バルクエッジ対応の物理の多様性と普遍性

Electronic structure of silicene in the extended Weaire-Thorpe model

Flat bands and Dirac cones

Y. Hatsugai
Univ. Tsukuba

Y.Hatsugai, K.Shiraishi, H. Aoki, New J. Phys. 17, 025009 (2015)
arXiv:1410.7885

科研費 KAKENHI

Plan

- Singular dispersions & silicene
  - "Topological" deformation of Takeda-Shiraishi's.
  - Flat bands in materials: counting dimensions
- Overlapping molecular orbitals & flat bands
  - Without translational invariance
  - Physical origin of (nearly) flat bands
- Weaire-Thorpe model and extension
  - 3D to 2D
  - Hydrogen termination
  - Buckling

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☆Silicene as a silicon analogue of graphene

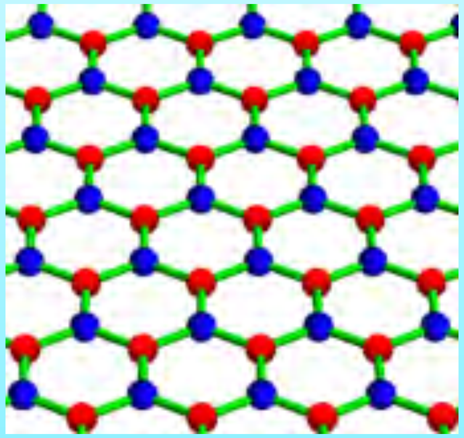
One line history of singular dispersions (Dirac cones)

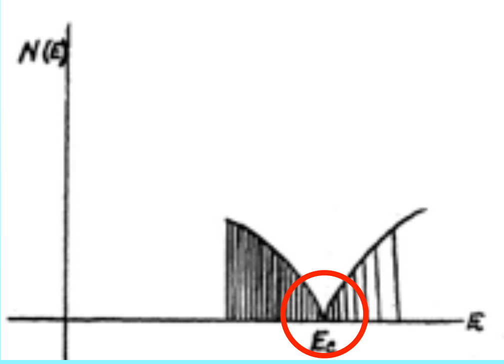
Graphene

Predicted in 1947, then, realized in 2004

Wallace

Novoselov-Geim et al.





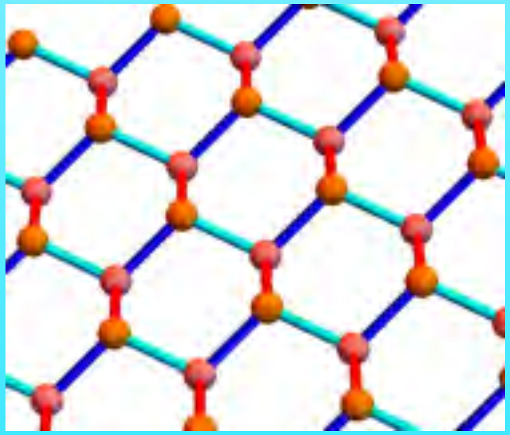
Wallace, Phys. Rev.71, 622 (1947)

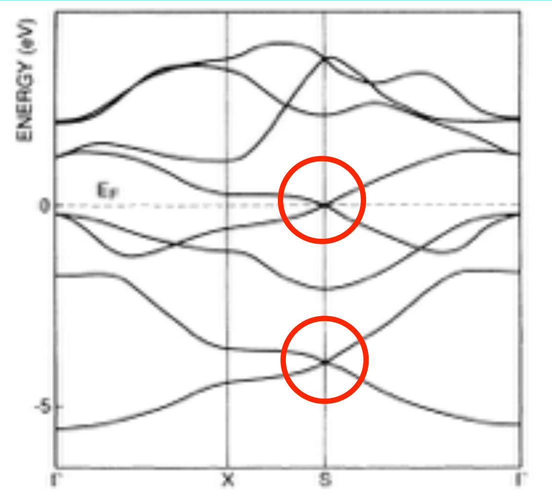
Silicene

Predicted in 1994, then, realized (??) in 2012

Takeda-Shiraishi

Lalmi et al./Vogt et al.



