Spontaneous Parity Breaking by Electron Correlations

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Acknowledgements : T. Arima, Y. Yanase, H. Harima, H. Tsunetsugu

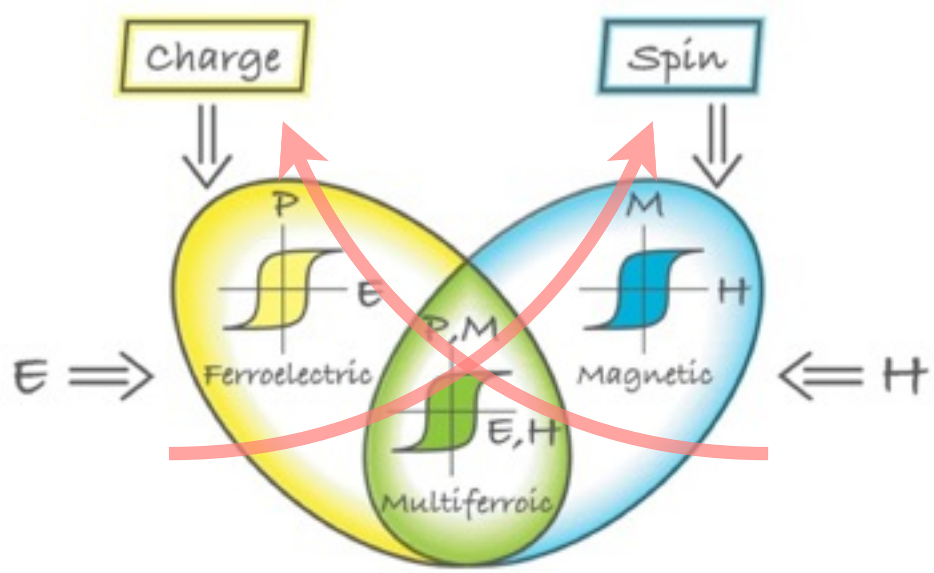
S. Hayami, HK and Y. Motome: arXiv:1406.2093
S. Hayami, HK and Y. Motome: arXiv:1404.1156

Recent Topics by Spin-Orbit Coupling

Various interesting phenomena caused by **spin-orbit coupling**,
especially **without spatial inversion symmetry**

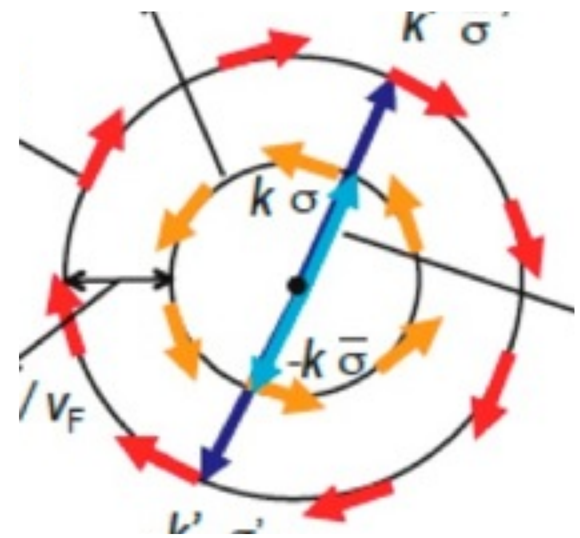
Magnetoelectric effects in multiferroics

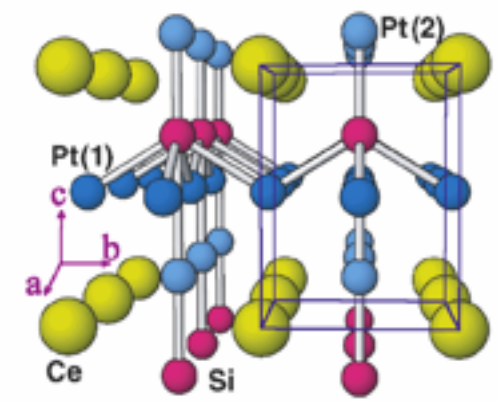
D. Khomskii: Physics **2** (2009) 20



Noncentrosymmetric superconductivity

S. Fujimoto

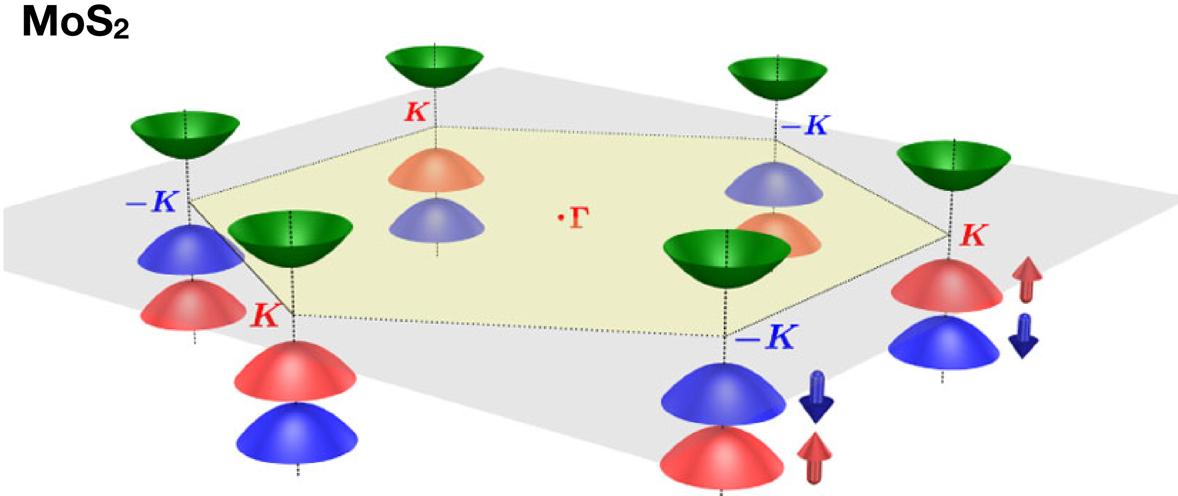




Anti-symmetric spin splitting in spin-orbit coupled systems

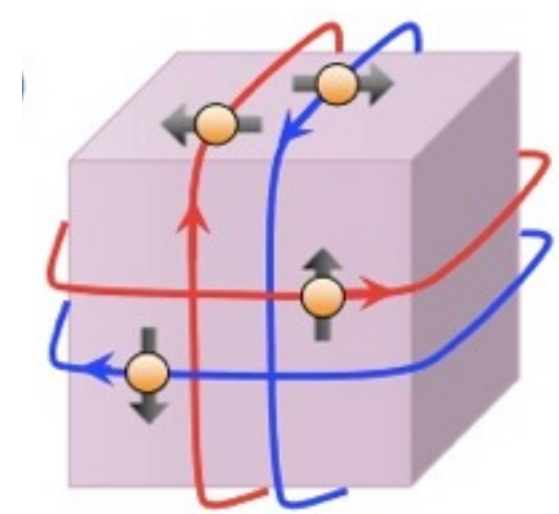
D. Xiao et al., PRL **108** (2012) 196802

monolayer
MoS_2



Spin-Hall effect in topological insulators

Y. Ando: JPSJ **82** (2013) 102001



Such interesting spin-orbital coupled systems can be created by spontaneous parity breaking ?

Degree of parity breaking is controllable

Parities and Band Structures

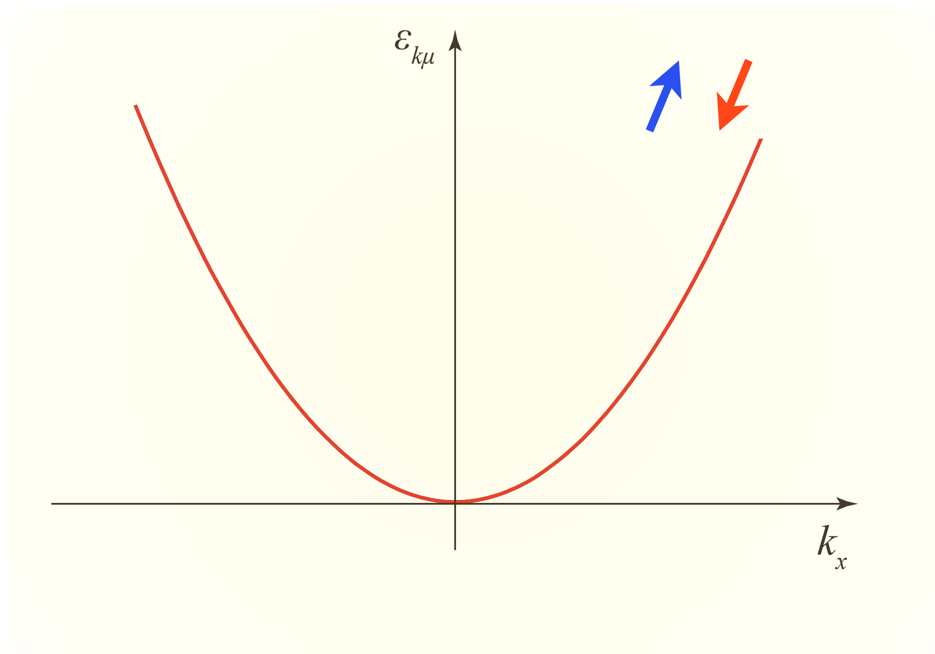
By symmetry argument

T $\quad (+\boldsymbol{k},\uparrow) \leftrightarrow (-\boldsymbol{k},\downarrow)$

