Pure Orbital Chern Insulators in Two-dimensional Phosphorene

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2025/Aug./21

Outline

- Hall effect

  Orbital Hall effect: metal and insulator

- Topological band theory

  Haldane model

  Feature Spectrum Topology (特徵譜拓撲)

- Orbital Hall insulator

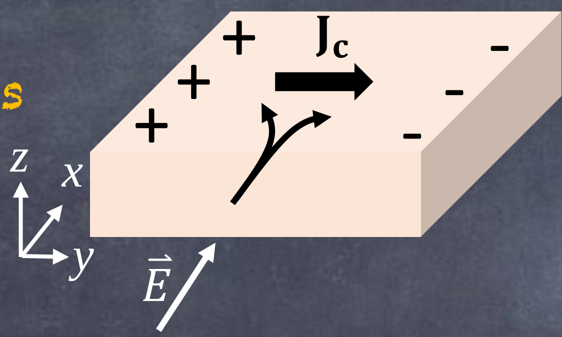
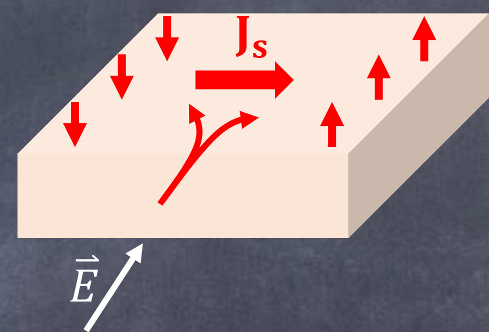
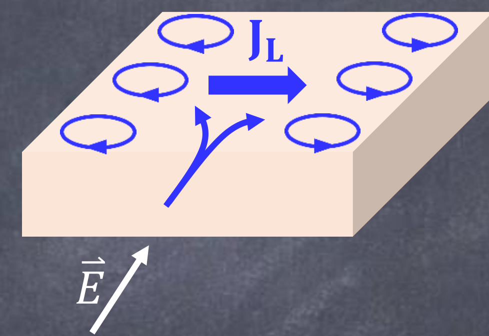
  Material: Phosphorene (磷烯)

  Orbital Chern number

  Boundary states

  Orbital Hall conductivity

Hall effect (metal)

Degree of freedom	Charge	Spin	Orbital
Hall responses	(Anomalous) Hall effect	Spin Hall effect	Orbital Hall effect
			
Material candidate	(1881) Fe Co_2MnGa $Co_3Sn_2S_2$ (Weyl) $Cr_2Ge_2Te_6$ (2D) …	(2004) Pt Bi_2Se_3 (TI) MoS_2 (2D) …	(2023) Cr, Ti

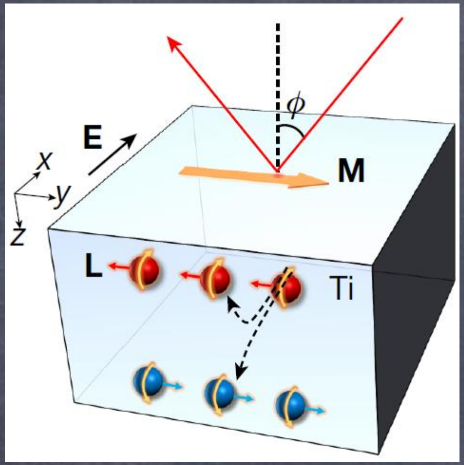
First theory:

B. A. Bernevig et al., PRL 95, 066601 (2005)
G.Y. Guo et al., PRL 94, 226601 (2005)

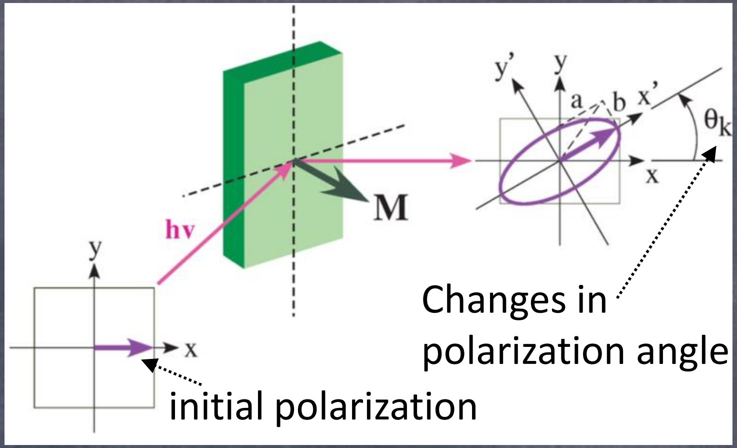
Orbital Hall effect (metal)

Ref: Y.-G. Choi et al., Nature 619, 52 (2023)

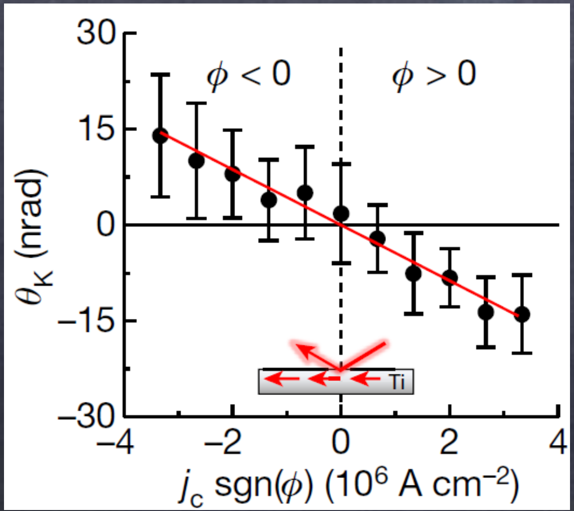
Accumulated orbital magnetization

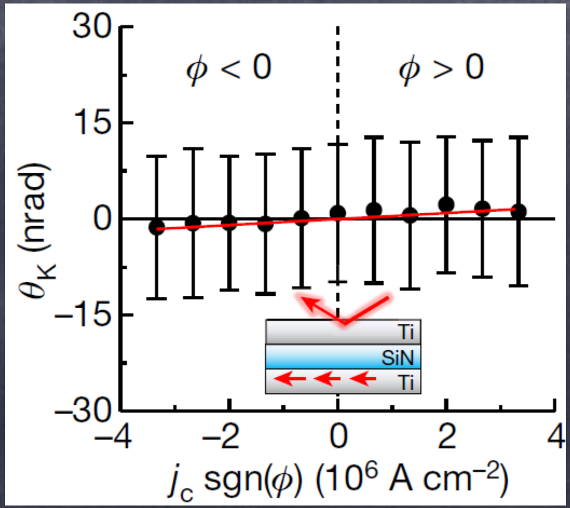


MOKE schematic



Magneto-optical Kerr effect (MOKE)





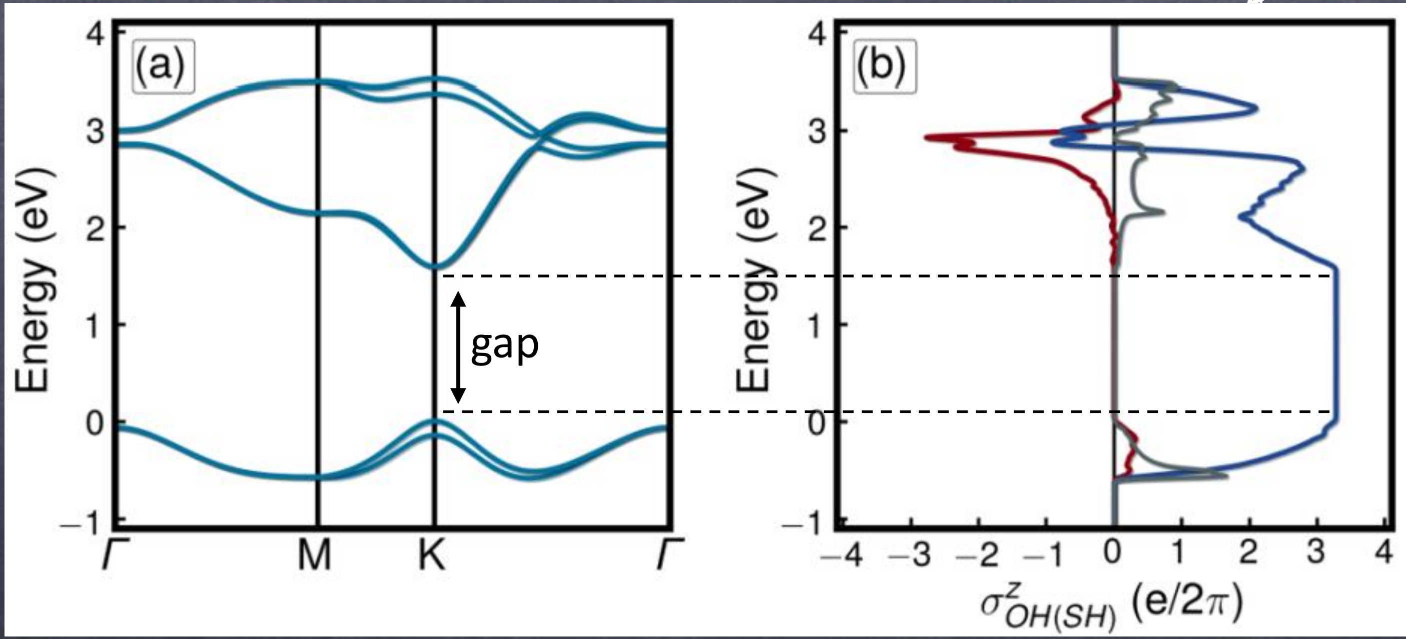
Orbital Hall effect (insulator)

Ref: PRB101, 161409(R) (2020)

Prior studies: orbital Hall effect in metals

Monolayer MoS_2
(2D insulator)

