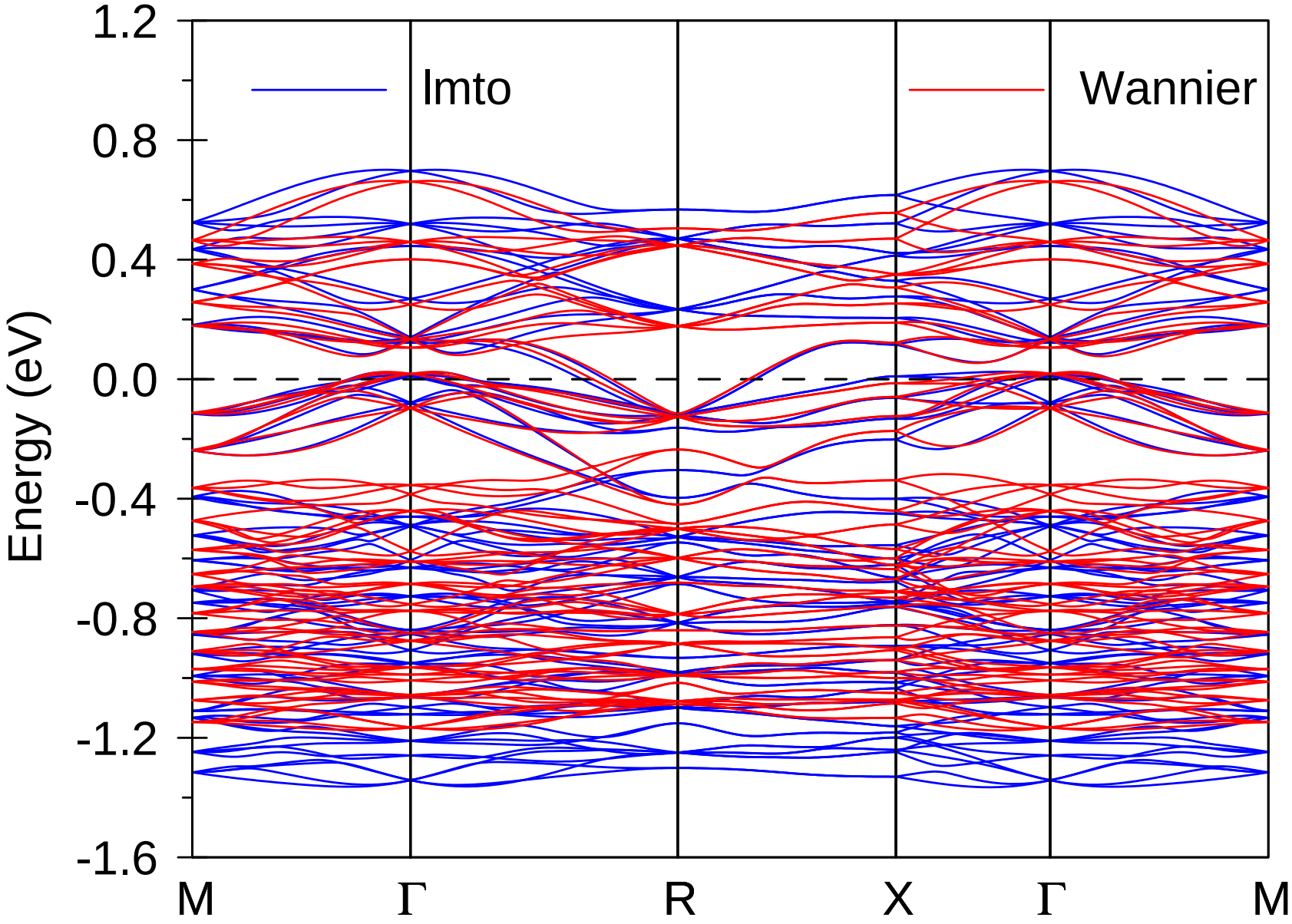


molecular orbitals

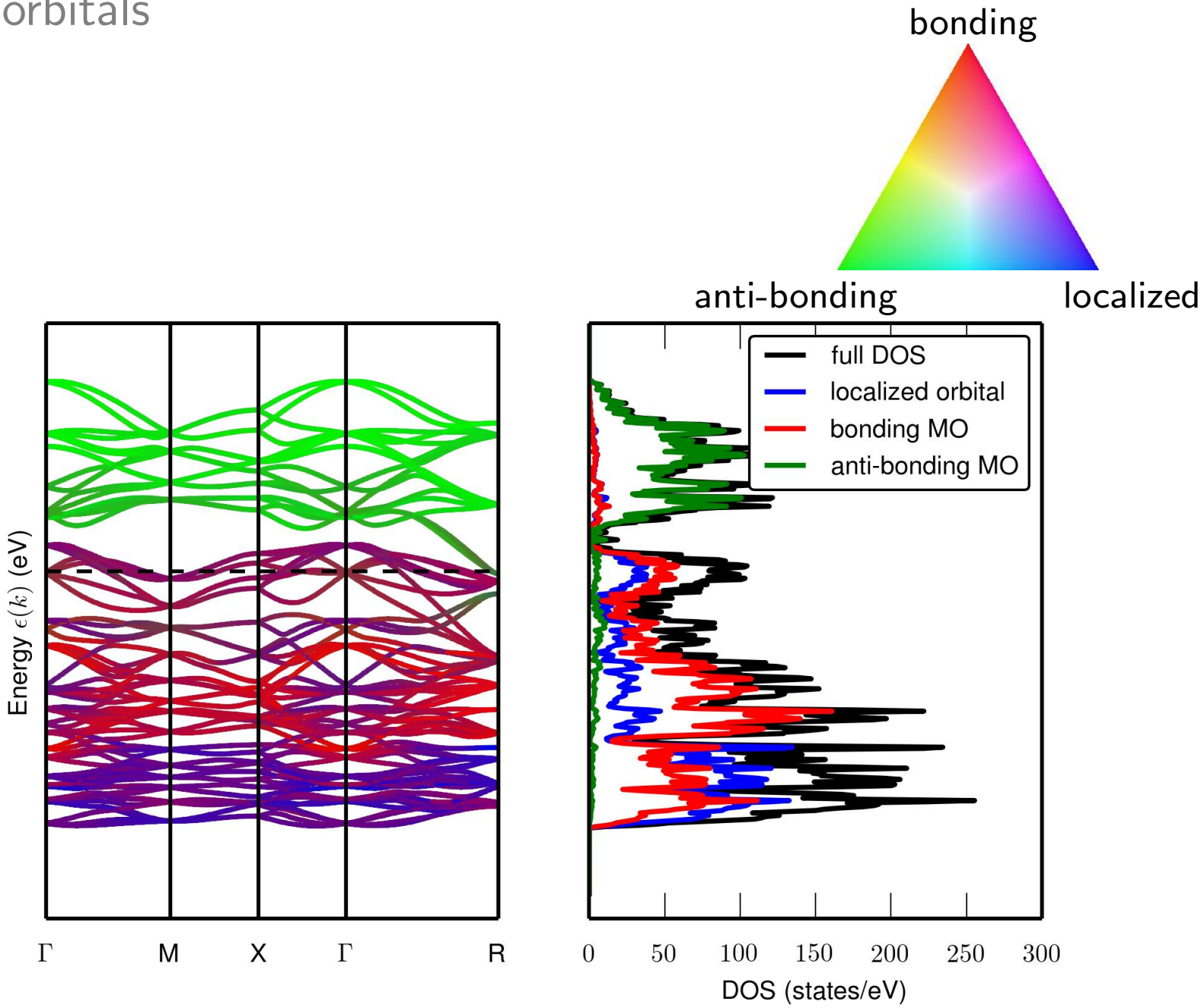


molecular orbitals

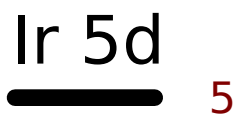



lmto
Wannier
Energy (eV)
1.2
0.8
0.4
0.0
-0.4
-0.8
-1.2
-1.6
M
Γ
R
X
Γ
M

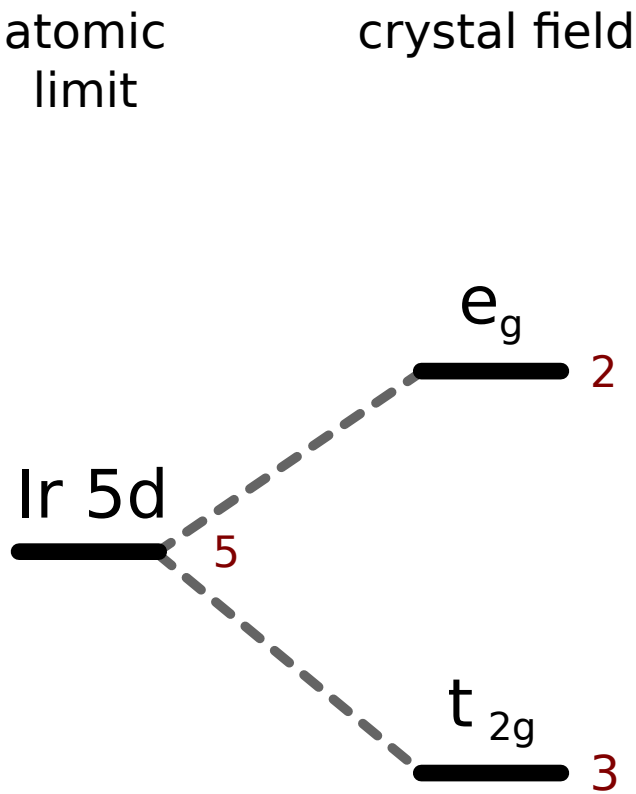
molecular orbitals



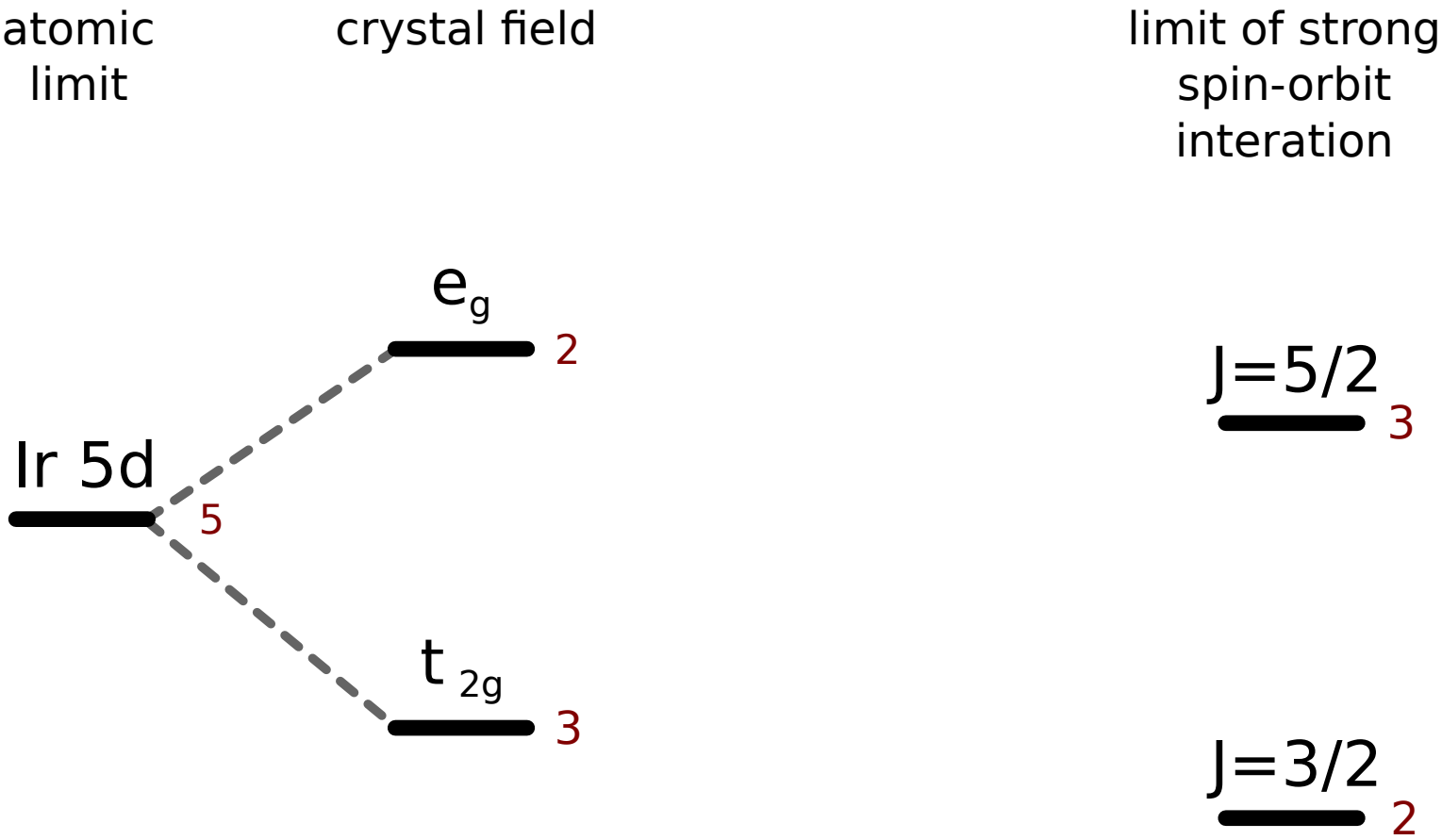
atomic
limit

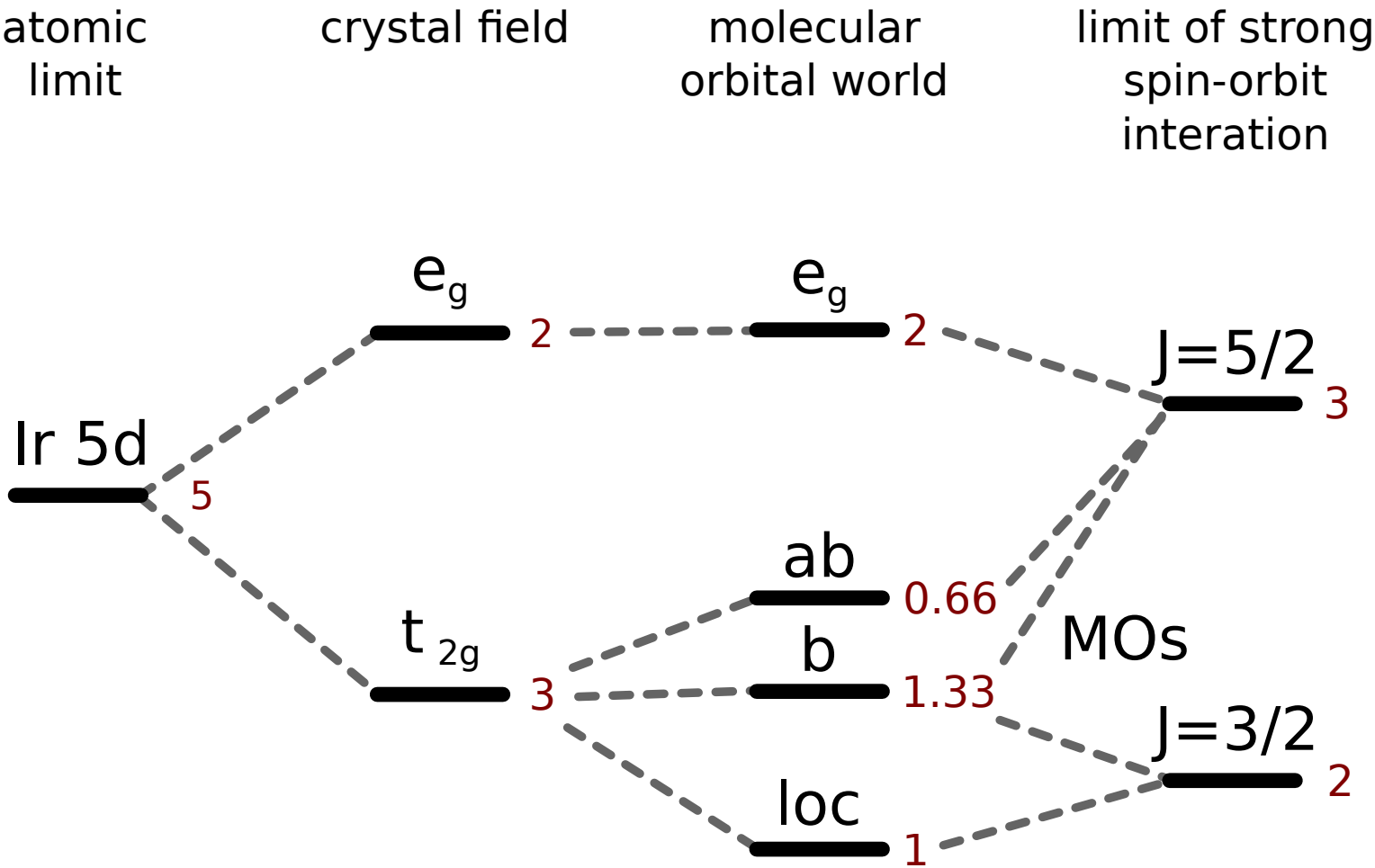