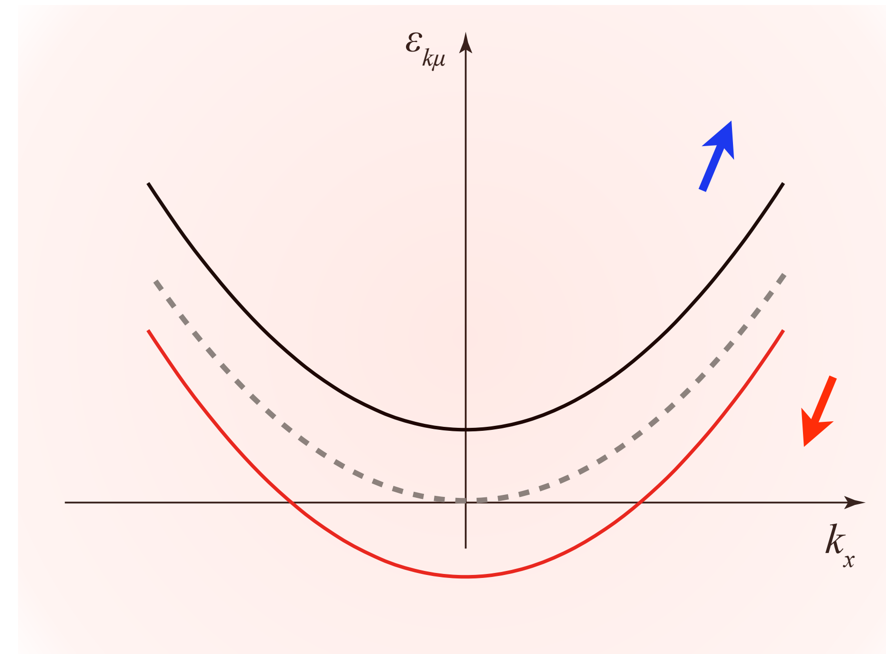
P $\quad (+\boldsymbol{k},\sigma) \leftrightarrow (-\boldsymbol{k},\sigma)$

TP $\quad (\pm\boldsymbol{k},\uparrow) \leftrightarrow (\pm\boldsymbol{k},\downarrow)$

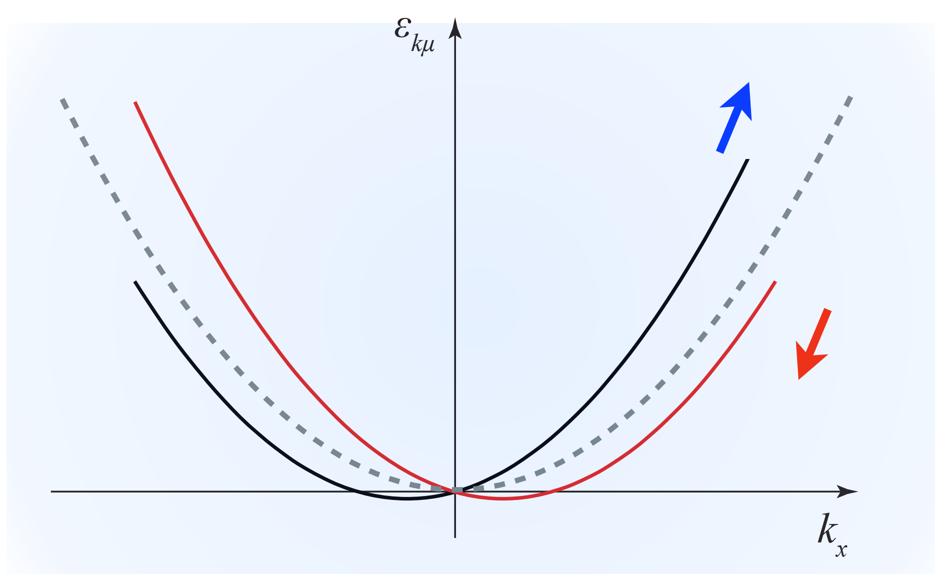
unbroken

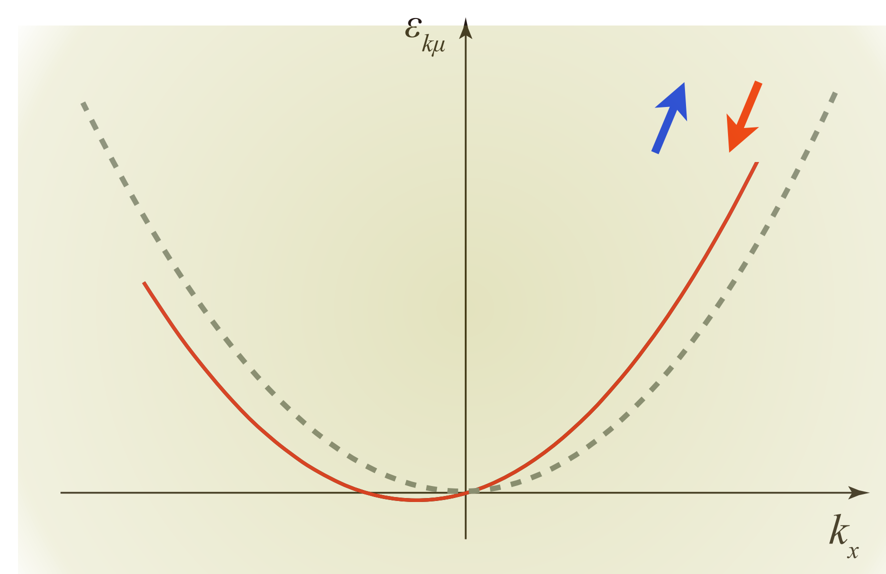


***T* broken**



***P* broken**





View from Microscopic Degrees of Freedom

One-particle Hamiltonian

$$H=\sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\alpha}[\varepsilon(\boldsymbol{k})1+\boldsymbol{f}(\boldsymbol{k})\cdot\boldsymbol{\sigma}]_{\alpha\beta}c_{\boldsymbol{k}\beta},$$

symmetric part | **anti-symmetric part**

charge sector $\varepsilon(\boldsymbol{k})=\xi(\boldsymbol{k})+\zeta(\boldsymbol{k}),$ $\qquad \xi(\boldsymbol{k})=\dfrac{k^2}{2m}$

spin sector $\boldsymbol{f}(\boldsymbol{k})=\boldsymbol{h}(\boldsymbol{k})+\boldsymbol{g}(\boldsymbol{k}).$

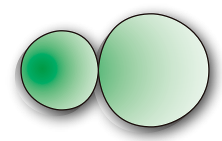
Simplest Examples

$\boldsymbol{h}(\boldsymbol{k})=h\boldsymbol{m}$ **magnetic dipole**

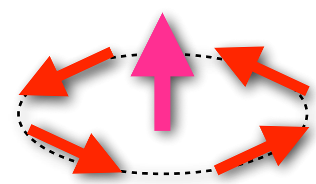
$\boldsymbol{m}\parallel y \qquad \boldsymbol{p}\parallel z \qquad \boldsymbol{t}\equiv\boldsymbol{p}\times\boldsymbol{m}\parallel x$

from SOC

$\boldsymbol{g}(\boldsymbol{k})=\alpha(\boldsymbol{p}\times\boldsymbol{k})$ **electric dipole**



$\zeta(\boldsymbol{k})=\beta(\boldsymbol{t}\cdot\boldsymbol{k})$ **toroidal dipole**



$$\varepsilon_{k\sigma}=\frac{k^2}{2m}-\beta k_x+\sigma\sqrt{(h+\alpha k_x)^2+\alpha^2k_y^2}$$

band shift **spin splitting**

lowest-order multipoles

	M-dipole	E-dipole	M-toroidal dipole	E-toroidal dipole
T	−	+	−	+
P	+	−	−	+
conj. field	$\boldsymbol{H}$	$\boldsymbol{E}$	$\boldsymbol{\nabla}\times\boldsymbol{H}$ $\quad \boldsymbol{j}$ $\quad \dfrac{\partial\boldsymbol{P}}{\partial t}$	$\boldsymbol{\nabla}\times\boldsymbol{E}$

Note that the momentum ***k*** has the same parities as M-toroidal dipole

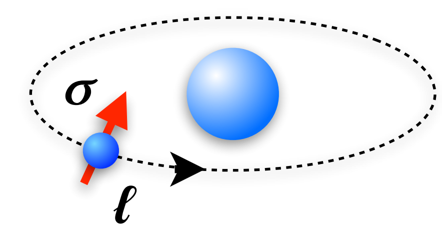
We can consider corresponding higher-rank multipoles, which couple with conjugate fields *in higher-order terms*

Minimal Ingredients for Parity Breaking

- **Spin-orbit coupling** — atomic origin (local)

$$\alpha$$

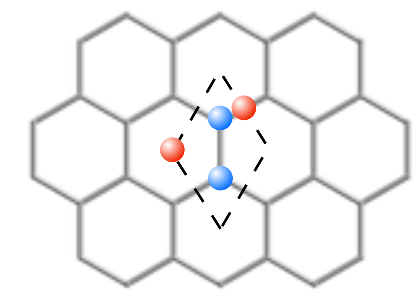
"magnetic field" without time-reversal breaking