Orbital Hall Conductivity



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  - Haldane model
  - Feature Spectrum Topology (特徵譜拓撲)
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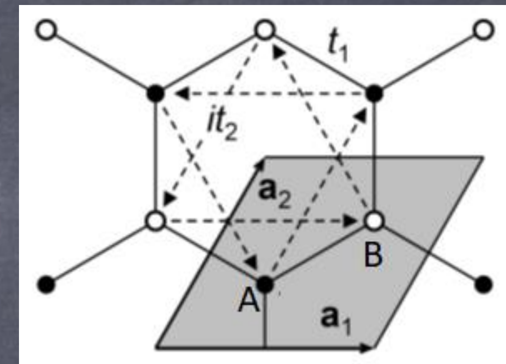
  - Orbital Chern number
  - Boundary states
  - Orbital Hall conductivity

Haldane model

Ref: PRL61, 2015 (1988)



Chern number

Topological invariant number $\frac{1}{2\pi}\sum_{m=occ}\int_{BZ} d^2k\,\Omega_m(k) = C$

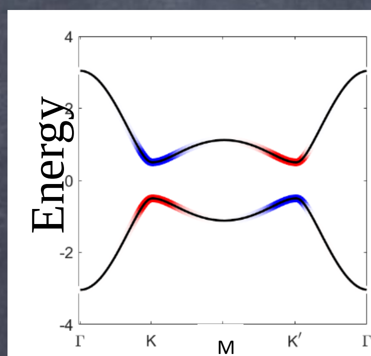
Berry curvature

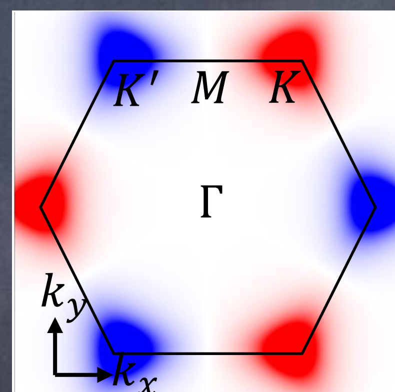
Haldane model:

$$H_{QAH} = \sum_i (-1)^{\tau_i} M c_i^\dagger c_i + t_1 \sum_{\langle ij\rangle}\left(c_i^\dagger c_j + h.c.\right) + t_2 \sum_{\langle\langle ij\rangle\rangle}\left(e^{i\phi_{ij}} c_i^\dagger c_j + h.c.\right)$$

Berry curvature Ω_k

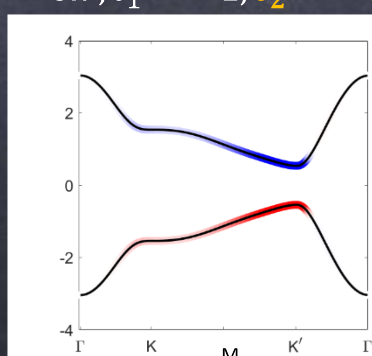
$M = 0.7, t_1 = -1, \boldsymbol{t_2 = 0}$

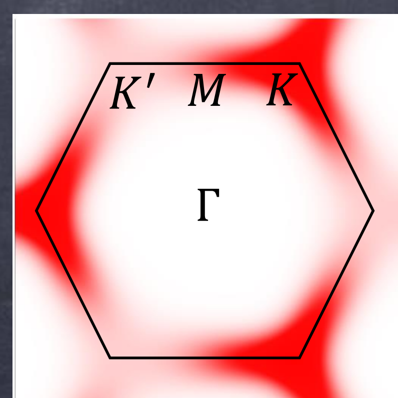




$C = 0$ Ordinary band insulator

$M = 0.7, t_1 = -1, \boldsymbol{t_2 = -0.2}$

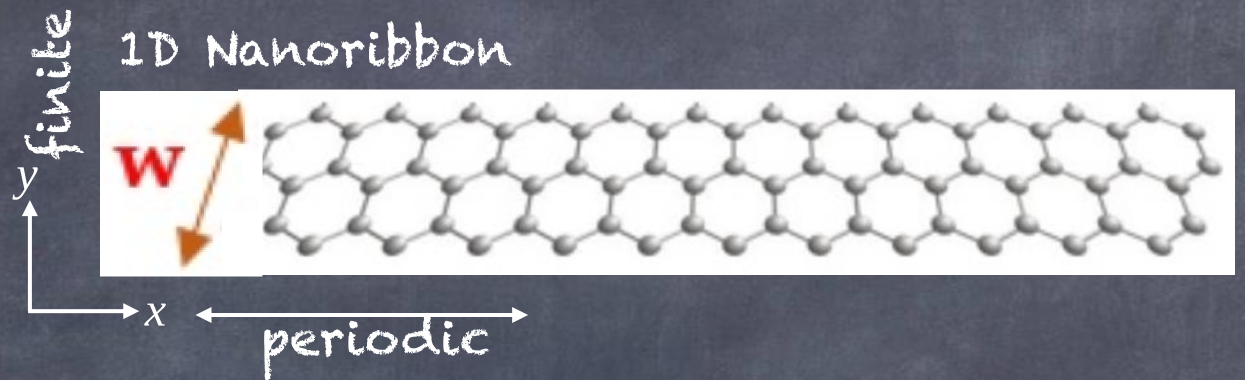




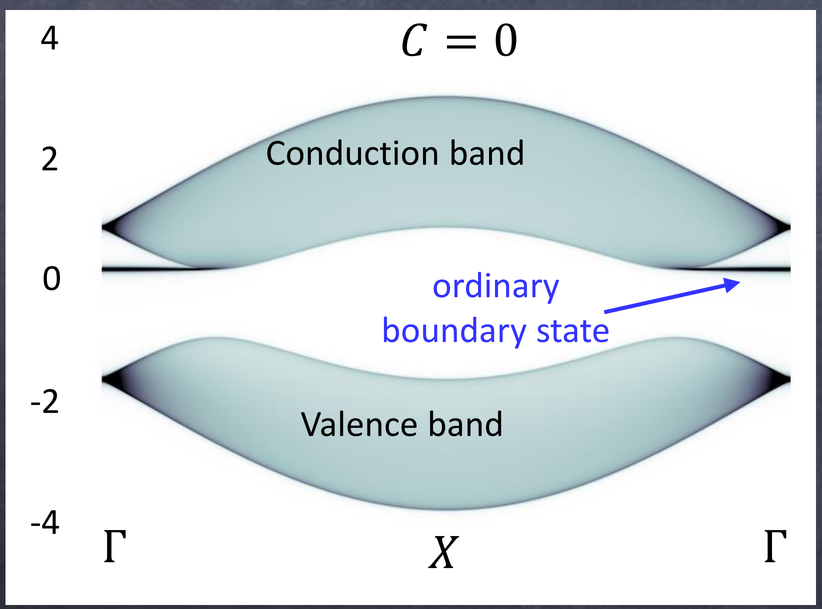
$C = 1$ Topological Chern insulator

Haldane model (2D honeycomb lattice)

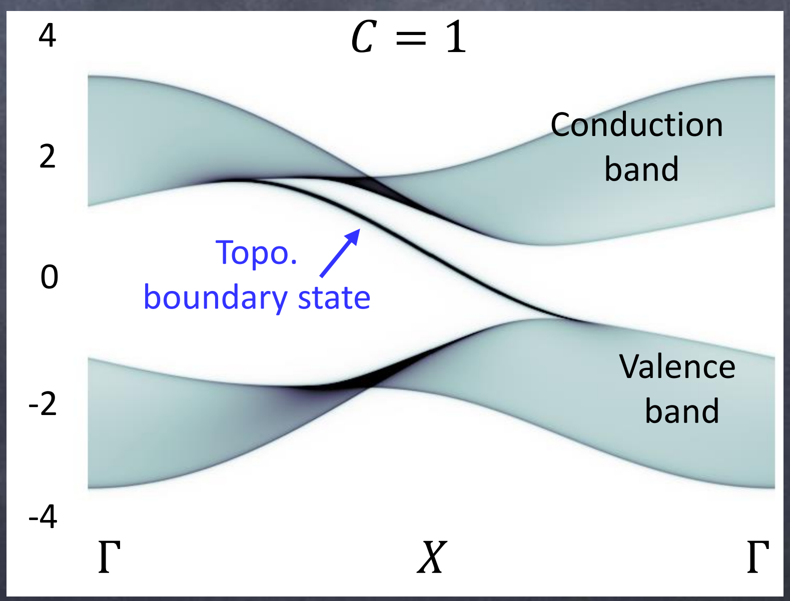
Bulk-Boundary Correspondence



$M = 0.7, t_1 = -1, \boldsymbol{t_2 = 0}$



$M = 0.7, t_1 = -1, \boldsymbol{t_2 = -0.2}$

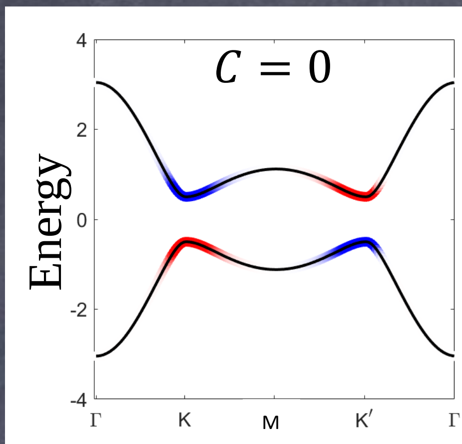


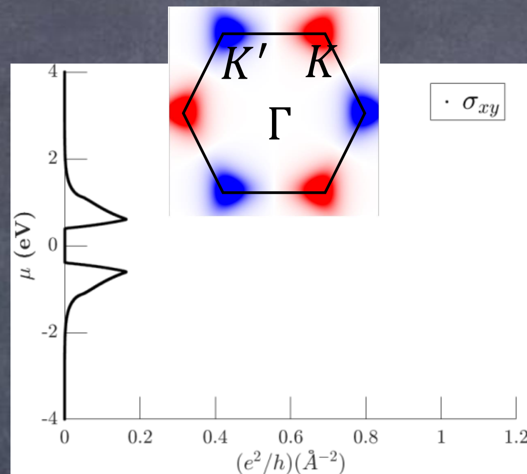
Haldane model (2D honeycomb lattice)

in gap Hall conductivity plateau σ_{xy}

Ref: PRL49, 405 (1982)