molecular orbitals

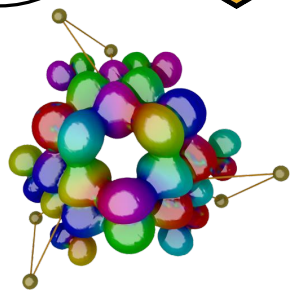


molecular orbitals

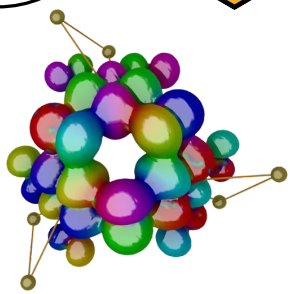



atomic limit
crystal field
molecular orbital world
limit of strong spin-orbit interation
Ir 5d
5
e_g
2
t_{2g}
3
e_g
2
ab
0.66
b
1.33
loc
1
MOs
J=5/2
3
J=3/2
2

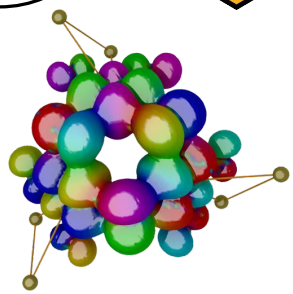
- ✓ Molecular orbital order renders $\mathrm{Na_3Ir_3O_8}$ a band insulator.