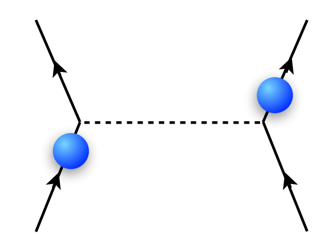
- **Local parity breaking** — exists intrinsically at atomic sites *in proper lattices*

$$d_i(Q)$$

"parity mixing" without *global* parity breaking



- **Electron correlations** — stabilize various electronic orders



$\Lambda_e(Q)$ electric orders

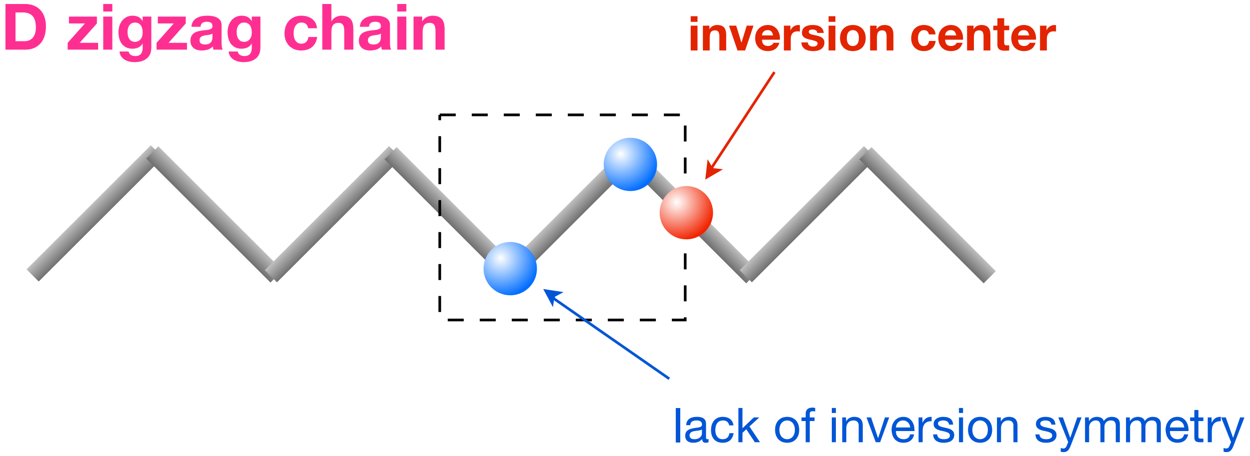
$\Lambda_m(Q)$ magnetic orders

Spontaneous parity breaking by electronic orders

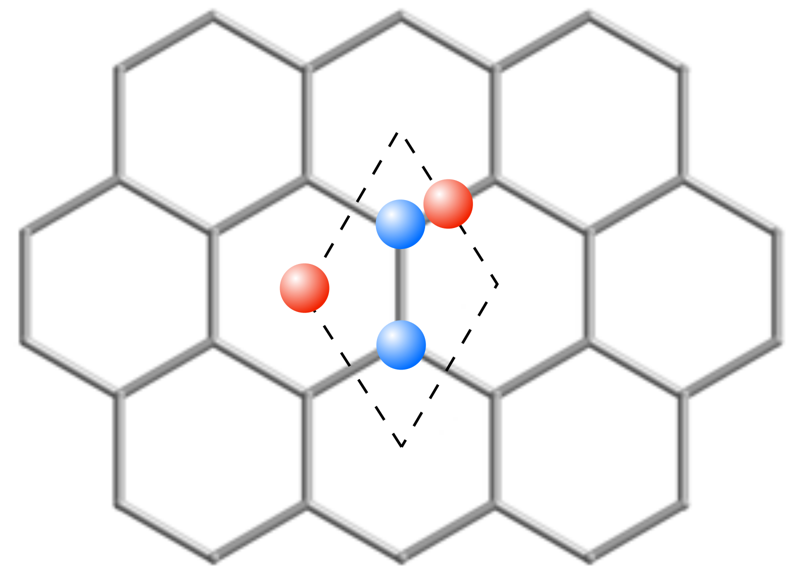
$$\mathcal{F}_{\mathrm{int}} = \alpha_1\, d_i(Q)\, \Lambda_e(Q) \underbrace{p_j(0)}_{\mathcal{P}\ \times} + \alpha_2\, d_i(Q) \Lambda_m(Q) \underbrace{t_k(0)}_{\mathcal{P}\&\mathcal{T}\ \times}$$