$M = 0.7, t_1 = -1, \boldsymbol{t_2 = 0}$





Hall conductivity:

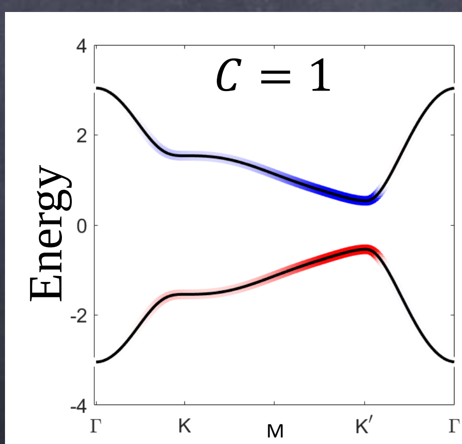
$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\sum_{m=occ}\int_{BZ} d^2k\, \Omega_m(k)$$

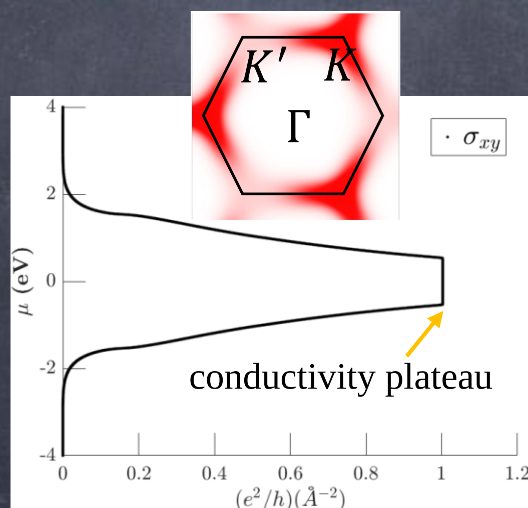
Berry curvature

$$= \frac{e^2}{h} C$$

Chern number

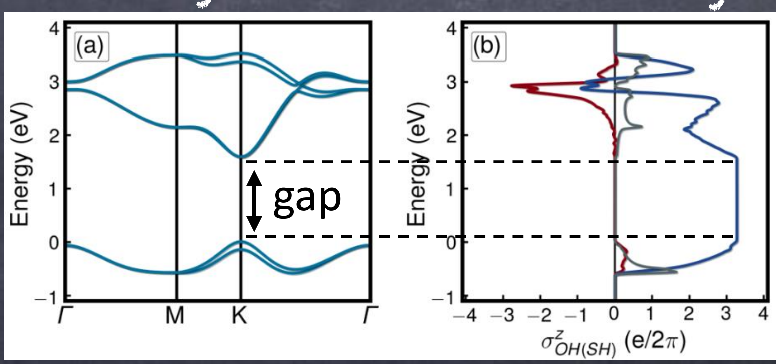
$M = 0.7, t_1 = -1, \boldsymbol{t_2 = -0.2}$





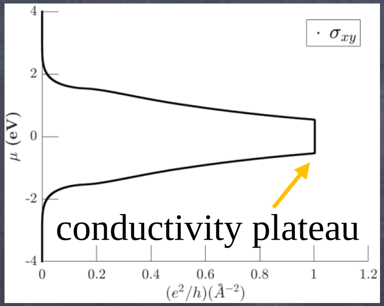
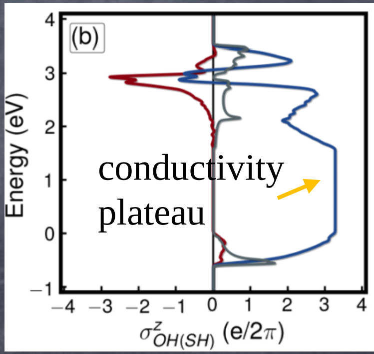
Monolayer MoS_2

Orbital Hall Conductivity



Orbital Chern insulator?

Haldane model

Degree of freedom	Charge	Orbital
Non-trivial insulators	Quantum anomalous Hall effect (Chern insulator)	Orbital Chern insulator
Hall responses		
Topological invariants	Chern number C	Orbital Chern number C_L

?

Topology: non-conserved quantity

PRB109, 155143 (2024)

S_z conserve

$$\begin{array}{ccc} & |\uparrow\rangle & |\downarrow\rangle \\ H_0 = & \begin{pmatrix} H_{QAH}^{+} & 0 \\ 0 & H_{QAH}^{-} \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Basis

H_{QAH} Haldane Hamiltonian (2x2 matrix)

Spin-up Chern number

$$H_{QAH}^{+} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega_m^{\uparrow}(k) = C_s^{\uparrow} = 1$$

Spin-down Chern number

$$H_{QAH}^{-} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega_m^{\downarrow}(k) = C_s^{\downarrow} = -1$$

Spin Chern number (C_s) : $C_s = \dfrac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1$

Topology: non-conserved quantity

PRB109, 155143 (2024)

S_z conserve

$$
\begin{array}{ccc}
 & |\uparrow\rangle & |\downarrow\rangle \ \text{Basis} \\
H_0 = & \begin{pmatrix} H^{+}_{QAH} & 0 \\ 0 & H^{-}_{QAH} \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array}
\end{array}
$$

H_{QAH} Haldane Hamiltonian
(2x2 matrix)

Spin-up Chern number

$$H^{+}_{QAH} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega^{\uparrow}_{m}(k) = C^{\uparrow}_{s} = 1$$

Spin-down Chern number

$$H^{-}_{QAH} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega^{\downarrow}_{m}(k) = C^{\downarrow}_{s} = -1$$

Spin Chern number (C_s) : $C_s = \dfrac{(C^{\uparrow}_{s} - C^{\downarrow}_{s})}{2} = 1$

S_z non-conserve

$$
\begin{array}{ccc}
 & |\uparrow\rangle & |\downarrow\rangle \ \text{Basis} \\
H_M = & \begin{pmatrix} H^{+}_{QAH} & -H_R \\ H_R & H^{-}_{QAH} \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array}
\end{array}
$$

Rashba SOC

H_{QAH} Haldane Hamiltonian

$|\uparrow\rangle_{VB}$ and $|\downarrow\rangle_{VB}$ mixed

How to define topological invariants?

We need a way to re-decompose the up and the down Berry curvature in the non-conserved quantity.

Feature Spectrum Topology

Redefine an operator to distinguish quantum numbers of the valence bands

Ref: E. Prodan PRB 80, 125327 (2009)
Ref: H. Lin arXiv:2310.14832v1 (2023)
YT Yao et al., PRB109, 155143 (2024)

Feature operator

$$\widehat{\mathbb{F}}_O|\tilde{\psi}_{mk}\rangle = (P\hat{O}P)|\tilde{\psi}_{mk}\rangle = O_{mk}|\tilde{\psi}_{mk}\rangle$$

$\hat{O}$ = quantum operator, e.g. $\hat{S}_z$, $\hat{L}_z \cdots$

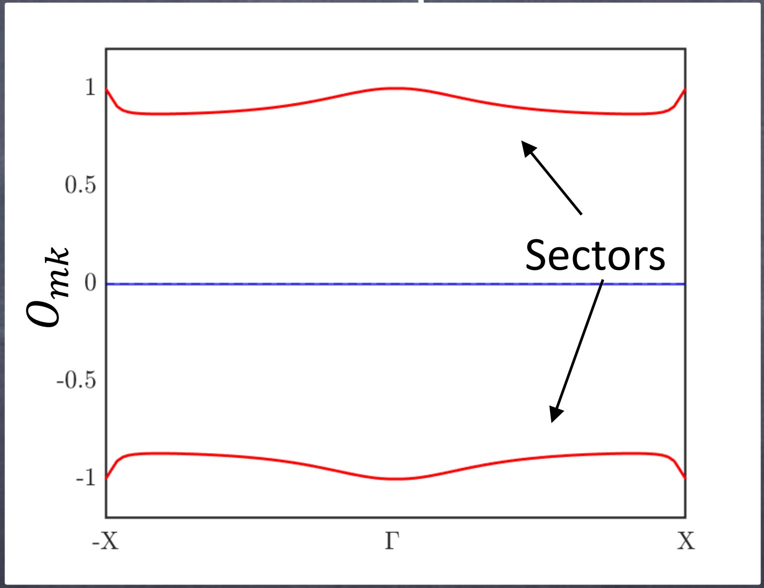
$P = \sum_{n\in occ.} |\psi_{nk}\rangle\langle\psi_{nk}|$ projector

O_{mk} = Feature eigenvalue

$|\tilde{\psi}_{mk}\rangle = \sum_{i=occ} a_i|\psi_i\rangle_{VB}$ Feature eigenstate

Bloch wavefunction of valence bands

Feature spectrum



Topological invariant number: Feature Chern number

Feature Spectrum Topology ($\hat{S}_z$)

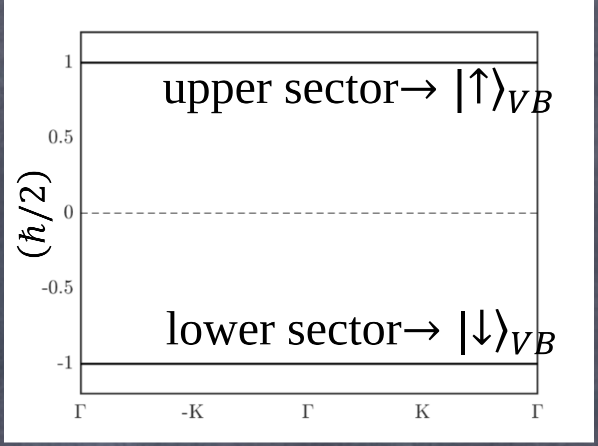
YT Yao et al., PRB109, 155143 (2024)