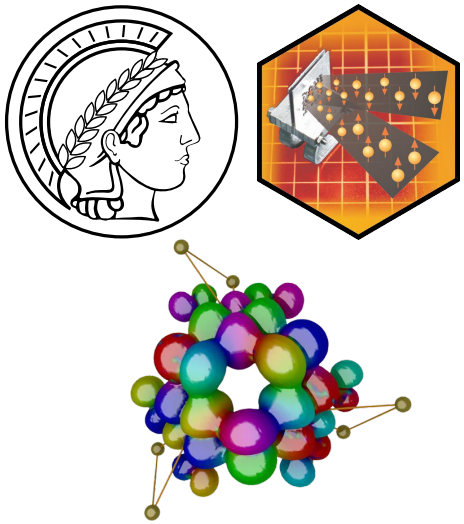


- ✓ Molecular orbital order renders $\mathrm{Na_3Ir_3O_8}$ a band insulator.
- ✓ Spin-orbit interaction introduces a coupling between MOs on neighboring triangles $\Rightarrow$ gap closure.



- ✓ Molecular orbital order renders $\mathrm{Na_3Ir_3O_8}$ a band insulator.
- ✓ Spin-orbit interaction introduces a coupling between MOs on neighboring triangles $\Rightarrow$ gap closure. *This is in stark contrast to* Sr_2IrO_4 *in which SOI creates/enhances the band gap.*





- ✓ Molecular orbital order renders $\mathrm{Na_3Ir_3O_8}$ a band insulator.
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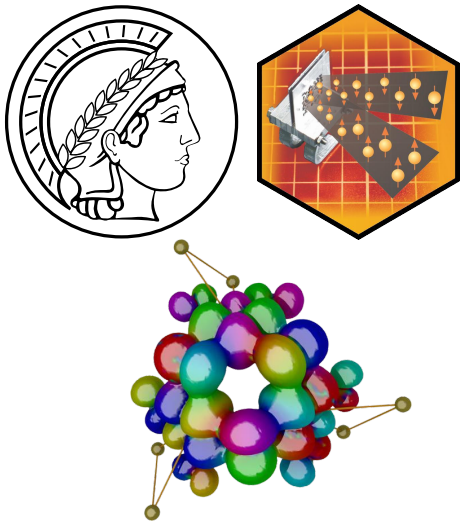
outlook: substitute Ir by Co or Rh to obtain an insulator tunable with pressure