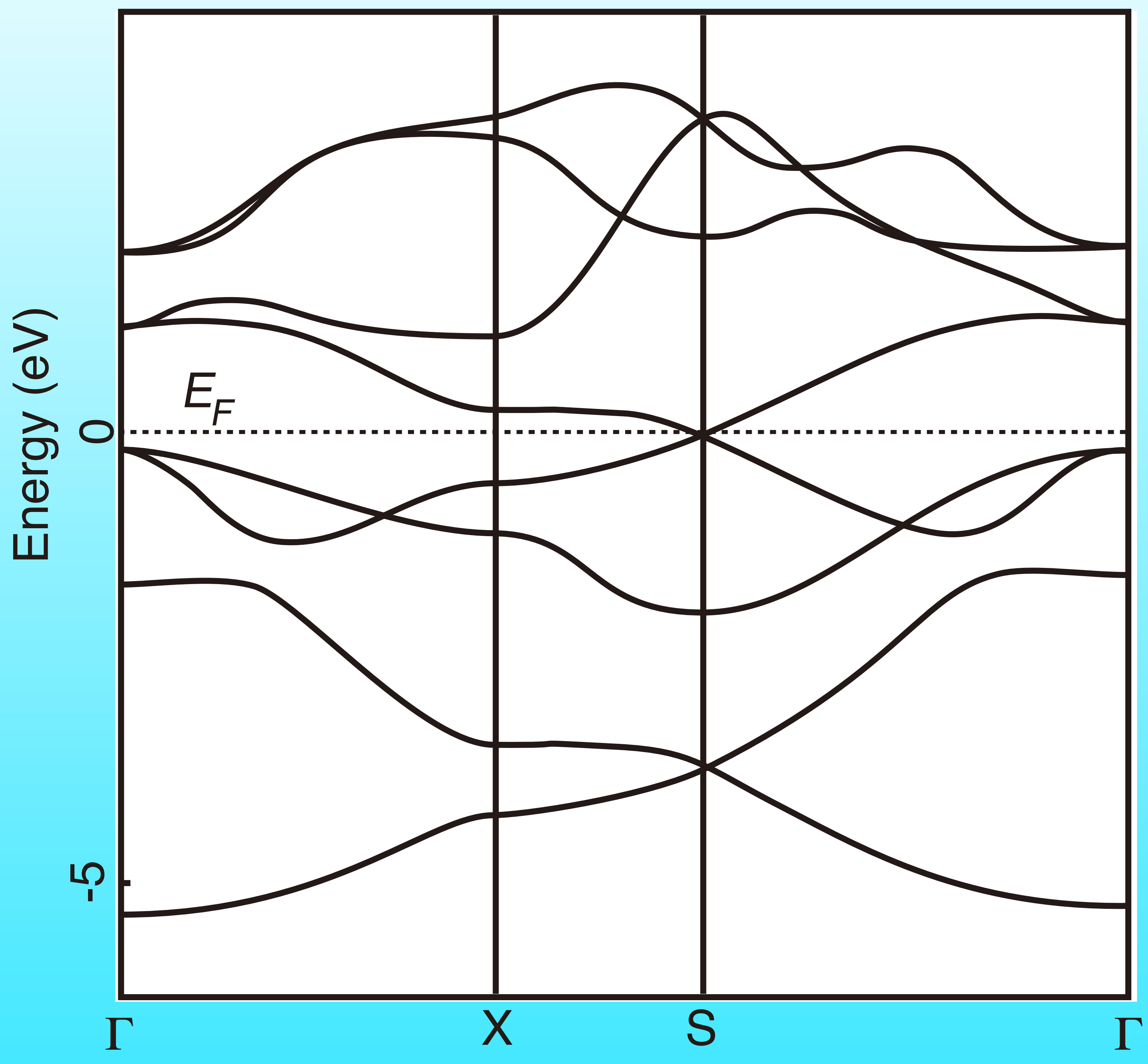


Takeda-Shiraishi,
Phys. Rev. B50, 14916 (1994)