Local Parity Breaking

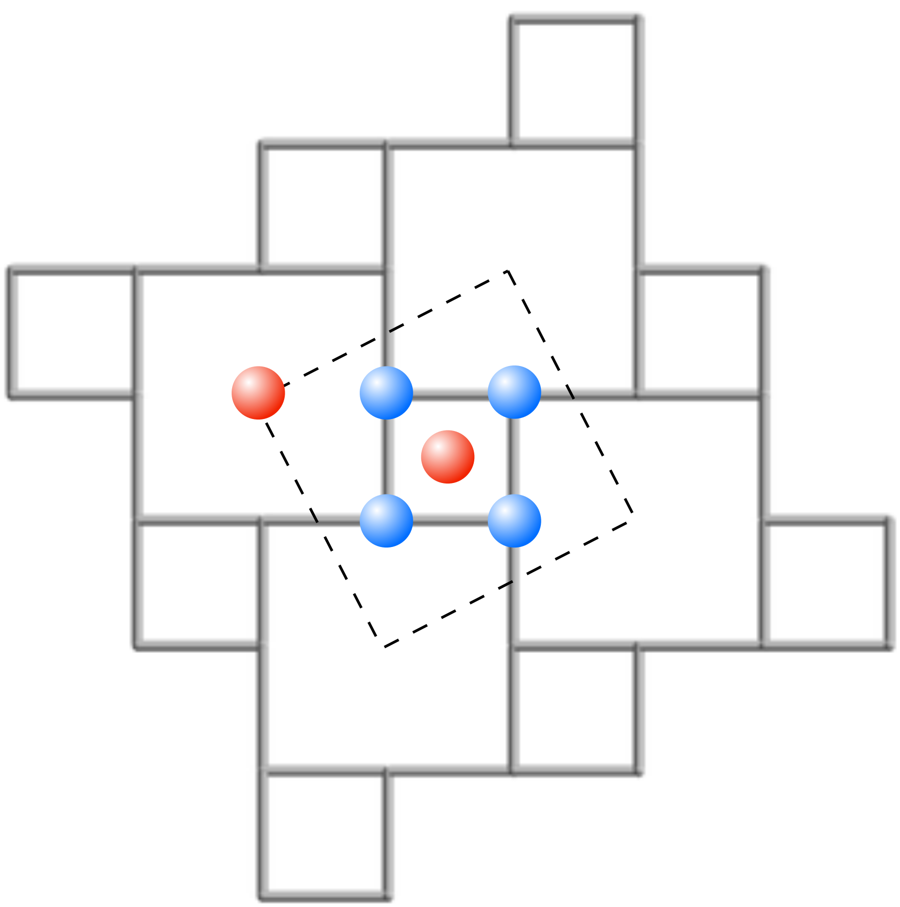
1D zigzag chain



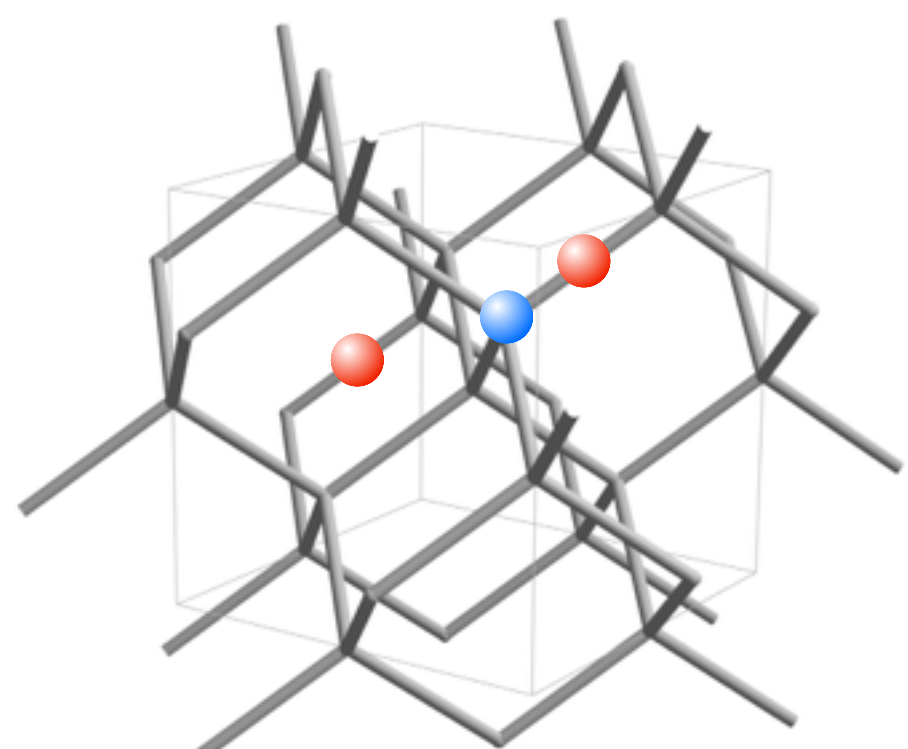
2D honeycomb lattice



2D 1/5-depleted square lattice



3D diamond lattice

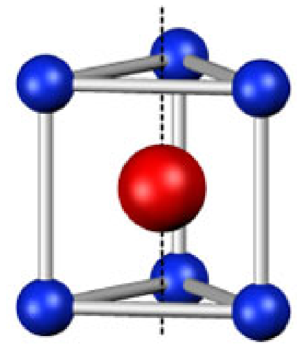


even number of lattice sites in a unit cell = global inversion symmetry

Two-Band Model on Honeycomb Lattice

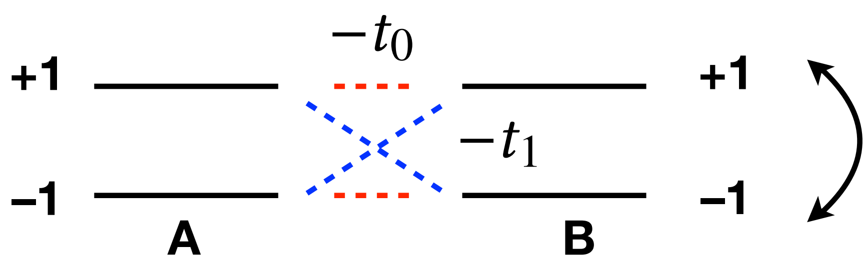
Basis & hoppings

$$|\pm 1\rangle = |xz\rangle \pm i\,|yz\rangle$$



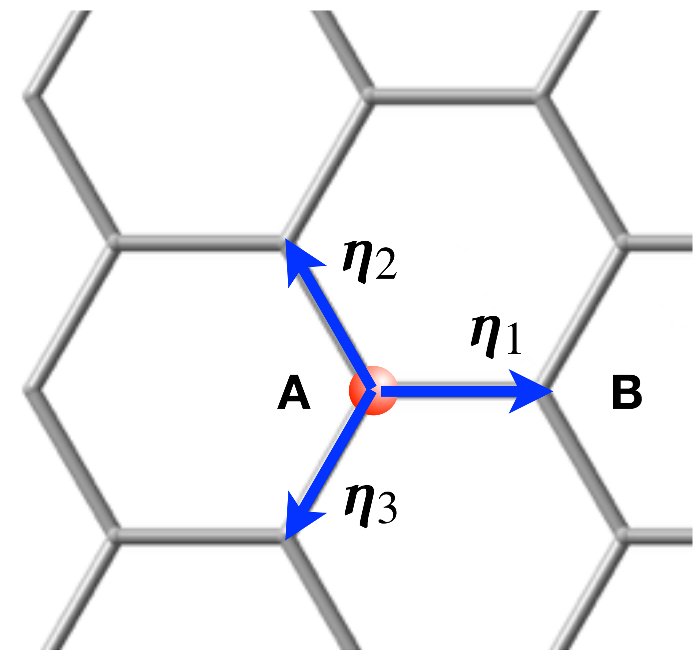
trigonal CEF

A:	z^2	m = 0
E:	(xz, yz)	±1
E':	(x^2-y^2, xy)	±2



spin-orbit coupling

$$\mathcal{H}_{\mathrm{SO}} = \lambda \ell_z \left(\frac{\sigma_z}{2}\right)$$



Non-interacting Hamiltonian

inversion symmetry exists

$$\mathcal{H}_0 = \begin{pmatrix} \frac{\lambda}{2}\sigma_z & -t_0\gamma_{0,k} - \frac{t_1}{2}(\gamma_{+1,k}\tau_+ + \gamma_{-1,k}\tau_-) \\ \text{h.c.} & \frac{\lambda}{2}\sigma_z \end{pmatrix}$$

A B

sublattice (A,B)	$\boldsymbol{\rho}$
orbital (+1,–1)	$\boldsymbol{\tau}$
spin (↑,↓)	$\boldsymbol{\sigma}$

$$\gamma_{n,k} = e^{i\boldsymbol{k}\cdot\boldsymbol{\eta}_1} + \omega^{-2n} e^{i\boldsymbol{k}\cdot\boldsymbol{\eta}_2} + \omega^{2n} e^{i\boldsymbol{k}\cdot\boldsymbol{\eta}_3}$$

additional phase factor
from angular-momentum transfer

$$\omega = e^{2\pi i/3}$$

Symmetry-breaking fields (AB-staggered type)

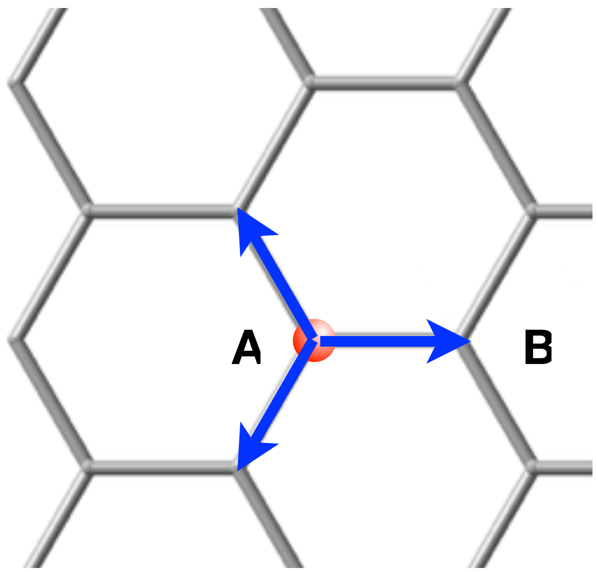
$$\mathcal{H}_1 = -h \sum_{s\boldsymbol{k}} \sum_{mm'\sigma\sigma'} c^{\dagger}_{s\boldsymbol{k}m\sigma} \left[p(s)\Lambda^{\alpha}_{\beta}\right]^{\sigma\sigma'}_{mm'} c_{s\boldsymbol{k}m'\sigma'}$$

$$p(A) = +1, \; p(B) = -1$$

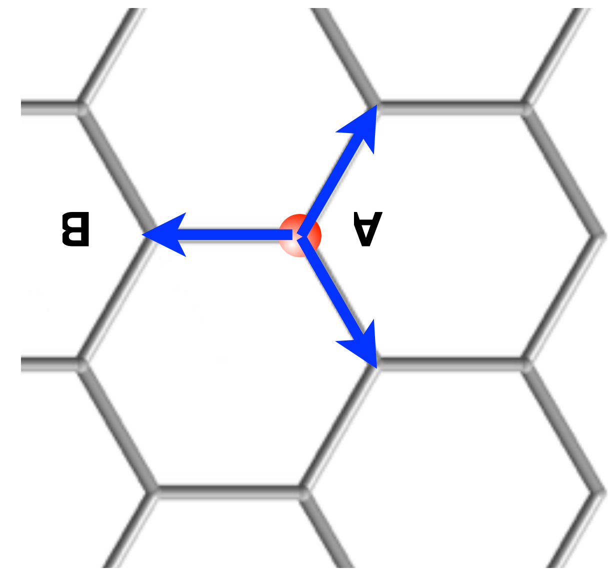
$$\Lambda^{\alpha}_{\beta} = \sigma_\alpha \tau_\beta$$

Symmetry Operations

in terms of $\boldsymbol{\rho},\ \boldsymbol{\tau},\ \boldsymbol{\sigma}$

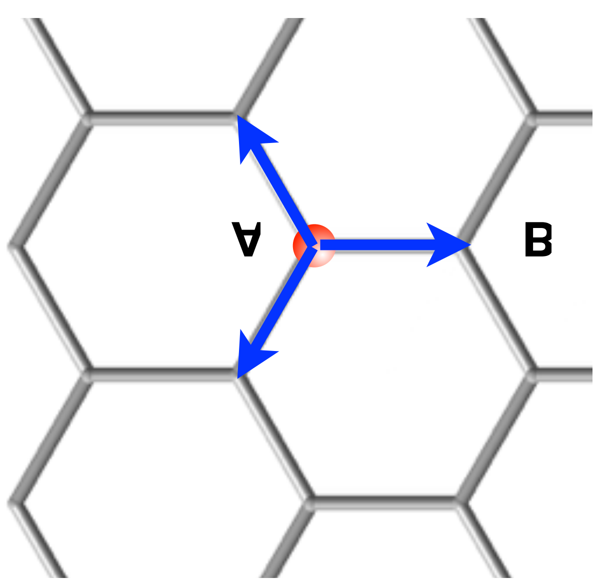


$E \quad \rho_0\sigma_0\tau_0$



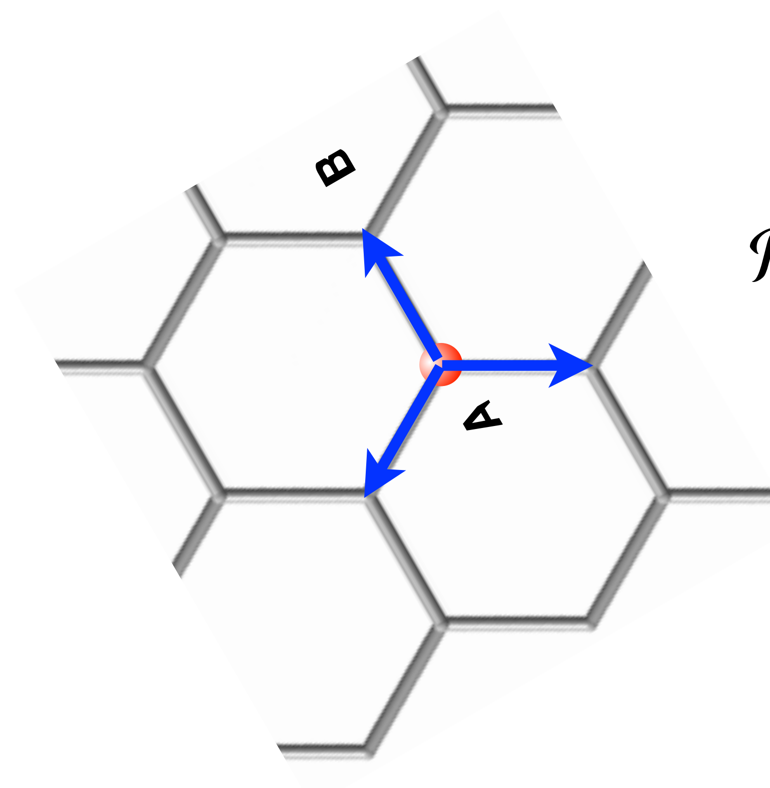
parity

$\mathcal{P} \quad \rho_x$



mirror
w.r.t. xz-plane

$\mathcal{M} \quad i\sigma_z$



120° rotation

$\mathcal{R} \quad \exp(2\pi i\tau_z/3)$

time reversal

$\mathcal{T} \quad i\sigma_y\tau_x K$

Possible Spin-Orbital Orders and ME effects

#	O.P.	$\mathcal{P}$	$\mathcal{T}$	$\mathcal{R}$	$\mathcal{M}$	ME(u)	ME(s)
1	CO, zz-SOO	×	○	○	○	—	—
2	x/y-OO	×	○	×	○	—	✓
3	xz/yz-SOO	×	○	○	×	—	—
4	z-SO, z-OO	×	×	○	○	—	—
5	zx/zy-SOO	×	×	×	○	—	✓
6	x/y-SO	×	×	○	×	—	—
7	$xx/yy/xy/yx$-SOO	×	×	×	×	✓	✓