Feature operator: $\widehat{\mathbb{F}}_O = P\hat{O}P \Rightarrow \widehat{\mathbb{F}}_{S_z} = P\hat{S}_zP$

S_z conserve

$$H_0 = \begin{array}{cc} \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \end{array} & \text{Basis} \\ \begin{pmatrix} H_{QAH}^{+} & 0 \\ 0 & H_{QAH}^{-} \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Feature spectrum



Eigenvalue of S_z
(S_z conserve)

$$\hat{S}_z|\psi_{nk}\rangle = \pm\frac{\hbar}{2}|\psi_{nk}\rangle$$

Feature Spectrum Topology ($\hat{S}_z$)

YT Yao et al., PRB109, 155143 (2024)

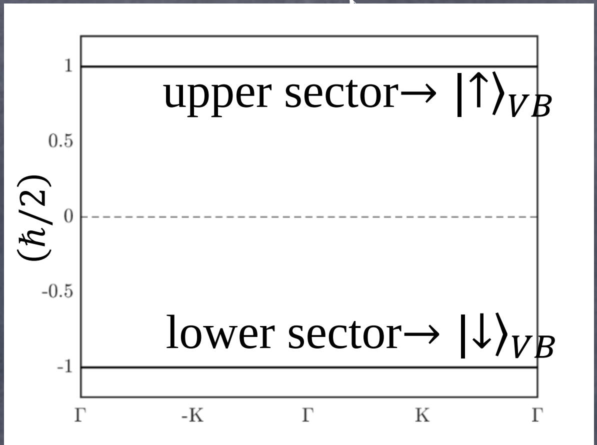
Feature operator: $\widehat{\mathbb{F}}_O = P\hat{O}P \Rightarrow \widehat{\mathbb{F}}_{S_z} = P\hat{S}_zP$

S_z conserve

$$H_0 = \begin{array}{cc|c} |\uparrow\rangle & |\downarrow\rangle & \text{Basis} \\ \end{array}$$

$$H_0 = \begin{pmatrix} H_{QAH}^{+} & 0 \\ 0 & H_{QAH}^{-} \end{pmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array}$$

Feature spectrum



Eigenvalue of S_z (S_z conserve)

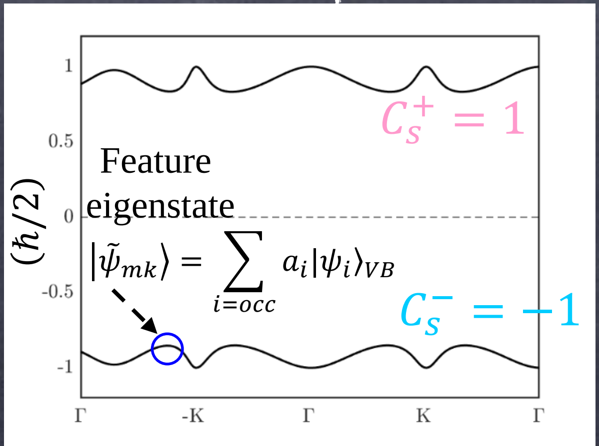
$$\hat{S}_z|\psi_{nk}\rangle = \pm\frac{\hbar}{2}|\psi_{nk}\rangle$$

S_z non-conserve

$$\begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \quad \text{Basis} \end{array}$$

$$H_M = \begin{pmatrix} H_{QAH}^{+} & -H_R \\ H_R & H_{QAH}^{-} \end{pmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array}$$

Feature spectrum



Feature Chern number

$$C_s = \frac{(C_s^+ - C_s^-)}{2} = 1$$

Feature Spectrum Topology $(\hat{L}_z)$

Orbital angular momentum in solid: non-conserved quantity

$$\Big\downarrow \; \widehat{\mathbb{F}}_{s_z} \to \widehat{\mathbb{F}}_{L_z}$$

Feature operator:

$$\widehat{\mathbb{F}}_{L_z} = P\hat{L}_z P$$

$$\Downarrow$$

Feature Chern number:

$$C_L = \frac{C_L^{\mathbb{I}+} - C_L^{\mathbb{I}-}}{2}$$

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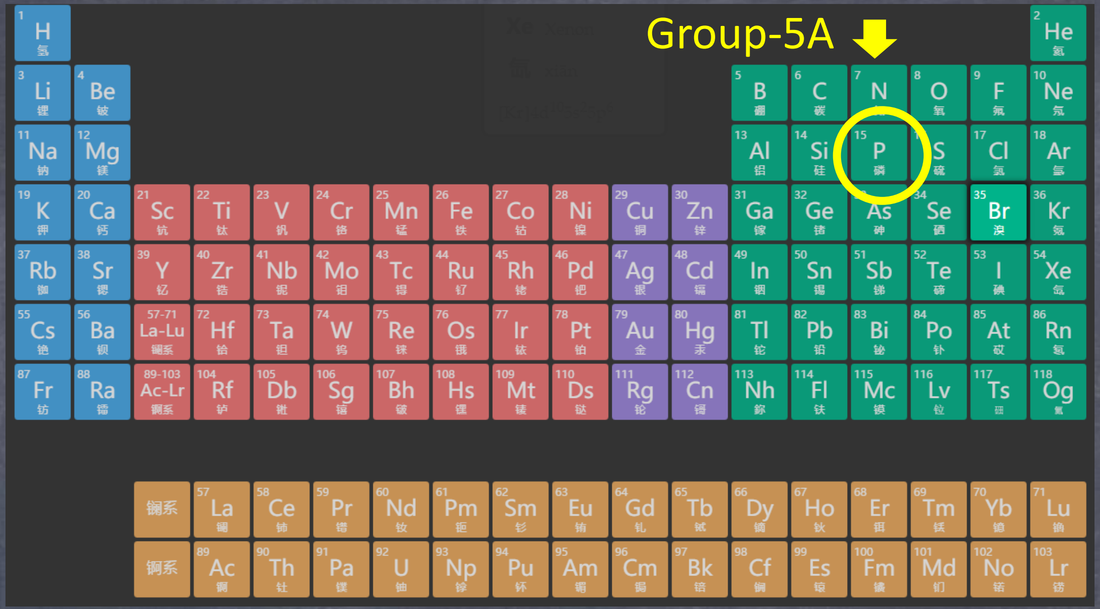
  Material: Phosphorene (磷烯)
  Orbital Chern number
  Boundary states
  Orbital Hall conductivity

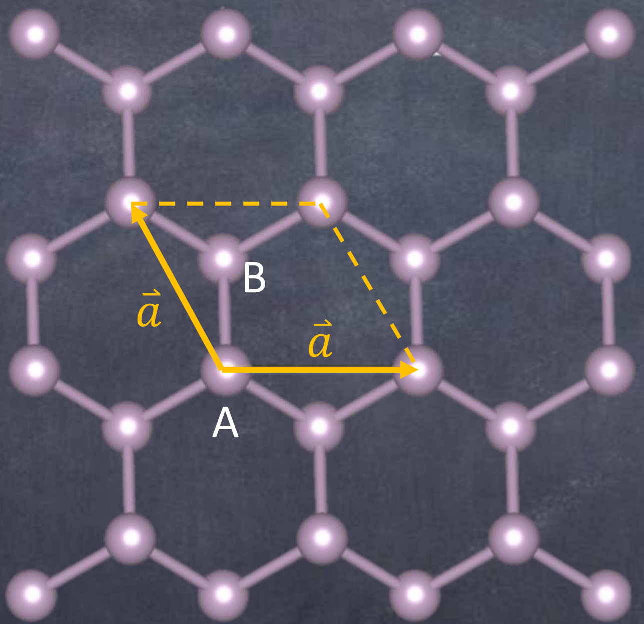
Phosphorene
(磷烯)

arXiv:2503.08138 (2025)

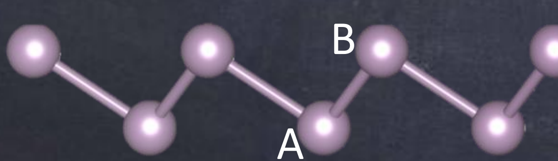


Buckled-Honeycomb Monolayer

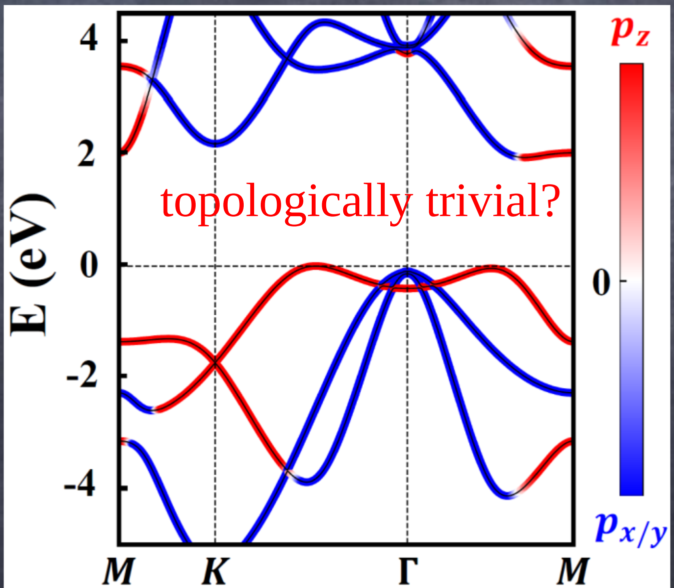
Top view



Side view



Band structure



Topological invariant: $\mathbb{Z}_2 = 0$

Orbital Hall insulator in Phosphorene

arXiv:2503.08138 (2025)

Feature Spectrum Topology

Orbital
Chern number

Gapless boundary states

Orbital Hall conductivity

Feature (orbital) Chern number

arXiv:2503.08138 (2025)

Spherical harmonics $Y_{l,m}$

$p_x \propto Y_{1,1} + Y_{1,-1}$

$p_y \propto i(Y_{1,1} - Y_{1,-1})$

$p_z \propto Y_{1,0}$

Feature operator:

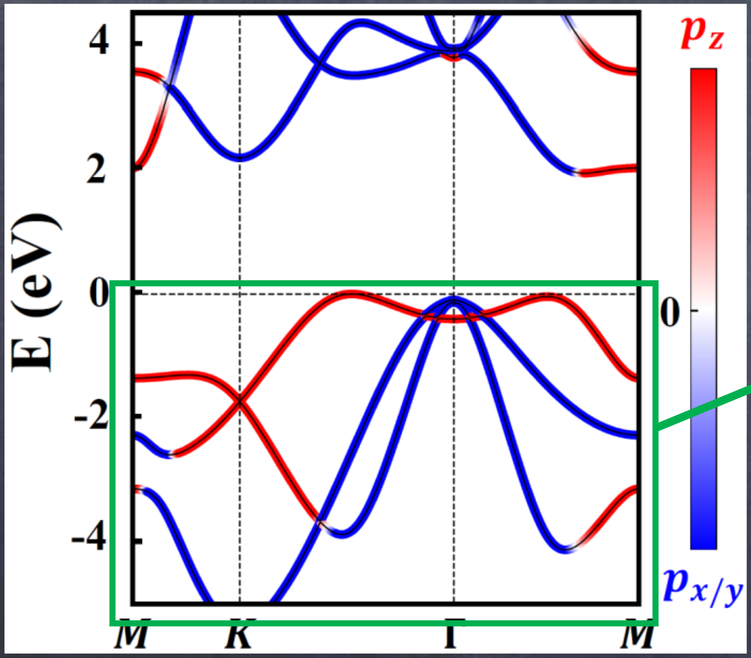
$$\hat{\mathbb{F}}_{L_z} = P\hat{L}_z P$$

Eigenvalue of L_z (L_z conserve)

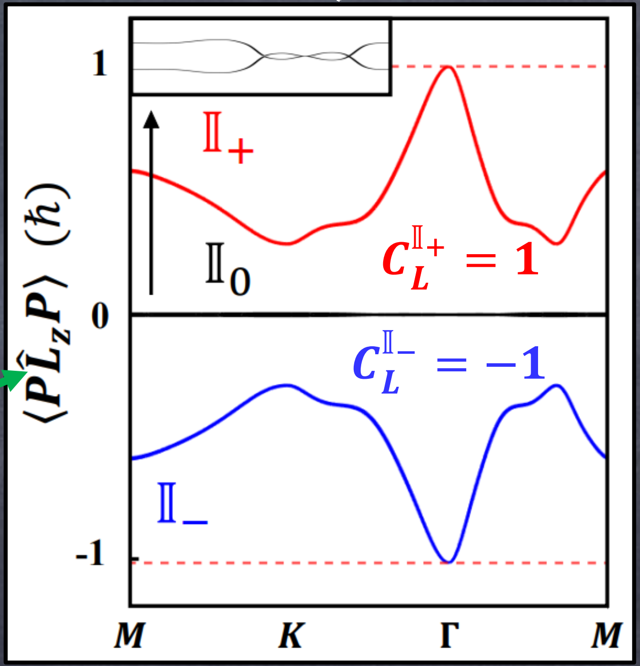
$$\hat{L}_z|\psi_{nk}\rangle = m\hbar|\psi_{nk}\rangle$$

$$m = 1, 0, -1$$

Band structure



Feature spectrum



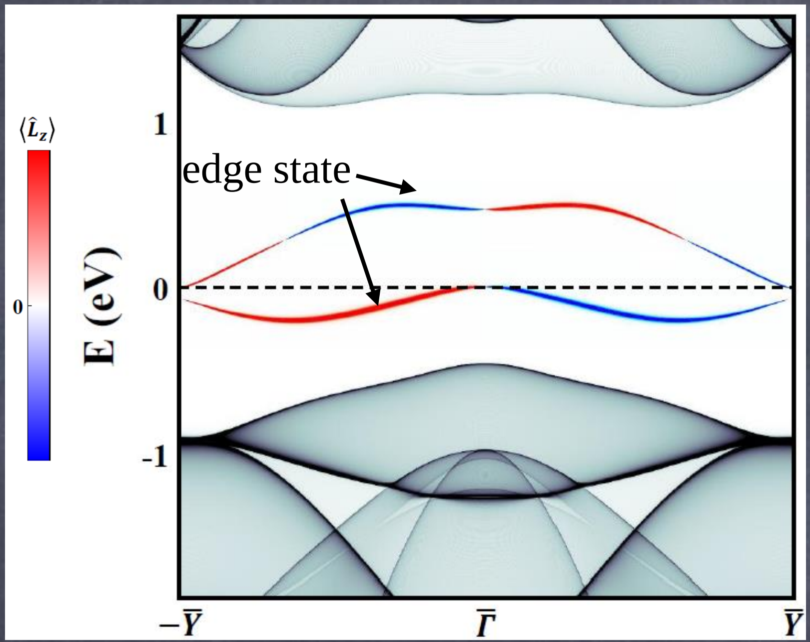
Feature (orbital) Chern number:

$$C_L = \frac{C_L^{\mathbb{I}_+} - C_L^{\mathbb{I}_-}}{2} = 1$$

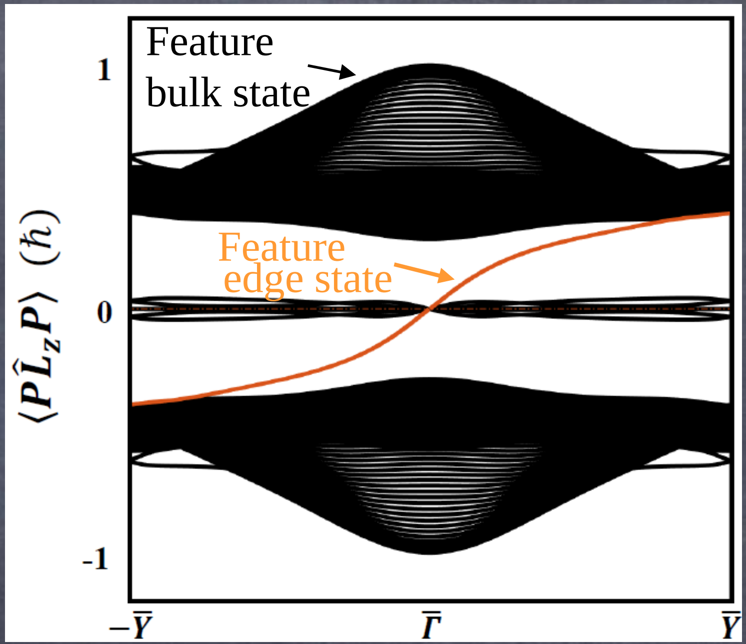
Bulk-Boundary Correspondence

arXiv:2503.08138 (2025)

Edge band structure



Edge feature spectrum



$$\mathbb{Z}_2 = 0$$

$$C_L = \frac{C_L^{\mathbb{I}+} - C_L^{\mathbb{I}-}}{2} = 1$$

Energy Feature

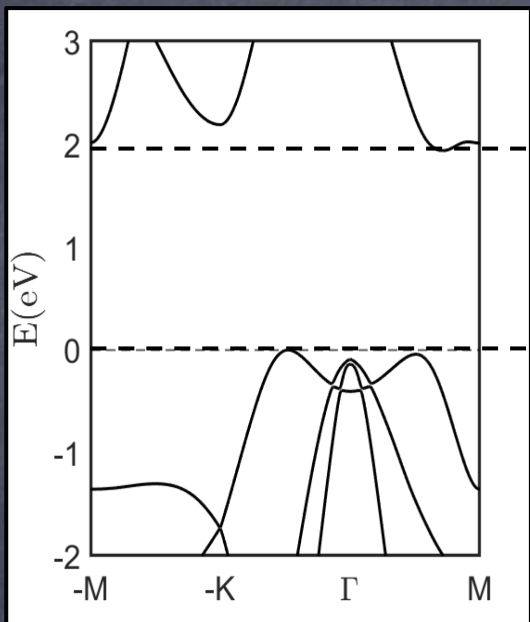
Feature-energy duality: $C_L^{\mu} = 0 + 1$

YT Yao et al., PRB109, 155143 (2024)

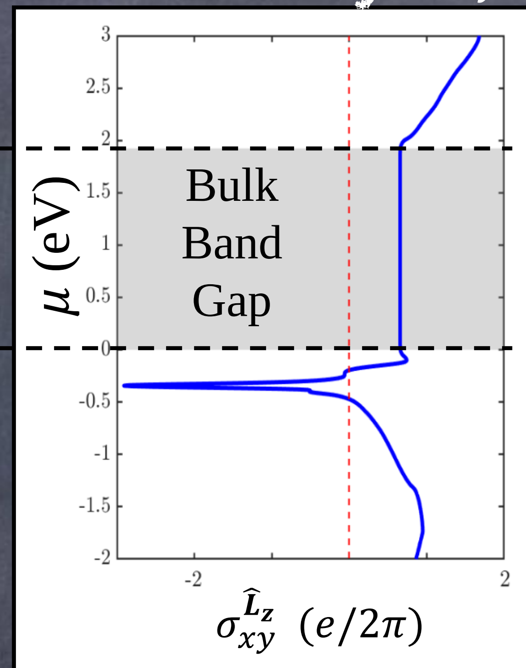
Orbital Hall conductivity

arXiv:2503.08138 (2025)