History repeats itself

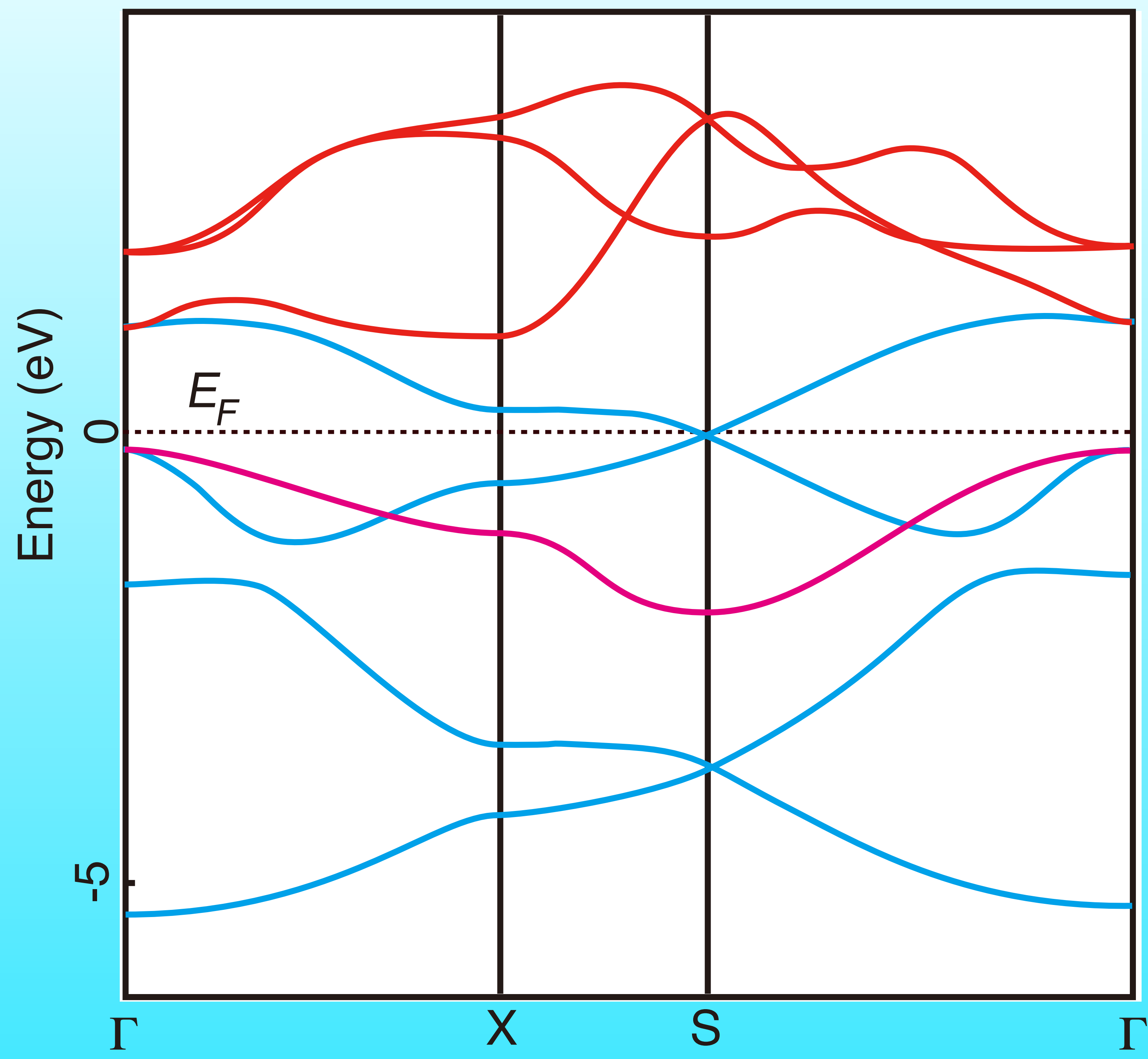
Dirac cones & something else, what ??

Revisiting Takeda-Shiraishi's



☆ Revisiting Takeda-Shiraishi's

"Topological" deformation of the bands



Classify into two: bands of Dirac fermions & else

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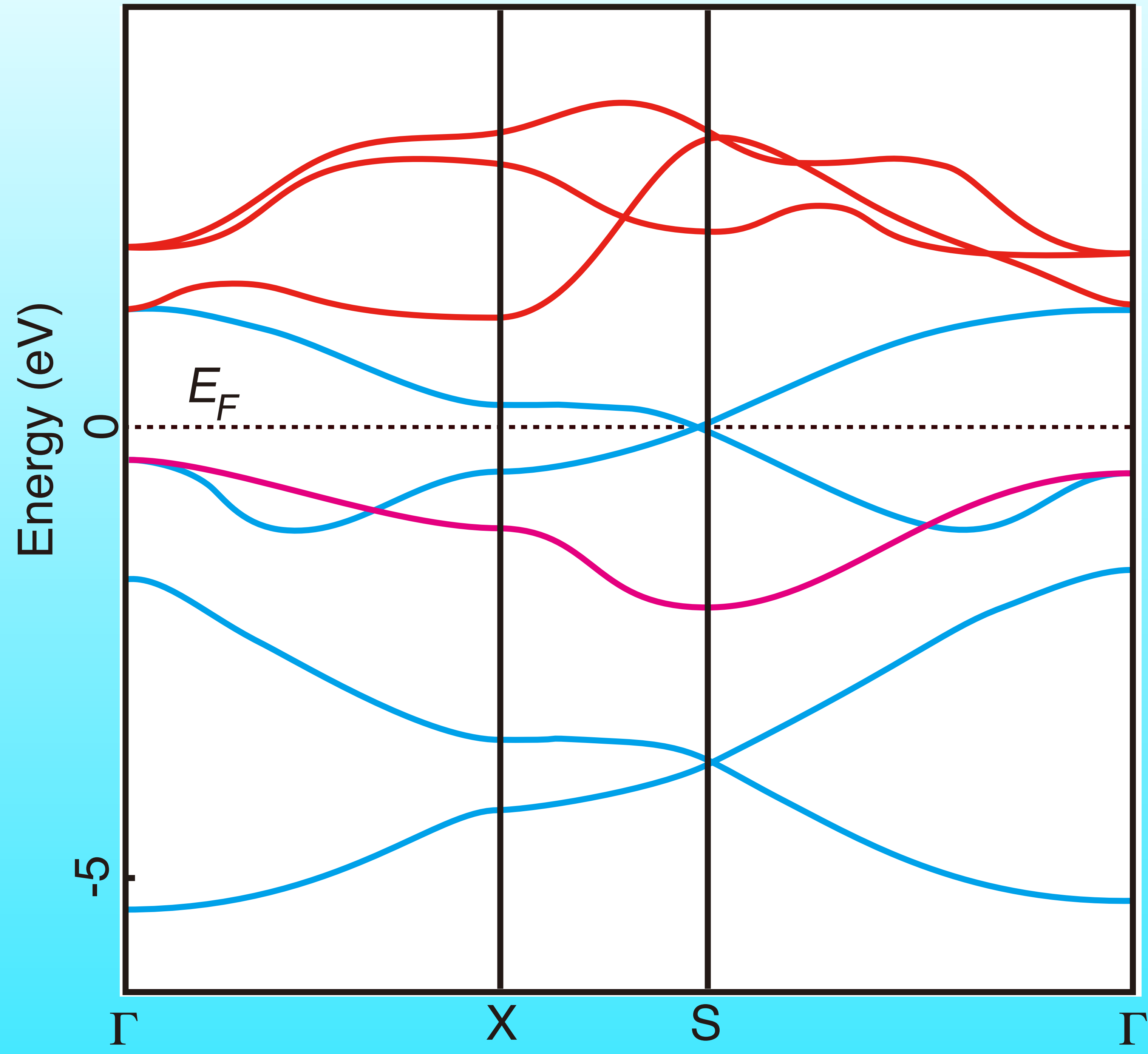