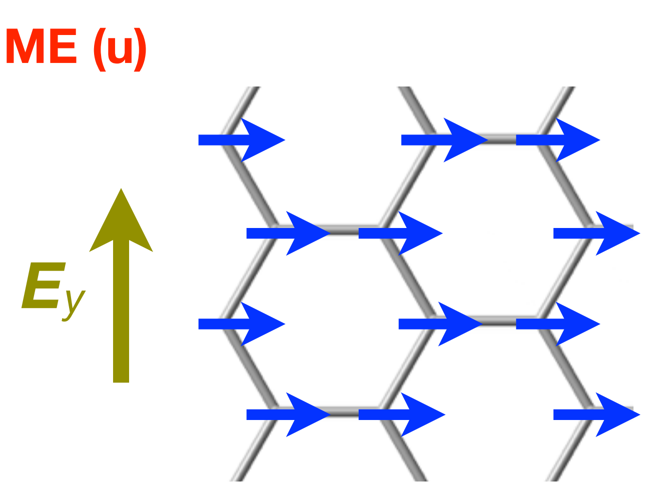
CO : charge order

SO : spin order

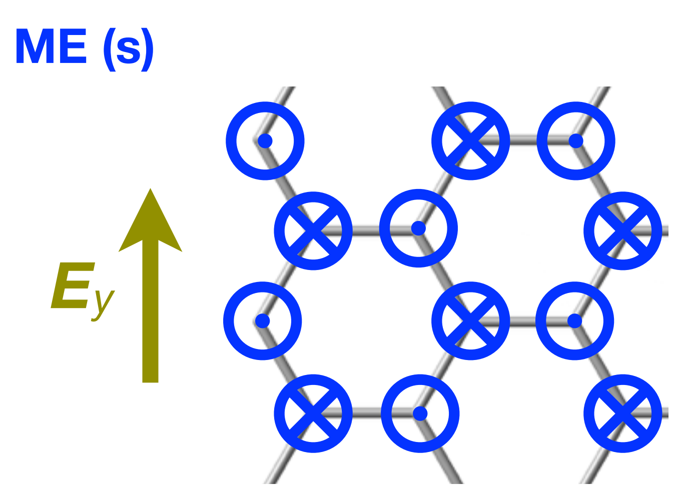
OO : orbital order

SOO : spin-orbital order

$$\Lambda^{\alpha}_{\beta} = \sigma_\alpha \tau_\beta$$



uniform $\boldsymbol{S}_x$

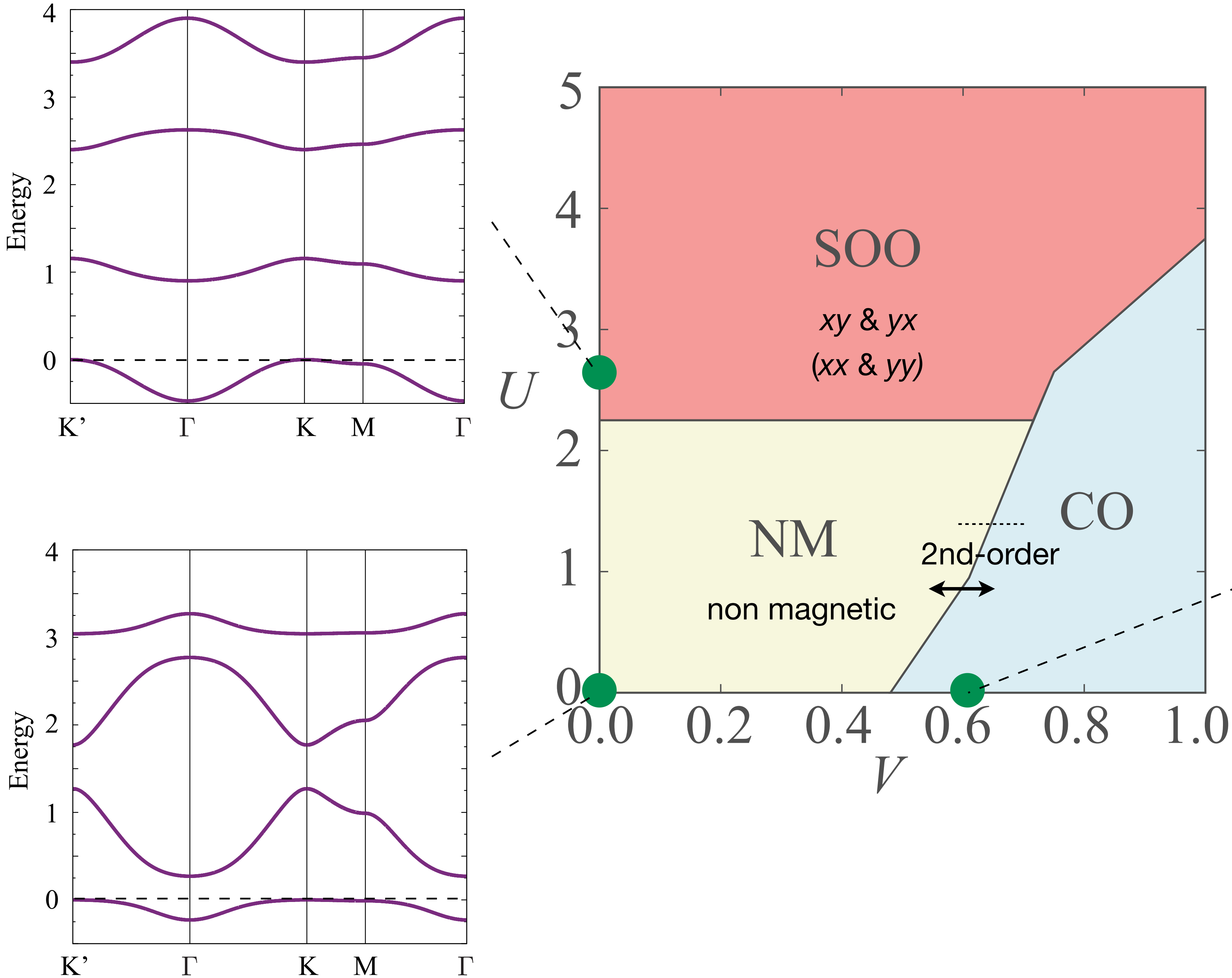


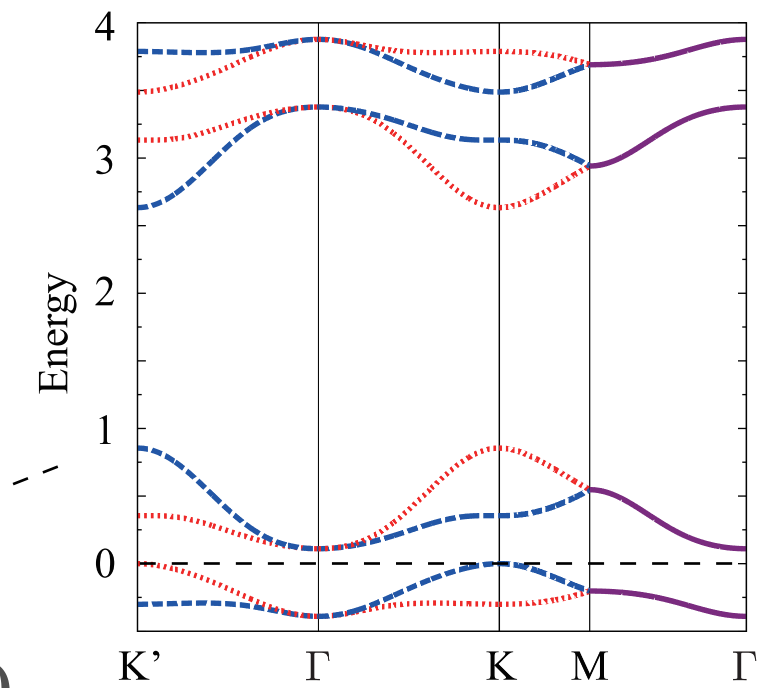
staggered $\boldsymbol{S}_z$

Phase Diagram at *T*=0 (1/4 filling)