Band Structure



Orbital Hall Conductivity ($\sigma_{xy}^{\hat{L}_z}$)



feature Chern number

$$C_L = 1$$

OHC Plateau

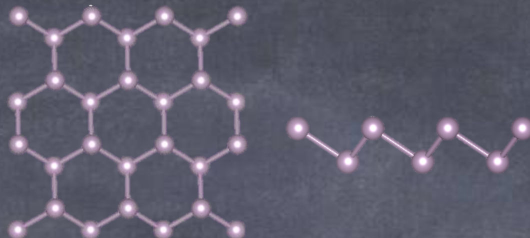
Kubo formula: $\sigma_{xy}^{\hat{L}_z} = 2e\hbar \int_{BZ} \frac{d^2\mathbf{k}}{(2\pi)^2} \sum_n f_n(\mathbf{k})\, \Omega_{n,xy}^{\hat{L}_z}(\mathbf{k})$

$$\Omega_{n,xy}^{\hat{L}_z}(\mathbf{k}) = \sum_{n\neq m} \mathrm{Im} \frac{\left\langle u_{n\mathbf{k}} \middle| \hat{J}_x^{\hat{L}_z} \middle| u_{m\mathbf{k}} \right\rangle \left\langle u_{m\mathbf{k}} \middle| \hat{v}_y \middle| u_{n\mathbf{k}} \right\rangle}{(E_{n\mathbf{k}} - E_{m\mathbf{k}})^2}$$

Take-home messages

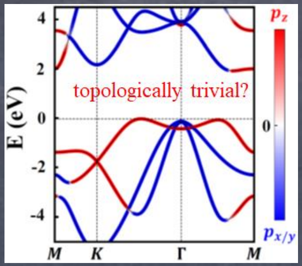
arXiv:2503.08138 (2025)

Phosphorene:



$\mathbb{Z}_2 = 0$

Topological band theory



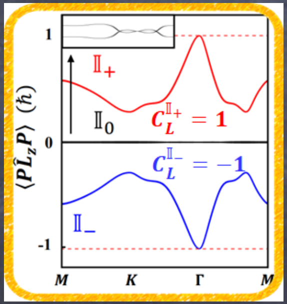
Ordinary band insulator

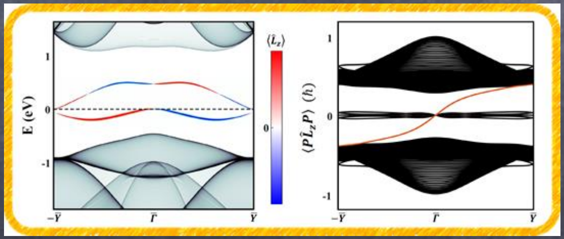
$\widehat{\mathbb{F}}_{L_z} = P\hat{L}_z P$

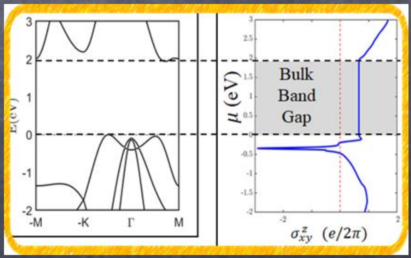
$C_L = 1$

Orbital Chern insulator

Feature Spectrum Topology







Orbital Hall effect in insulators originates from the band topology

Acknowledgements

arXiv > cond-mat > arXiv:2503.08138

Condensed Matter > Materials Science

[Submitted on 11 Mar 2025]

Topological Nature of Orbital Chern Insulators

arXiv:2503.08138 (2025)

My students

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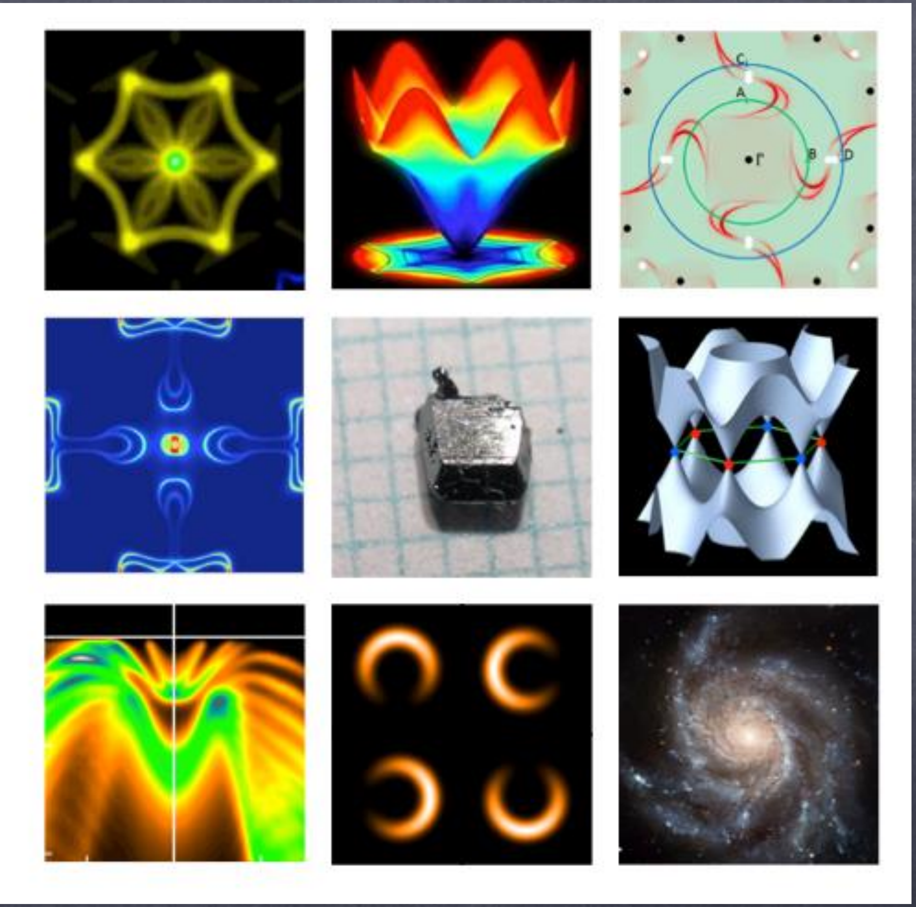
Collaborator

Hsin Lin (Sinica)

Thank you !

To see a world in a grain of sand … —William Blake



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1931

前沿量子科技研究中心
Center for Quantum Frontiers of Research & Technology

NCTS
Physics Division

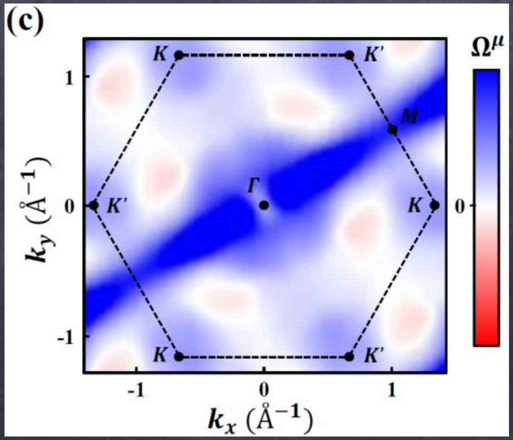
APPENDIX

projector $P = \sum_{n\in occ} |u_{nk}\rangle\langle u_{nk}|$

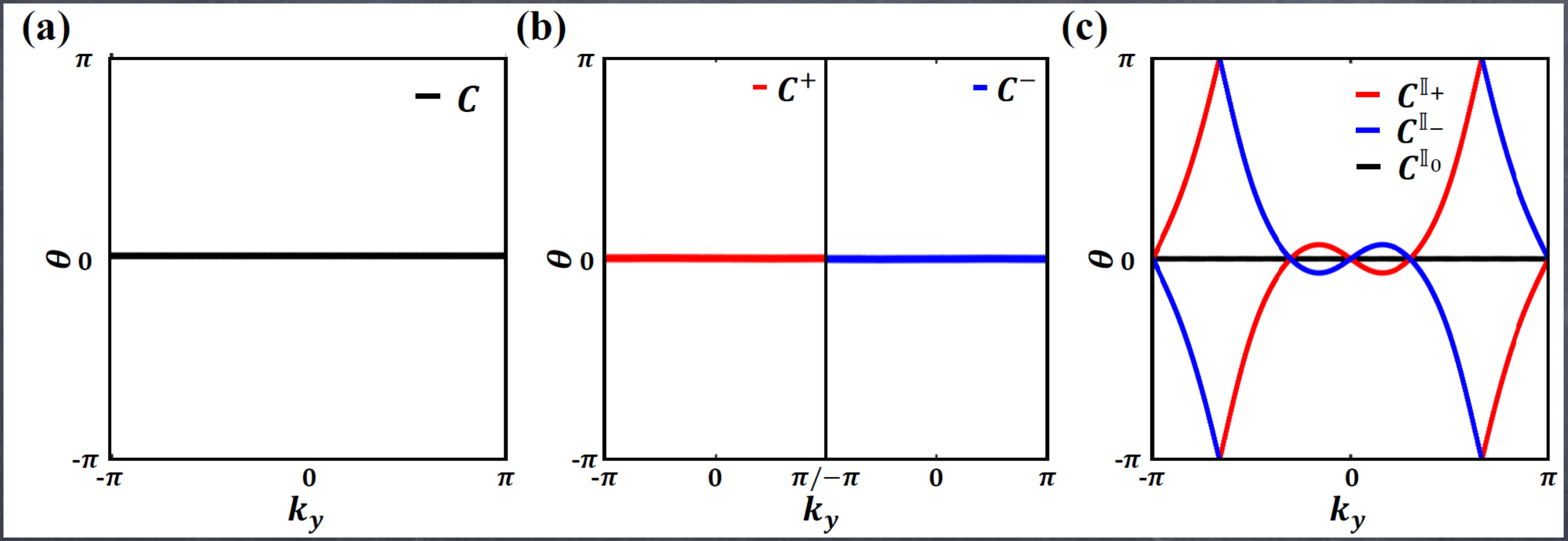
Berry curvature $\Omega = i\mathrm{Tr}\left(P\left[\partial_{k_x}P, \partial_{k_y}P\right]\right) d_{k_x}\wedge d_{k_y}$