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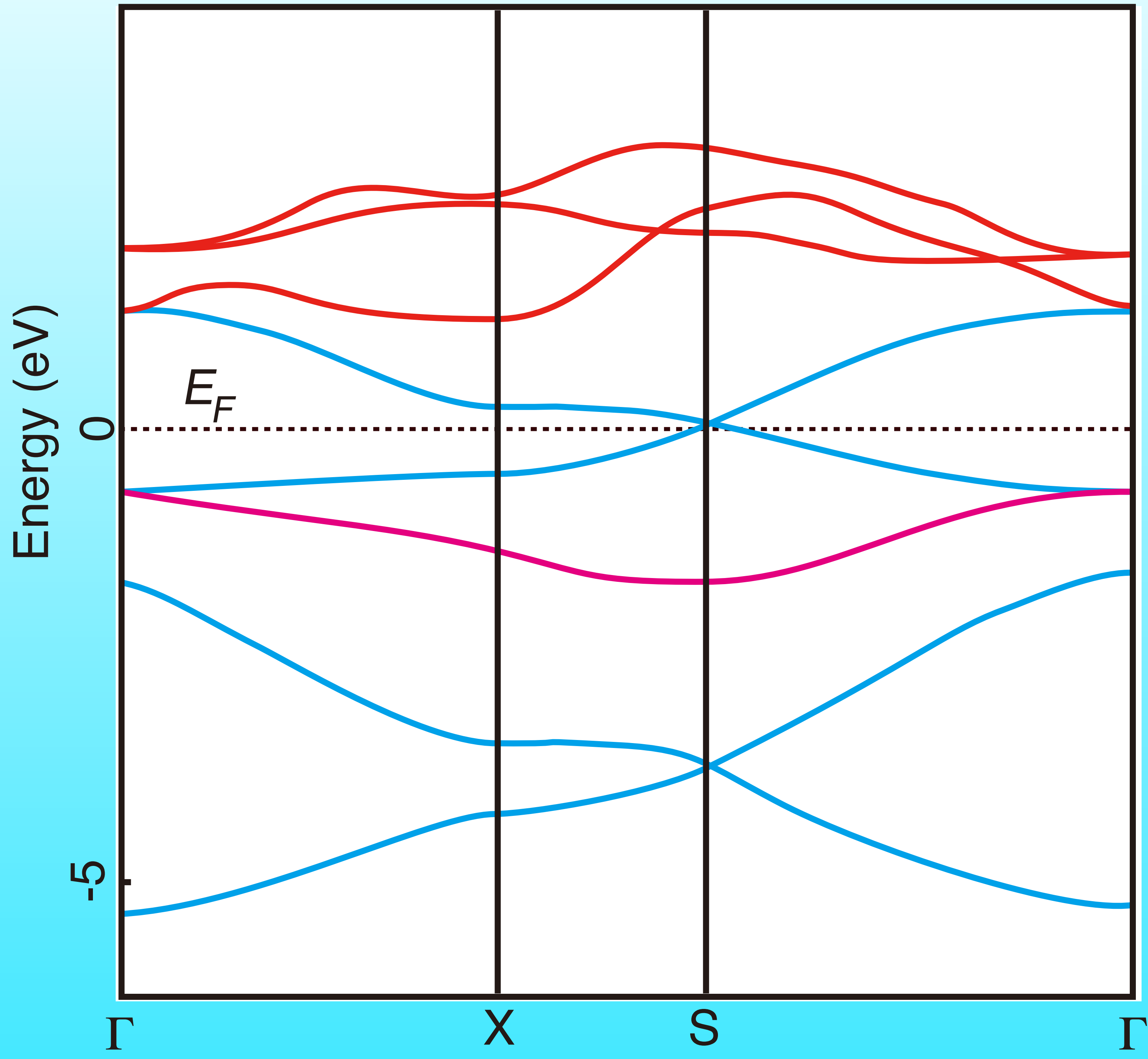