n_e=1 (1/4 filling)
$t_0 = t_1 = \lambda = 0.5$
$J_H = 0.1U$

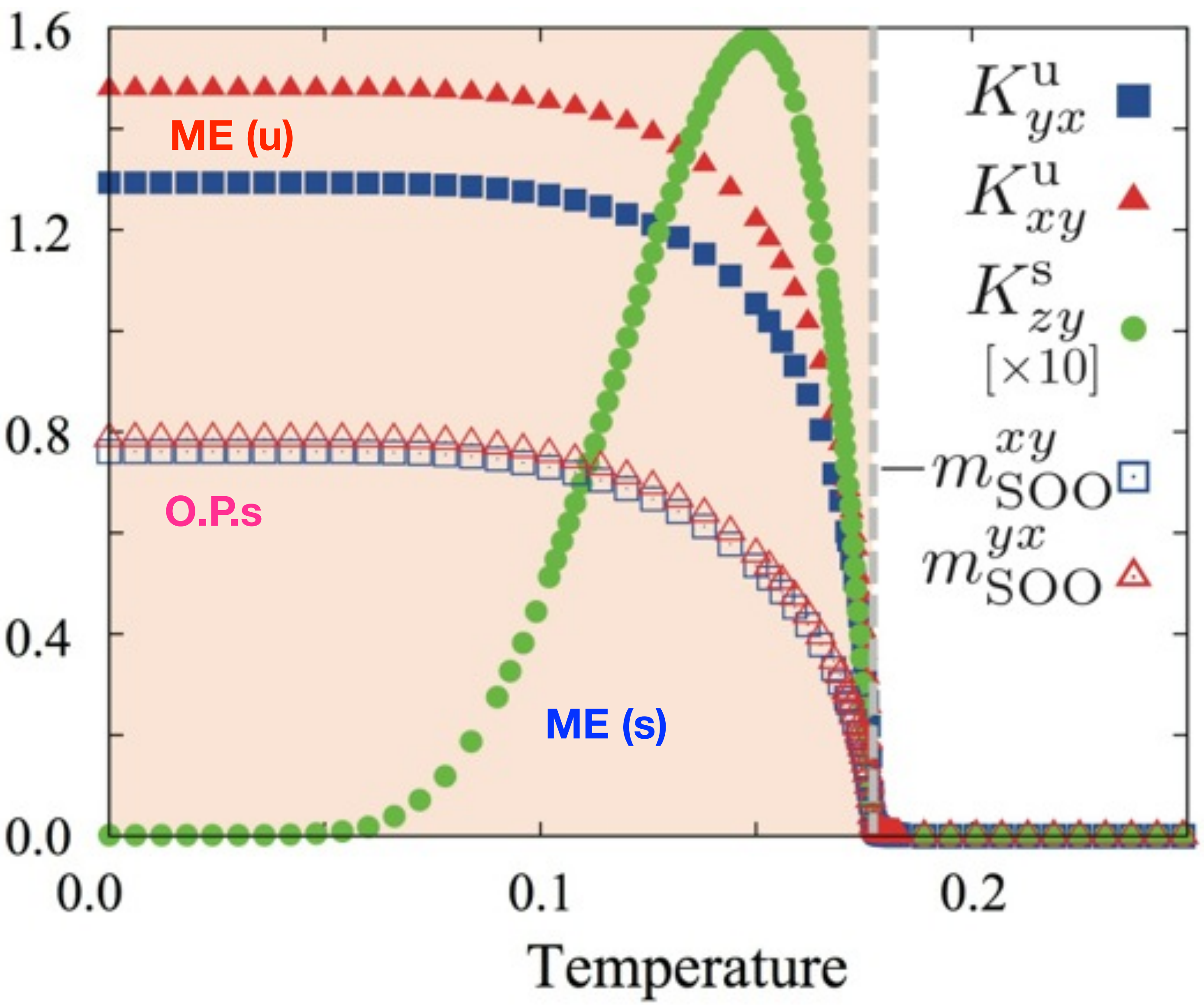
U : on-site repulsion
V : n.n. repulsion





Note: all cases are insulators

ME responses in SOO state

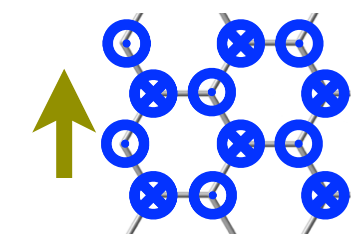


#	O.P.	$\mathcal{P}$	$\mathcal{T}$	$\mathcal{R}$	$\mathcal{M}$	ME(u)	ME(s)
1	CO, zz-SOO	×	◯	◯	◯	—	—
2	x/y-OO	×	◯	×	◯	—	✓
3	xz/yz-SOO	×	◯	◯	×	—	—
4	z-SO, z-OO	×	×	◯	◯	—	—
5	zx/zy-SOO	×	×	×	◯	—	✓
6	x/y-SO	×	×	◯	×	—	—
7	$xx/yy/xy/yx$-SOO	×	×	×	×	✓	✓

$\mathcal{R}$ × ME (s) linear coupling

SOC around Γ point

$$\mathcal{H}^{\text{eff}}_{\text{SO}} \sim \text{Re}[\gamma^{*}_{0,k}\left(\gamma_{+1,k} - \gamma_{-1,k}\right)]\sigma\Lambda$$
$$\sim k_y \sigma \Lambda$$



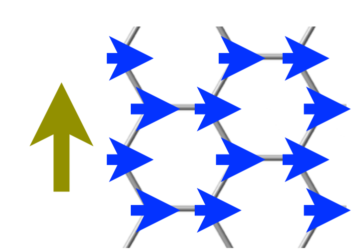
$\mathcal{R}$ ◯ no linear coupling in ME response

e.g. for CO

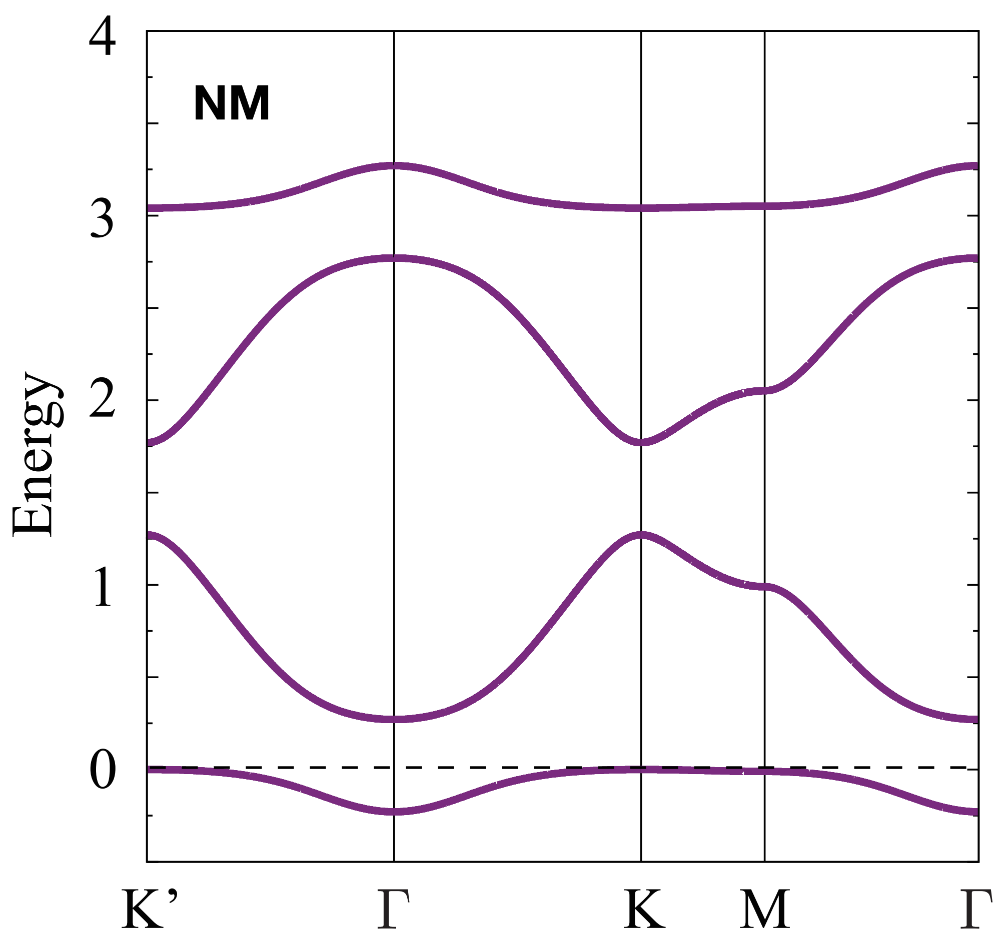
$$\mathcal{H}^{\text{eff}}_{\text{SO}} \sim \left(|\gamma_{+1,k}|^2 - |\gamma_{-1,k}|^2\right)\sigma\Lambda$$
$$\sim k_y(3k_x^2 - k_y^2)\sigma\Lambda$$

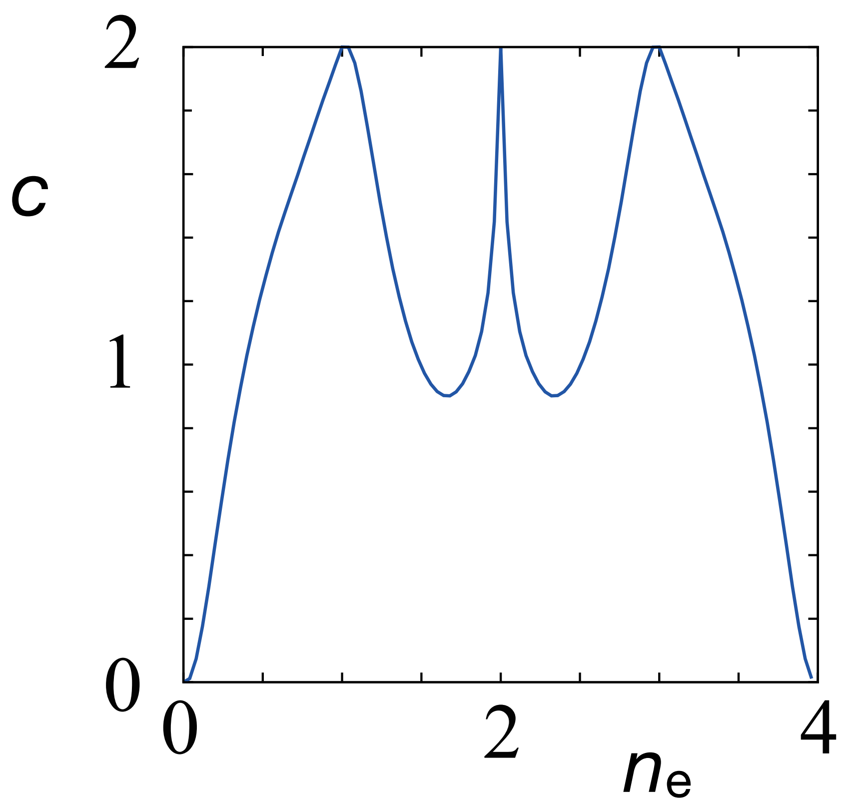
$\mathcal{R}$ × , $\mathcal{T}$ × ME (u) T_z toroidal dipole exists