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Get decent spaghetti: ask (yourself or your favorite theoretician) for a physical interpretation of the presented *ab-initio* solutions of your problem. Don't be satisfied with "blackbox" results.

supplementary

JJ Randall et al. JACS **79**, 266-267 (1957)
MK Crawford et al. PRB **49**, 9198 (1994)
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BJ Kim et al. Science **323**, 1329-1332 (2009)
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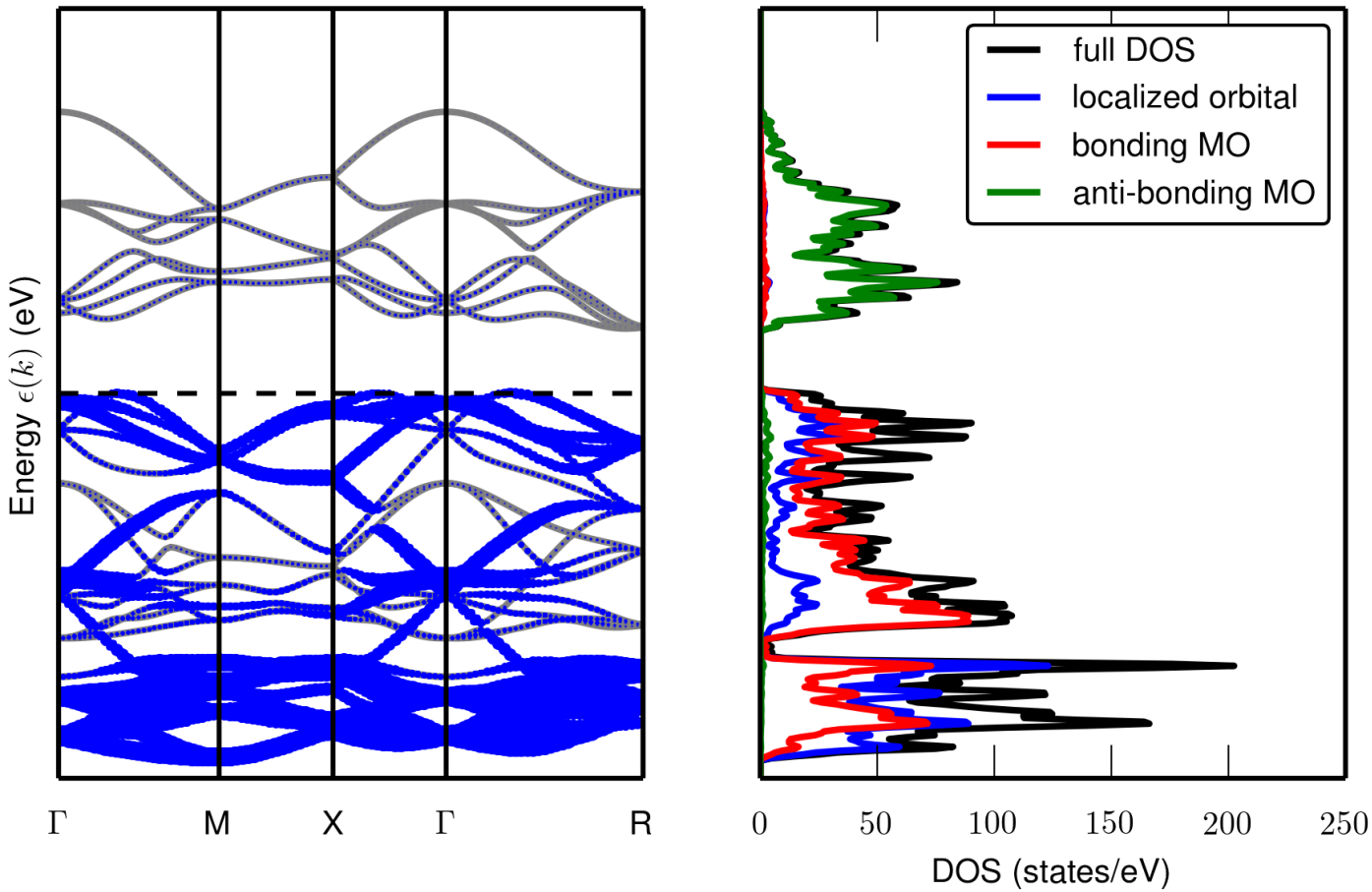
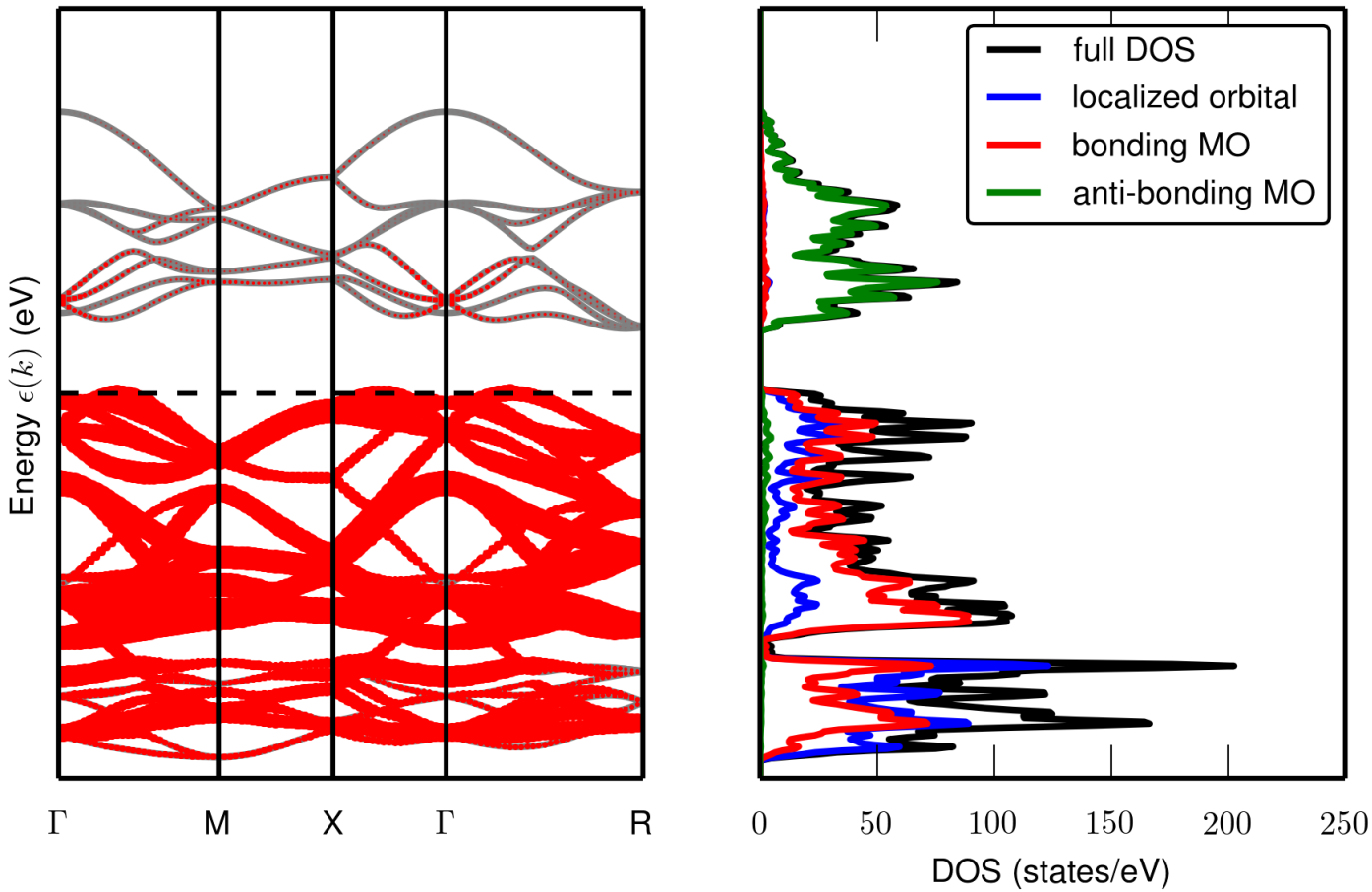