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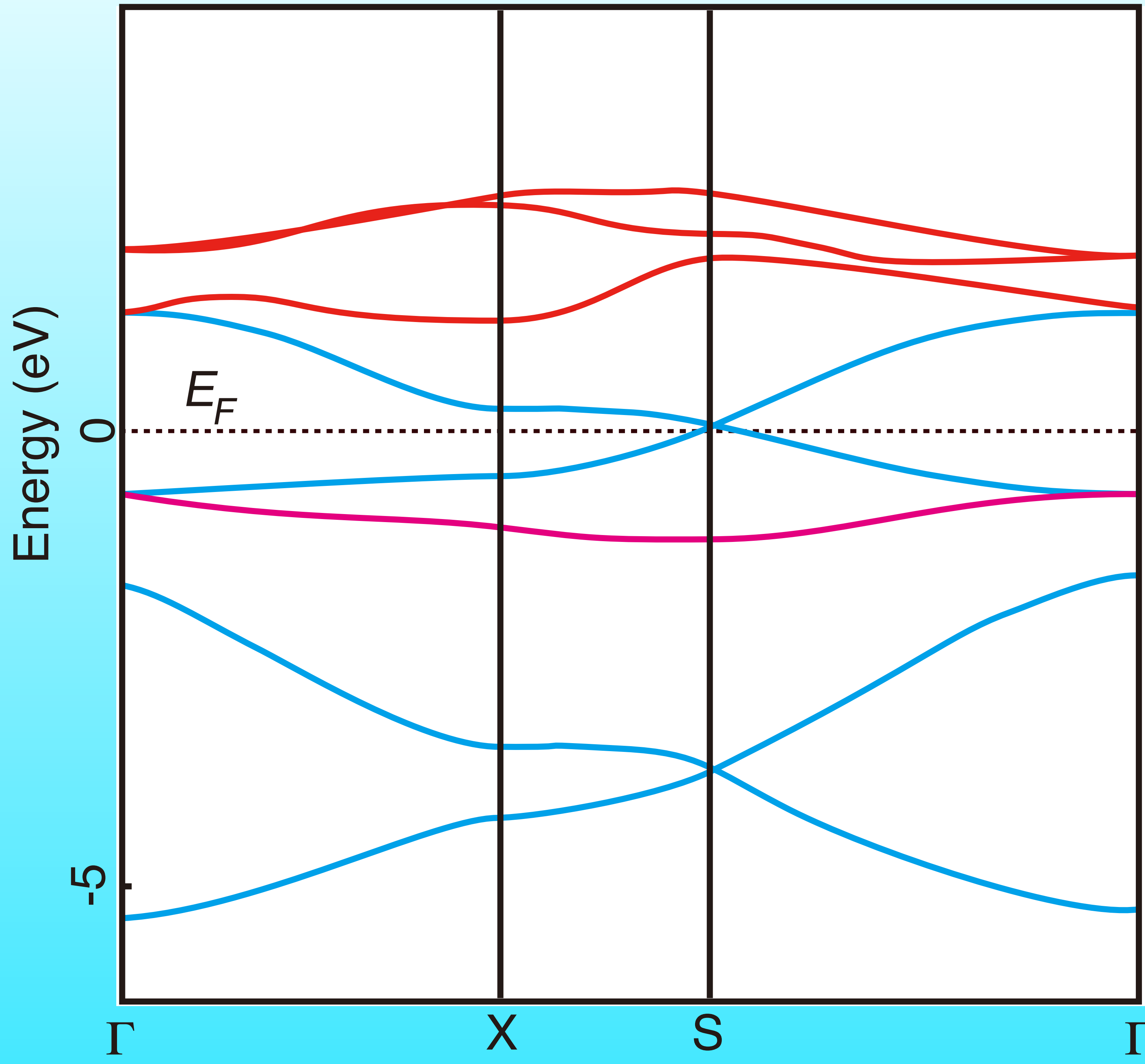