$$M = T \times E$$



Non-Magnetic State

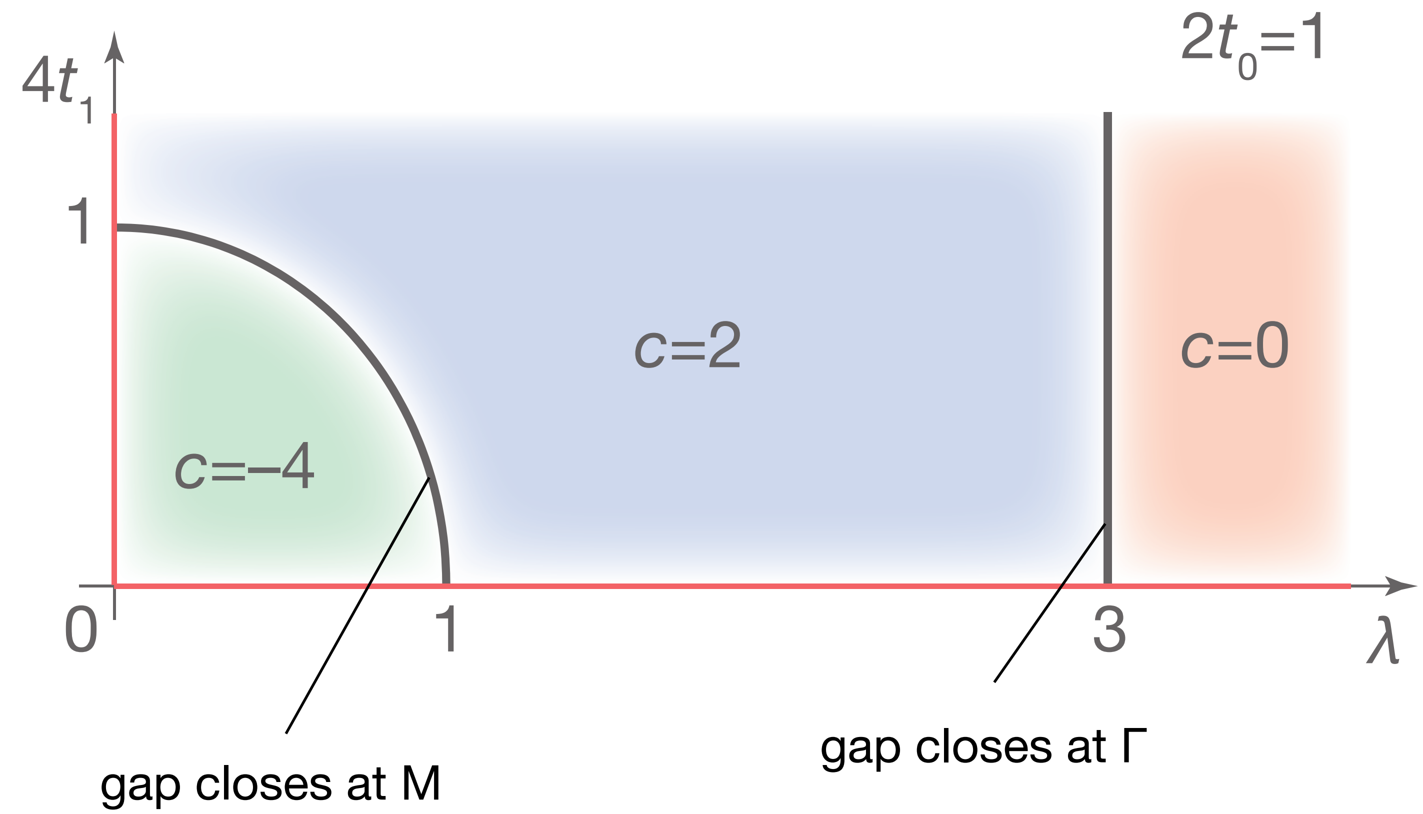




Quantum spin-Hall insulator

$$c \equiv \frac{\sigma_{xy}^z}{e/2\pi}$$

half filling



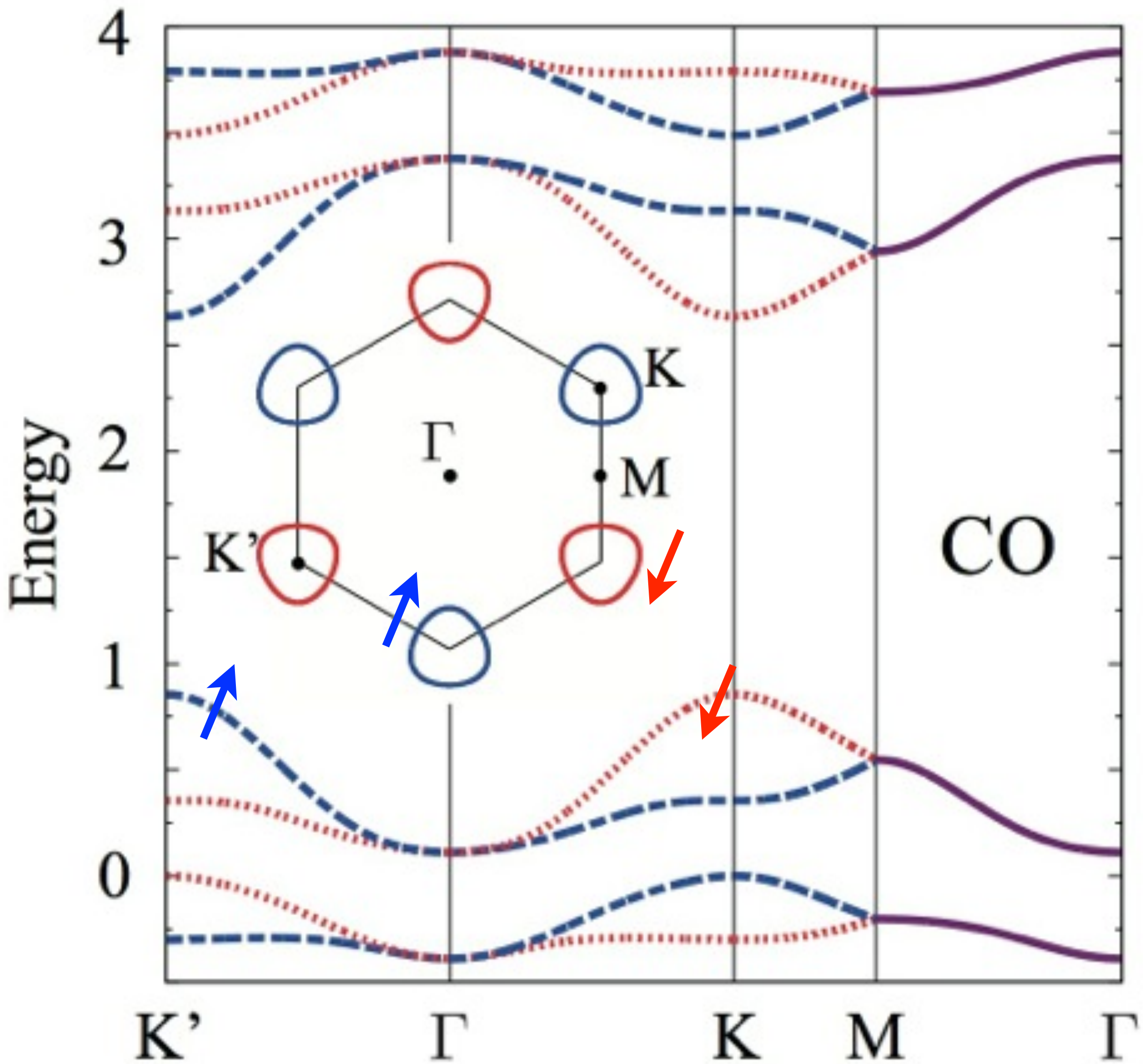
1/4 filling (for insulating parameters)

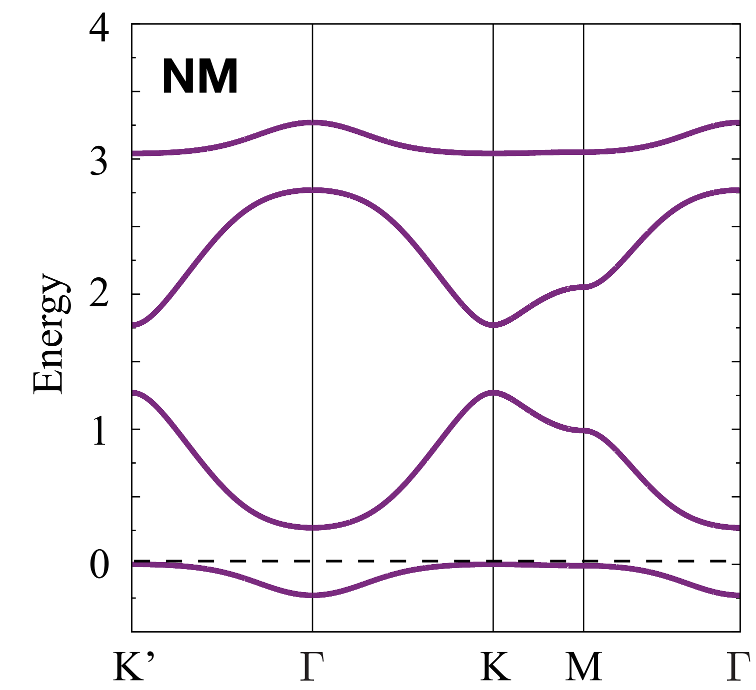
$$c = 2$$

cf. single-band Hubbard model with n.n.n. imag. hopping

C.L. Kane and E.J. Mele, PRL **95** (2005) 226801
(F.D. Haldane, PRL **61** (1988) 2015)