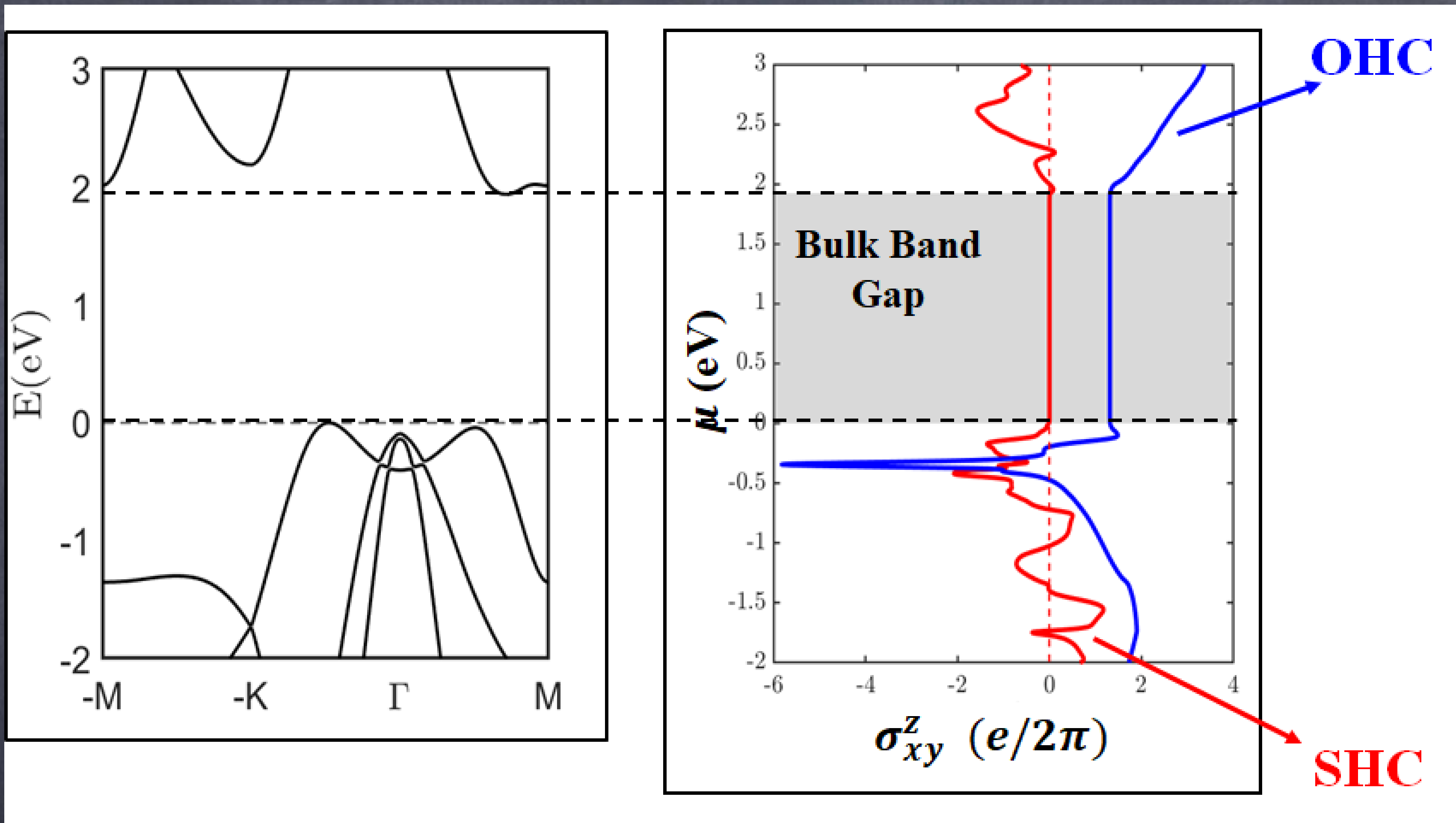
Feature Berry curvature $\Omega^{\mu} = i\mathrm{Tr}\left(P^{\mu}\left[\partial_{k_x}P^{\mu}, \partial_{k_y}P^{\mu}\right]\right) d_{k_x}\wedge d_{k_y}$

$$P^{\mu} = \sum_{m} |u_{mk}^{\mu}\rangle\langle u_{mk}^{\mu}| \qquad \mu = \text{sector}$$

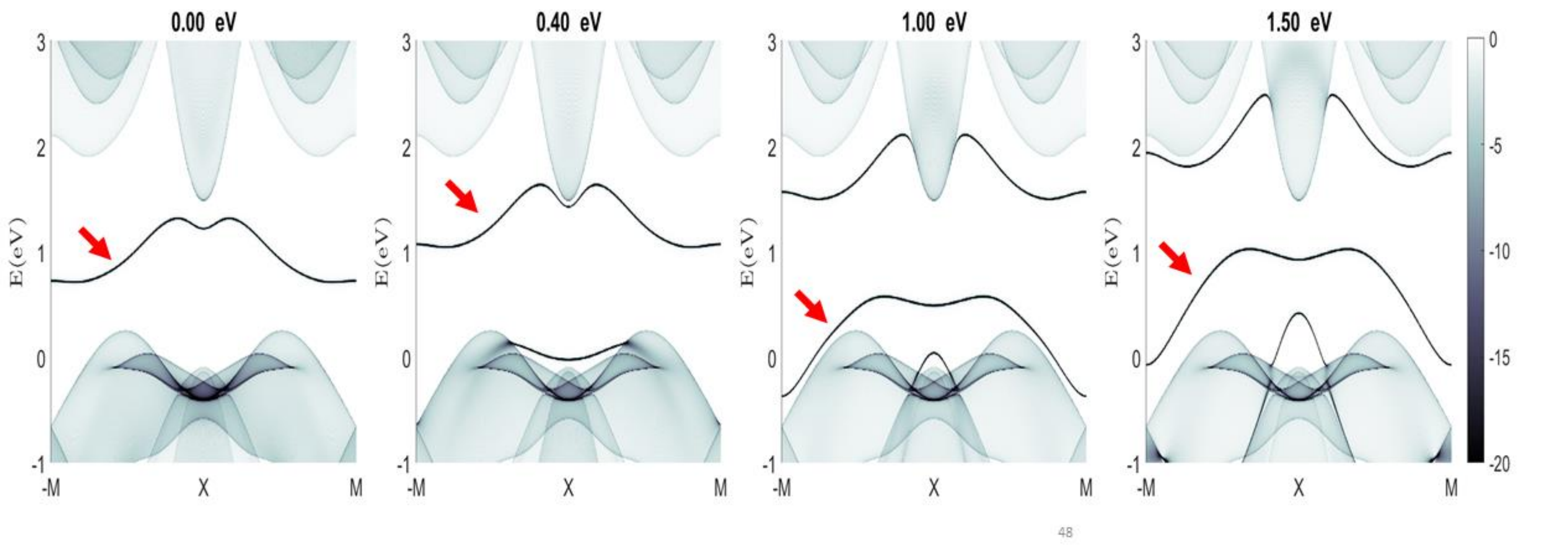


Chern number Spin Chern number Orbital Chern number

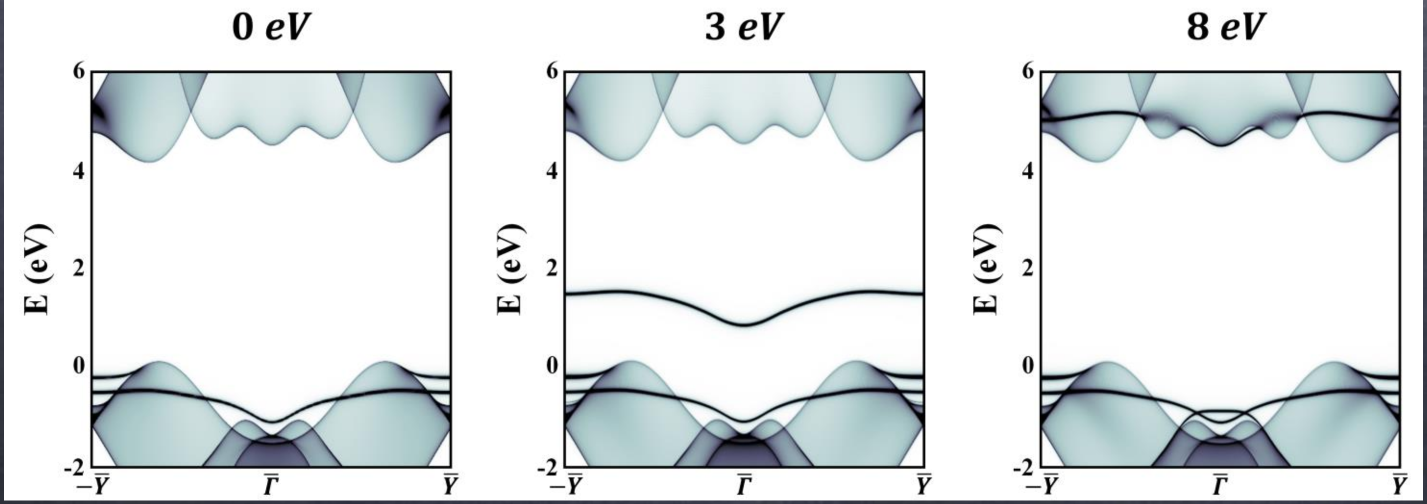


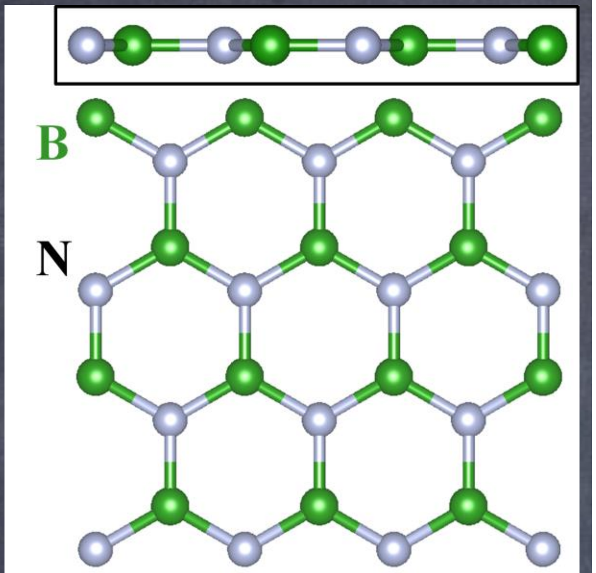

3
2
1
0
-1
-2
E(eV)
-M
-K
Γ
M
OHC
Bulk Band Gap
μ (eV)
σ^z_{xy} $(e/2\pi)$
SHC
3
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-6
-4
-2
0
2
4