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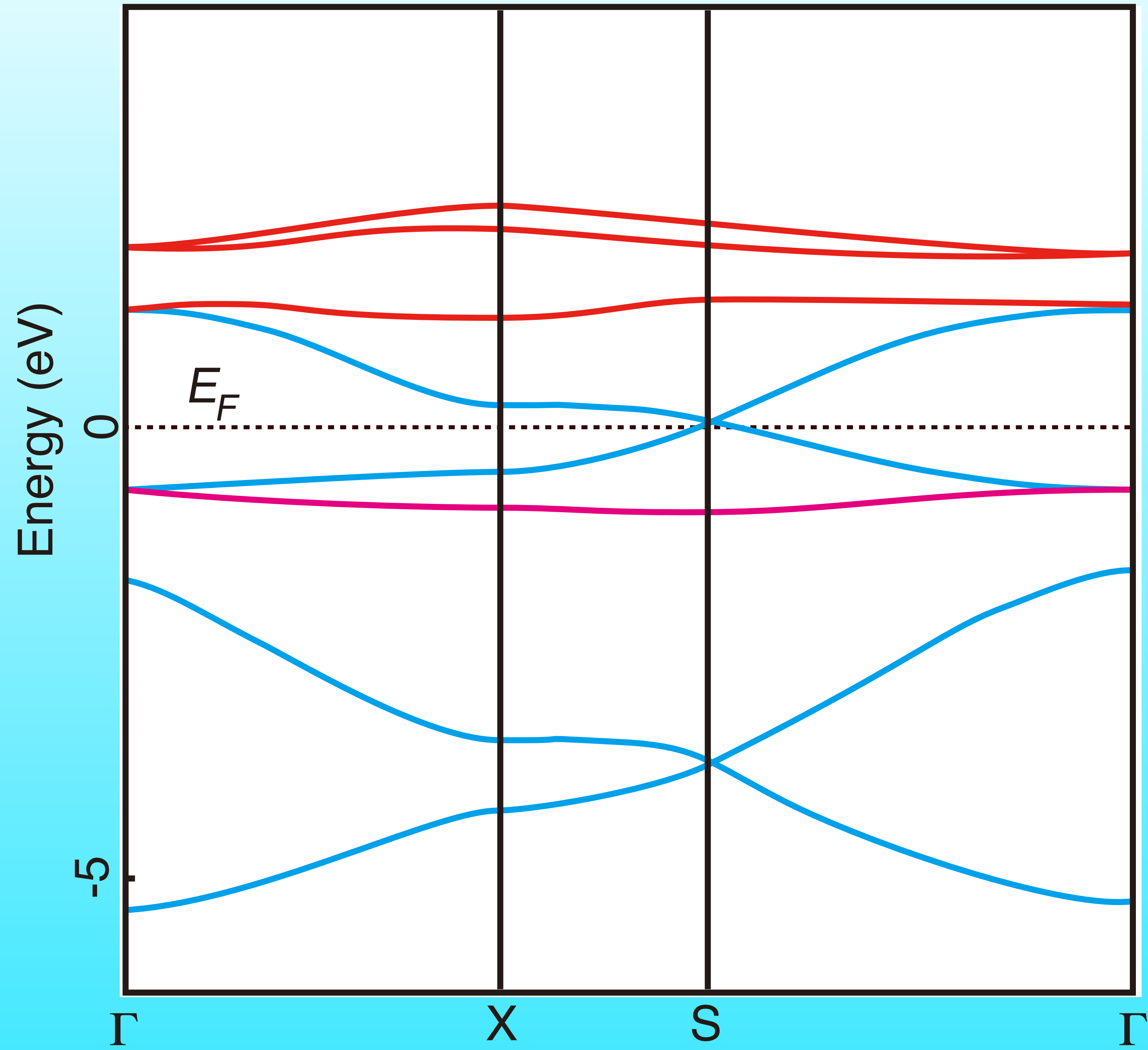