Charge Ordered State





increasing *V* in CO state (topological switching)

gap closes at K and K' points

The quantized value of σ^z_{xy} changes from 2 to 0

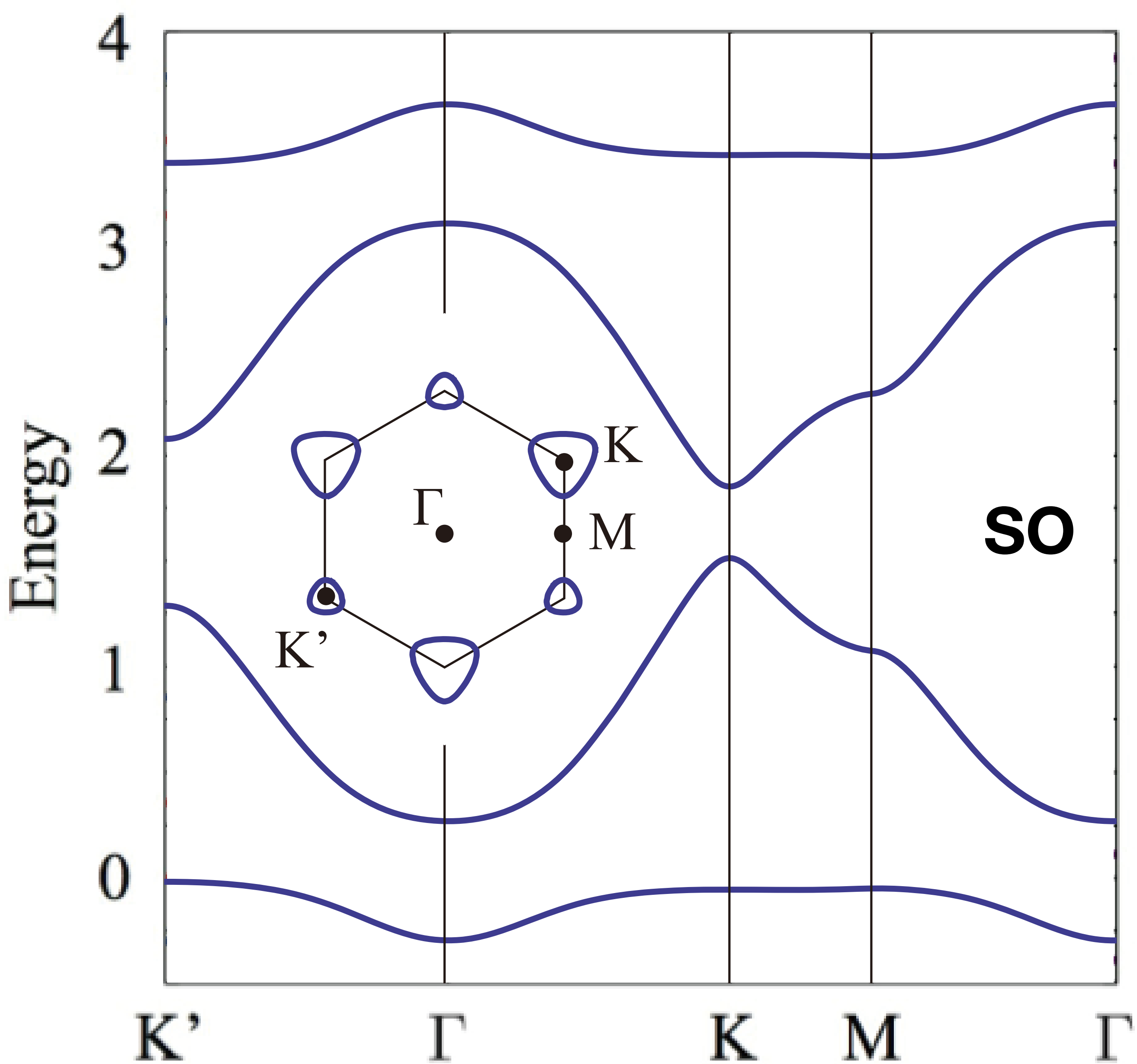
anti-symmetric spin splitting occurs

(energy contour at $\mu = -0.05$)

$$\mathcal{H}_{\rm SO}^{\rm eff} \sim \left(|\gamma_{+1,k}|^2 - |\gamma_{-1,k}|^2\right)\sigma\Lambda_0^0$$
$$\sim k_y(3k_x^2 - k_y^2)\sigma\Lambda_0^0$$

cf. electronic structure is similar to monolayer dichalcogenides, MoS_2

Spin Ordered State

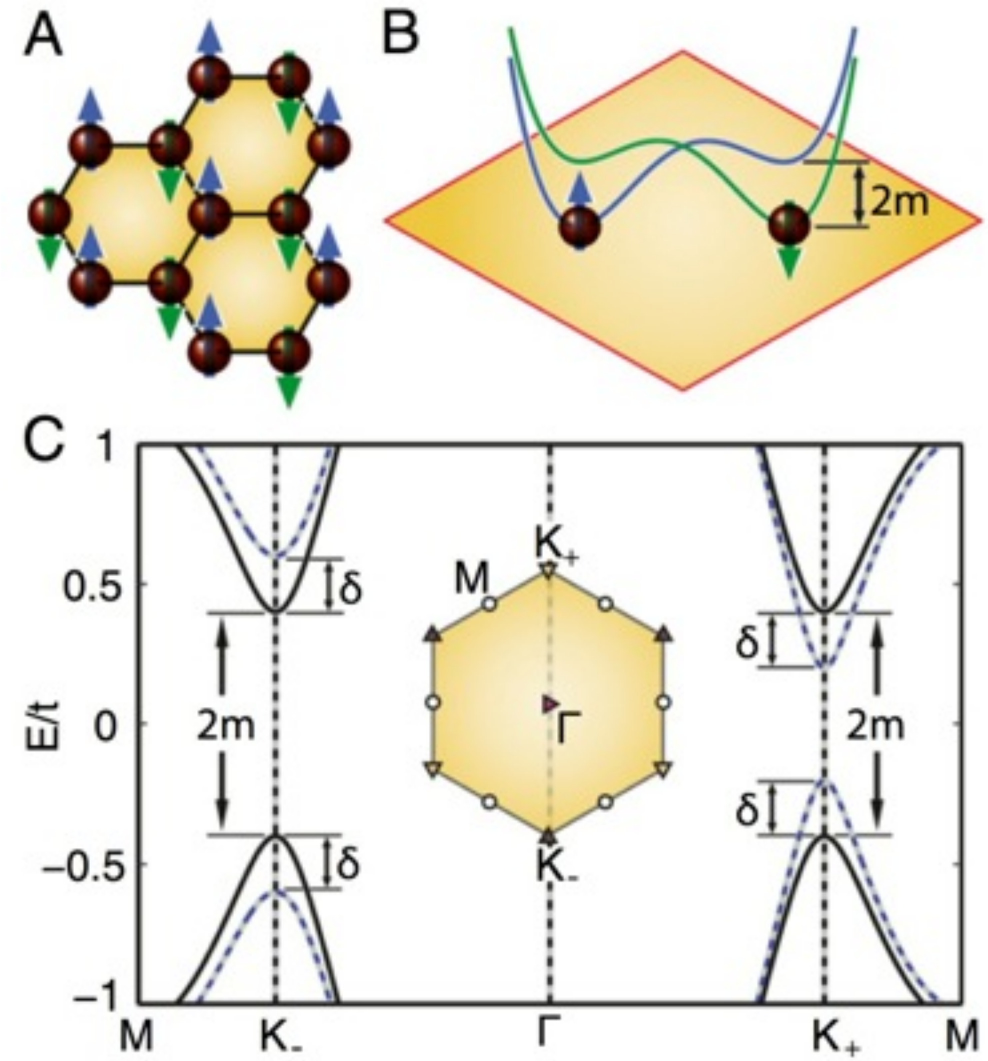


anti-symmetric band deformation occurs

(energy contour at μ = 1)

cf. electronic structure is similar to monolayer $MnPX_3$ (X=S, Se) under AFM

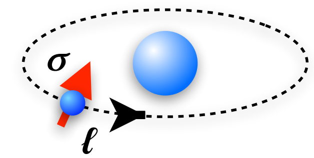
X. Li et al., PNAS, doi/10.1073/pnas.1219430110 (2013)

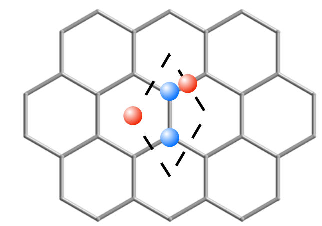


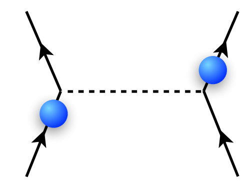
Summary

Minimal ingredients for spontaneous parity breaking

- **Spin-orbit coupling** ... for spin-orbital entanglement
- **Local parity breaking** ... seed for parity breaking
- **Electron correlations** ... origin of electronic orders



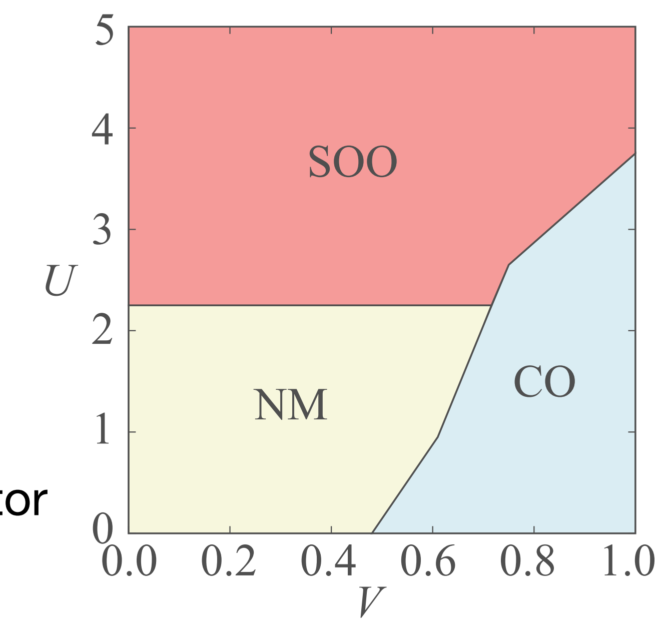




Two-band system on honeycomb lattice

orbitals + honeycomb + orders
= treasure of SO physics

two types of ME effects triggered by SOO orders



quantum spin-Hall insulator

anti-symmetric spin splitting

topological switching

possibly
spin-valley selective spin-Hall effect & optics
cf. MoS_2

SO: anti-symmetric band deformation
cf. $MnPX_3$ (X=S, Se)