Energy $\epsilon(k)$ (eV)
Γ
M
X
Γ
R
full DOS
localized orbital
bonding MO
anti-bonding MO
0
50
100
150
200
250
DOS (states/eV)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Γ
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0
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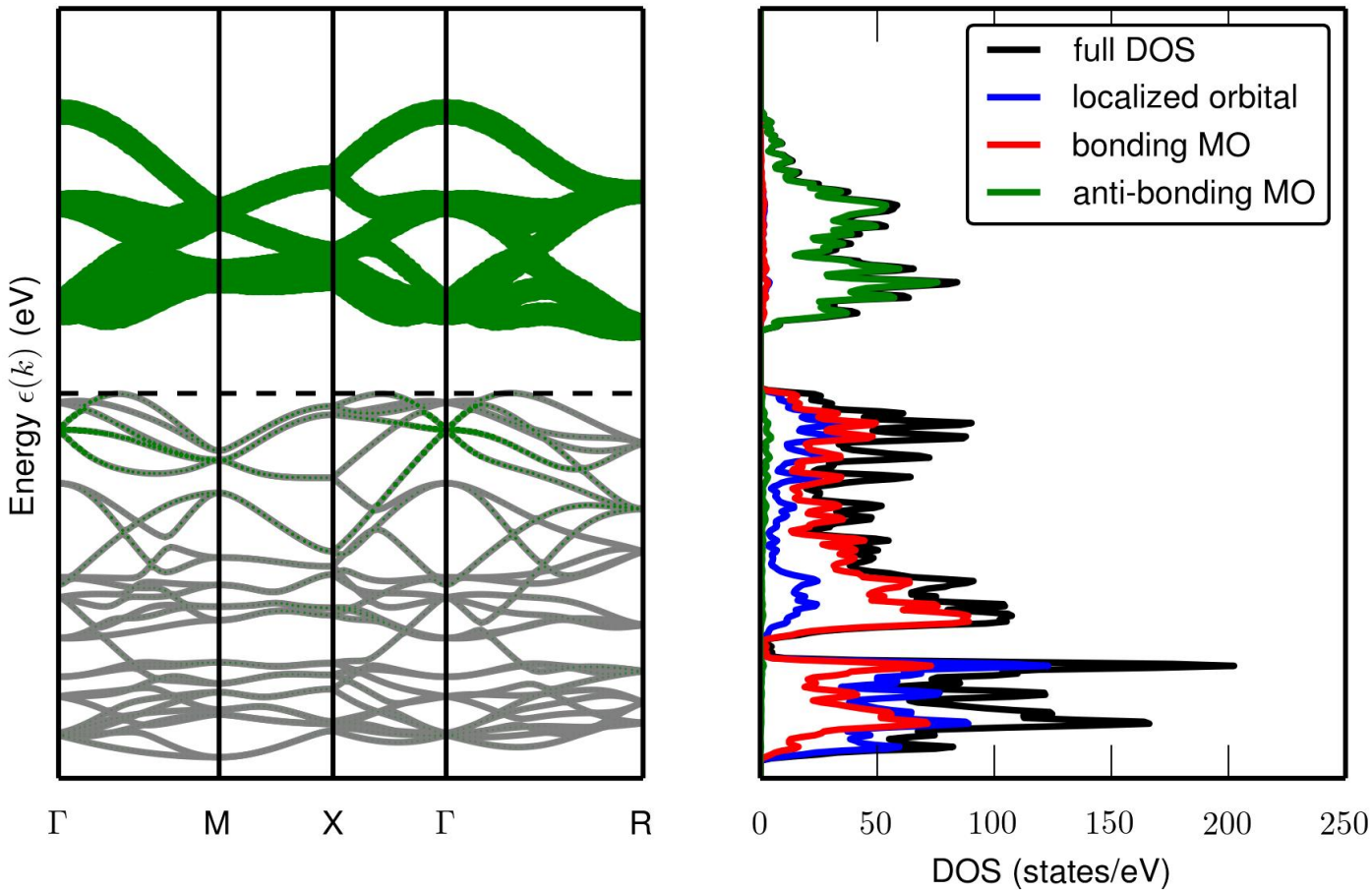
DOS (states/eV)