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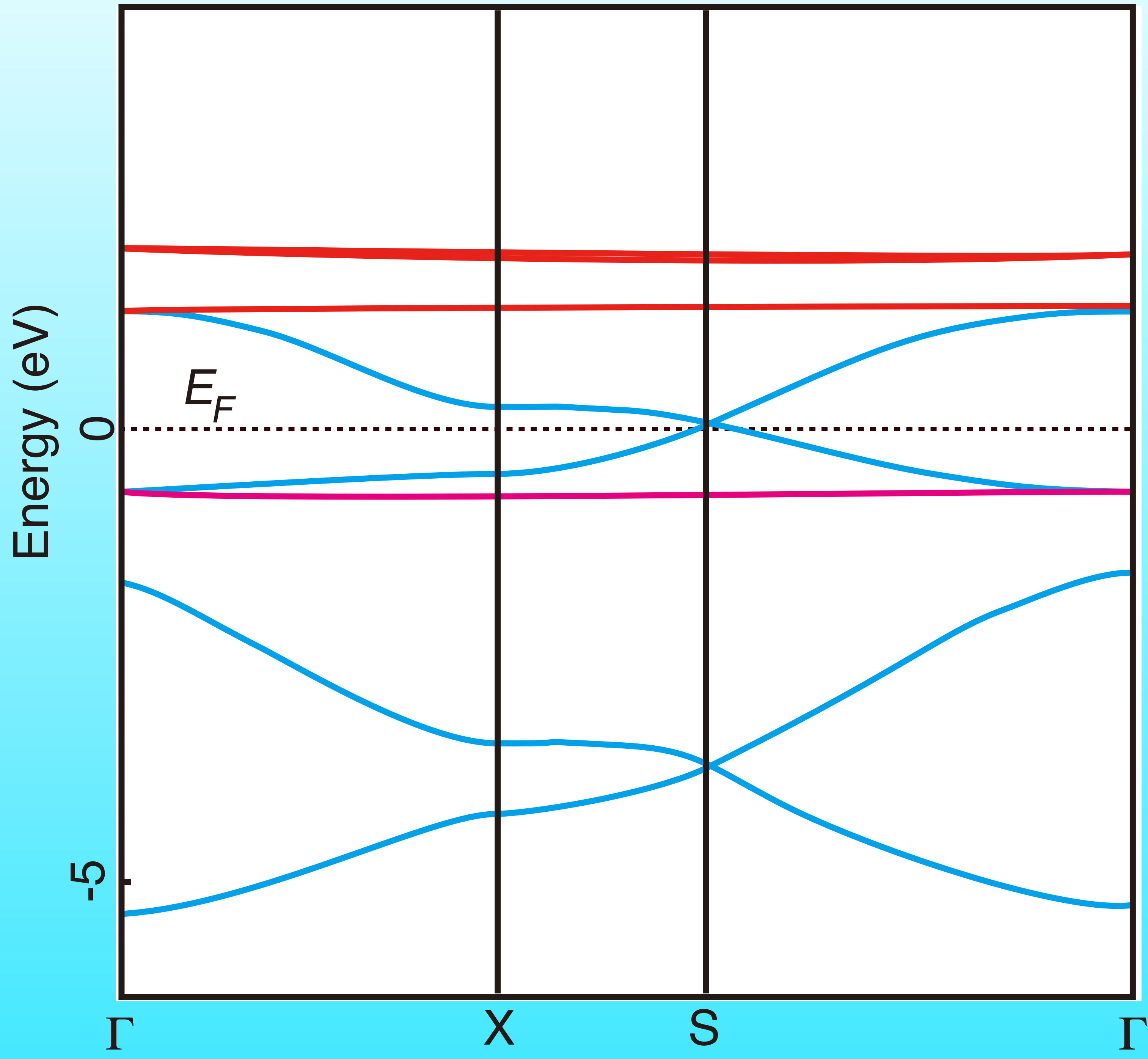

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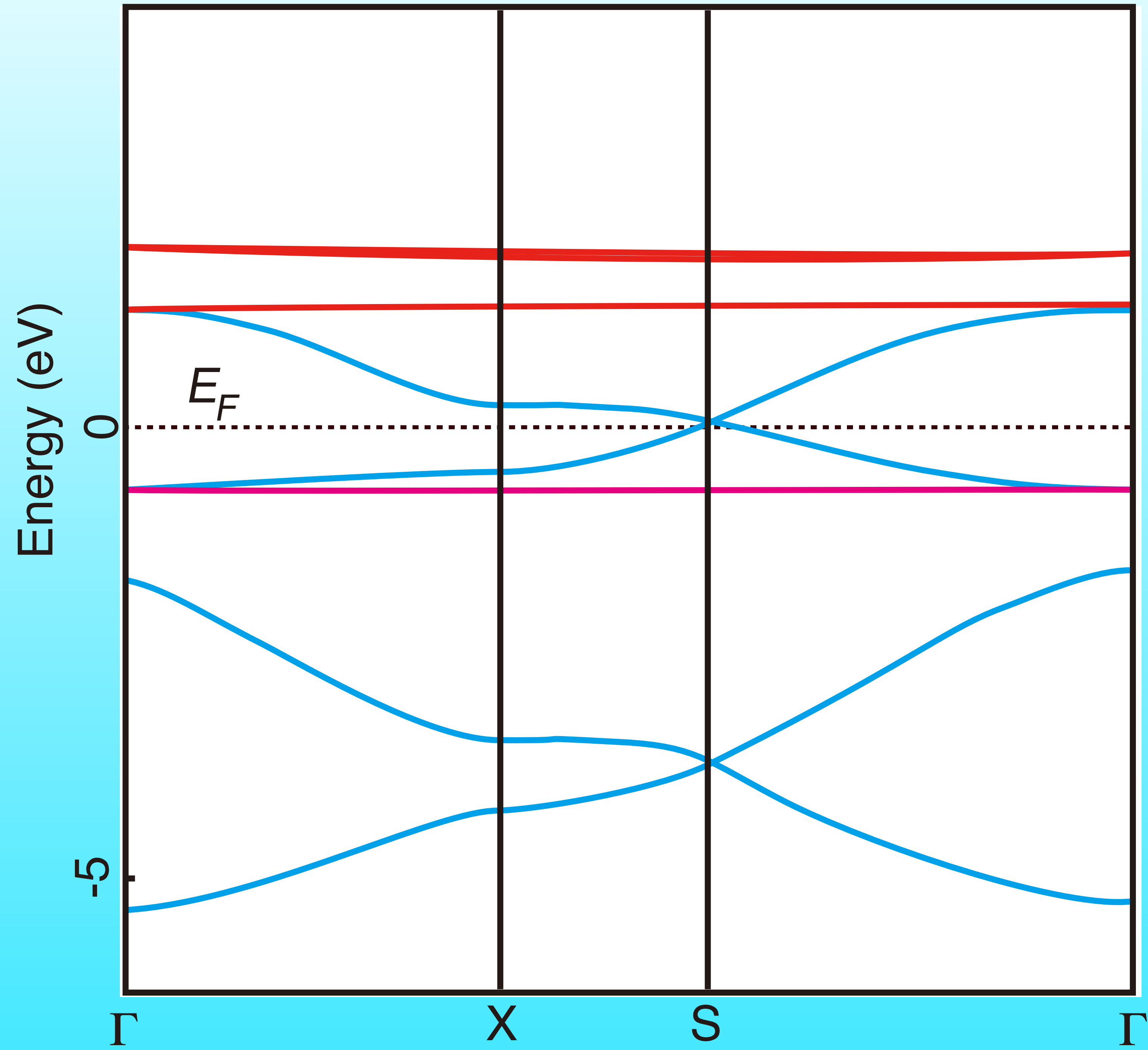