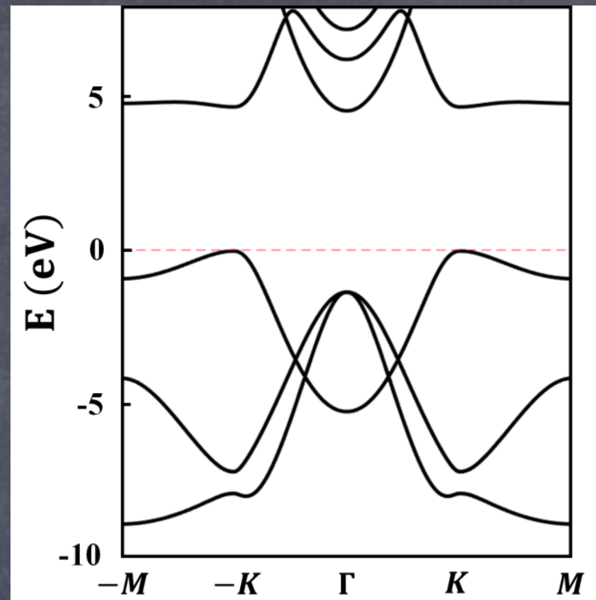
Phosphorene

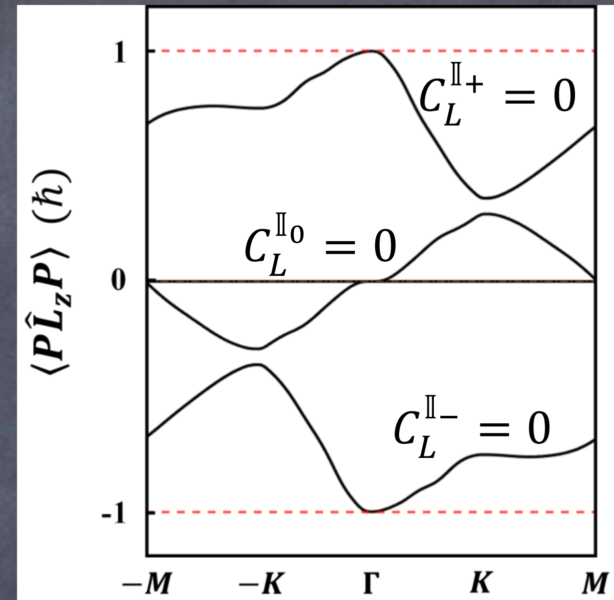


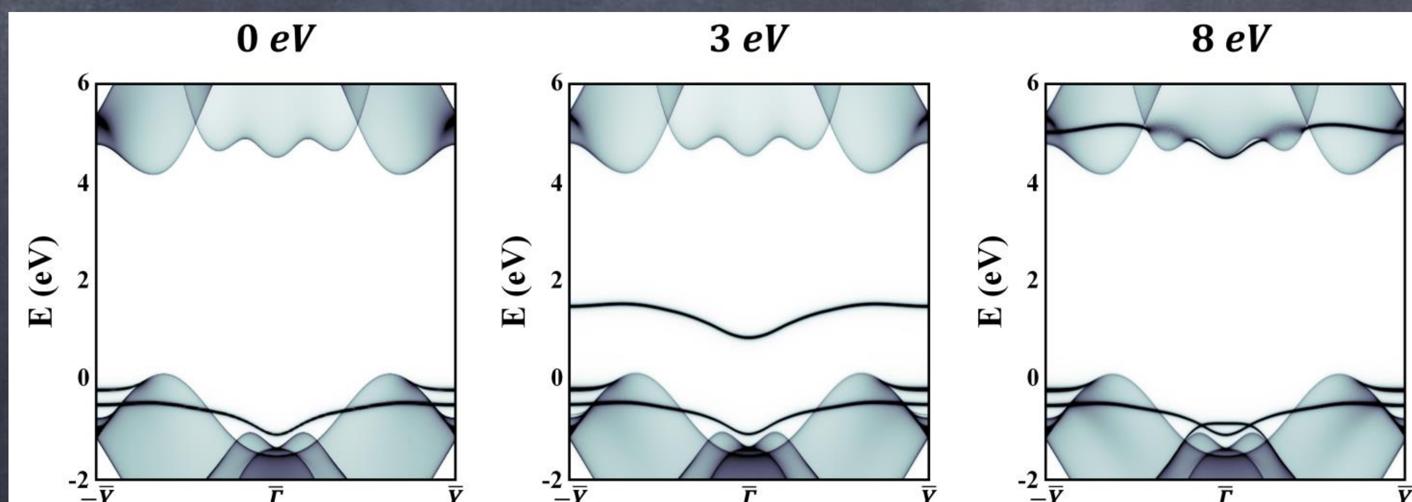
h-BN

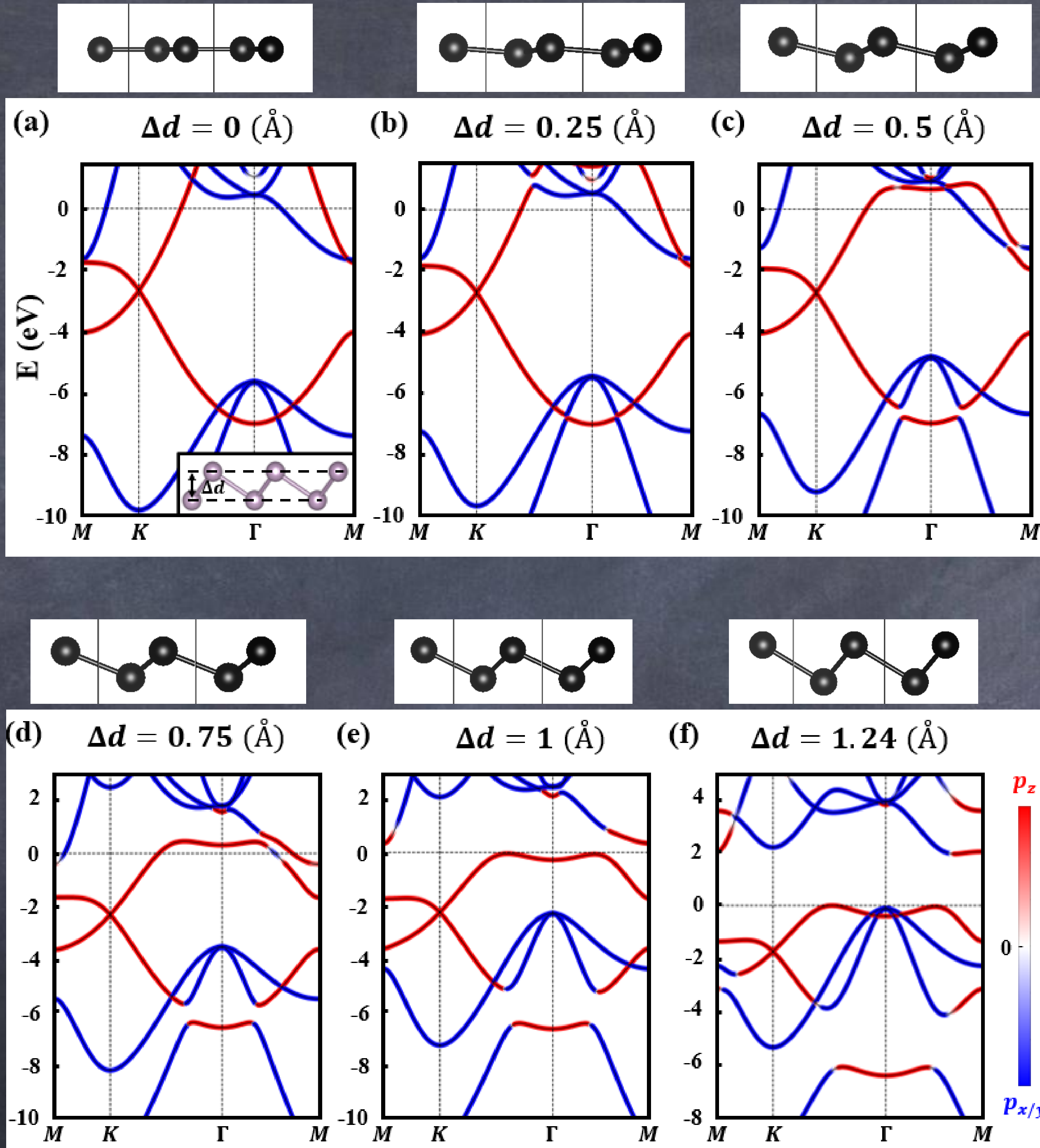



B
N


E (eV)
5
0
-5
-10
$-M$
$-K$
Γ
K
M


$\langle P\hat{L}_z P\rangle\ (\hbar)$
1
0
-1
$C_L^{\mathbb{I}+} = 0$
$C_L^{\mathbb{I}0} = 0$
$C_L^{\mathbb{I}-} = 0$
$-M$
$-K$
Γ
K
M


0 eV
3 eV
8 eV
E (eV)
6
4
2
0
-2
$-\overline{Y}$
$\overline{\Gamma}$
$\overline{Y}$



(a)
$\Delta d = 0$ (Å)
(b)
$\Delta d = 0.25$ (Å)
(c)
$\Delta d = 0.5$ (Å)
E (eV)
Δd
M K Γ M
(d)
$\Delta d = 0.75$ (Å)
(e)
$\Delta d = 1$ (Å)
(f)
$\Delta d = 1.24$ (Å)
p_z
$p_{x/y}$