Energy $\epsilon(k)$ (eV)
Γ
M
X
Γ
R
full DOS
localized orbital
bonding MO
anti-bonding MO
0
50
100
150
200
250
DOS (states/eV)

$$\hat{H}_{SO} = \xi \hat{\mathbf{s}} \cdot \hat{\mathbf{l}} = \frac{\xi}{2} \begin{pmatrix} \hat{l}_z & \sqrt{2}\hat{l}_- \\ -\sqrt{2}\hat{l}_+ & -\hat{l}_z \end{pmatrix}; \quad \xi_d = 0.6\text{eV}$$

mixes t_{2g} states at each Ir site

$$\langle \sigma | l_z | \sigma \rangle = \begin{pmatrix} yz & xy & zx \\ \hline 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad \pm\sqrt{2}\langle -\sigma | l_{\mp} | \sigma \rangle = \left(\begin{array}{ccc|c} yz & xy & zx & \\ \hline 0 & \mp 1 & 0 & yz \\ \pm 1 & 0 & -i & xy \\ 0 & i & 0 & zx \end{array}\right)$$

to form a Γ_8 ($j_{\text{eff}} = 3/2$) quartet and a Γ_6 ($j_{\text{eff}} = 1/2$) doublet.

d_{yz} and d_{zx} orbitals are coupled by SOC $\Rightarrow$
molecular orbitals on two corner sharing triangles start to interact

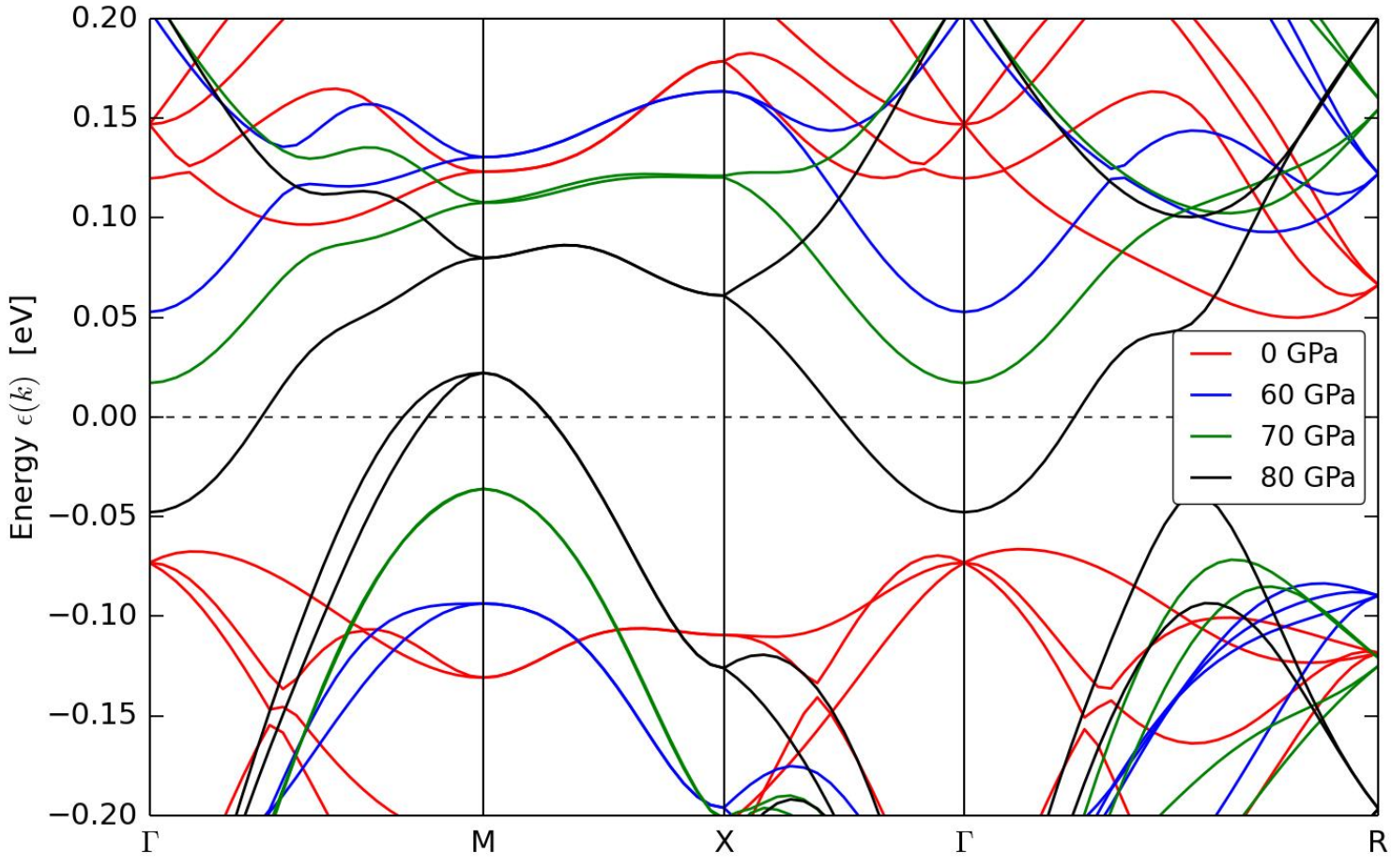
$$\chi_{\Gamma_8} = \begin{cases} \sqrt{\frac{5}{6}}\chi_{\frac{5}{2}\pm\frac{5}{2}} + \sqrt{\frac{1}{6}}\chi_{\frac{5}{2}\mp\frac{3}{2}} \\ \chi_{\frac{5}{2}\pm\frac{1}{2}} \end{cases}$$

$$\chi_{\Gamma_6} = \sqrt{\frac{1}{6}}\chi_{\frac{5}{2}\pm\frac{5}{2}} - \sqrt{\frac{5}{6}}\chi_{\frac{5}{2}\mp\frac{3}{2}}$$

or

$$\chi_{\Gamma_6} = \sqrt{\frac{1}{3}}\left[d_{xy}\chi_{\mp\frac{1}{2}} \mp d_{yz}\chi_{\pm\frac{1}{2}} + i d_{zx}\chi_{\pm\frac{1}{2}}\right]$$

$Na_3Rh_3O_8$


0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
Energy $\epsilon(k)$ [eV]
Γ
M
X
Γ
R
0 GPa
60 GPa
70 GPa
80 GPa

	t_{2g}			e_g	
1 \ 1	d_{xy}	d_{xz}	d_{yz}	d_{3z^2-1}	$d_{x^2-y^2}$
d_{xy}	−2.35367	0.02875	−0.05588	0.12330	0.33642
d_{xz}		−2.65602	−0.02875	−0.22377	−0.38758
d_{yz}			−2.35367	−0.22969	−0.27499
d_{3z^2-1}				1.26341	0.06304
$d_{x^2-y^2}$					1.33621

1 \ 2	d_{xy}	d_{xz}	d_{yz}	d_{3z^2-1}	$d_{x^2-y^2}$
d_{xy}	0.02870	0.00911	0.07228	0.02506	0.00750
d_{xz}	0.04264	0.16388	0.02192	−0.12583	−0.46722
d_{yz}	0.26937	0.08265	0.01002	0.00007	0.03223
d_{3z^2-1}	0.04220	−0.30436	−0.03500	0.13097	−0.18045
$d_{x^2-y^2}$	0.05333	−0.30554	0.00814	−0.10799	−0.07450

1 \ 3	d_{xy}	d_{xz}	d_{yz}	d_{3z^2-1}	$d_{x^2-y^2}$
d_{xy}	0.16388	0.08265	0.00911	0.41678	−0.11081
d_{xz}	0.02192	0.01002	0.07228	0.01045	−0.03438
d_{yz}	0.04264	0.26937	0.02870	−0.06728	0.00988
d_{3z^2-1}	0.46754	−0.02794	−0.01902	−0.14804	0.01937
$d_{x^2-y^2}$	0.12463	−0.01606	0.01795	−0.05309	0.20450

1 \ 4	d_{xy}	d_{xz}	d_{yz}	d_{3z^2-1}	$d_{x^2-y^2}$
d_{xy}	0.02870	−0.26937	0.04264	−0.04220	0.05333
d_{xz}	−0.07228	0.01002	−0.02192	−0.03500	−0.00814
d_{yz}	0.00911	−0.08265	0.16388	0.30436	−0.30554
d_{3z^2-1}	−0.02506	0.00007	0.12583	0.13097	0.10799
$d_{x^2-y^2}$	0.00750	−0.03223	−0.46722	0.18045	−0.07450