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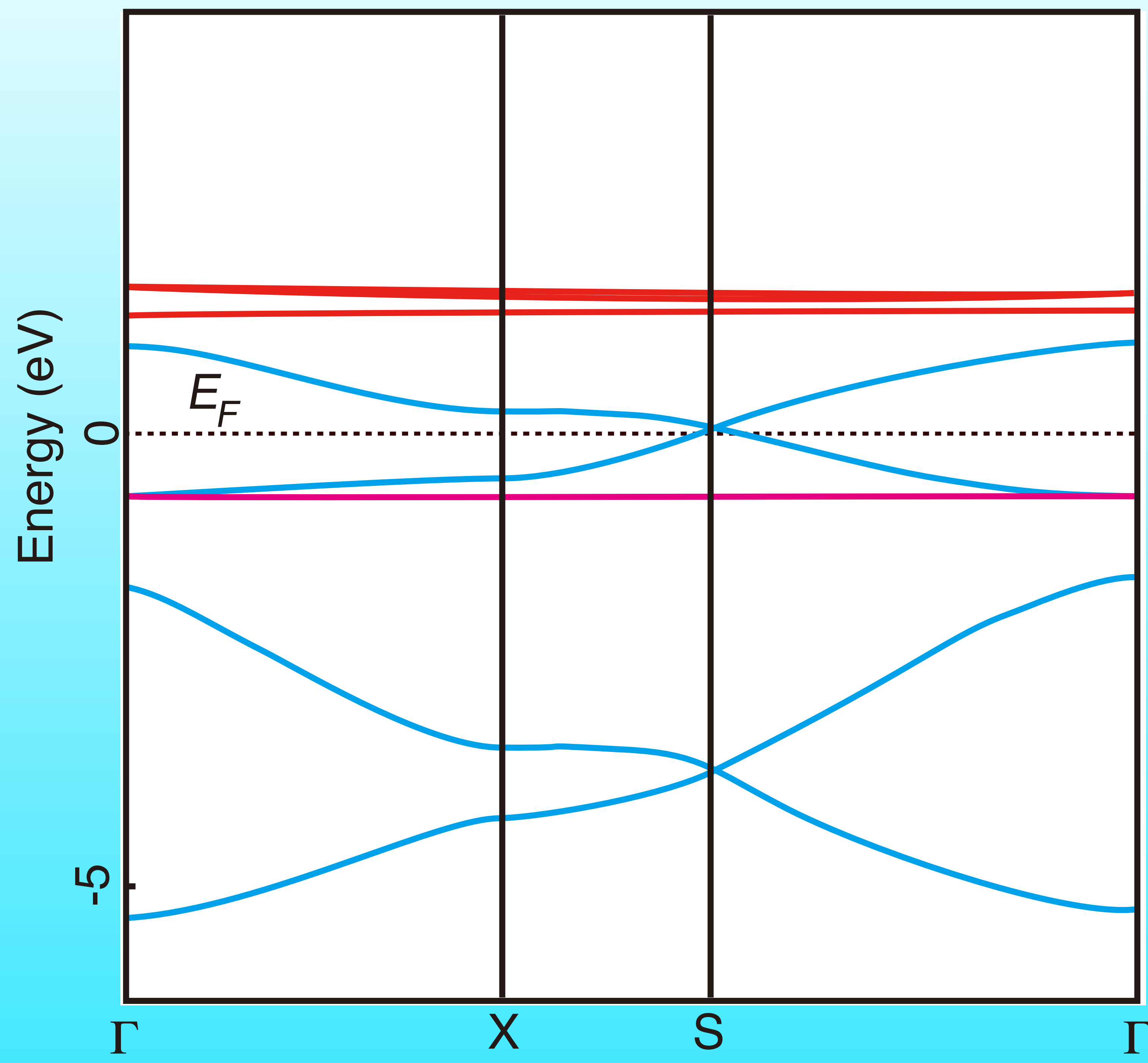

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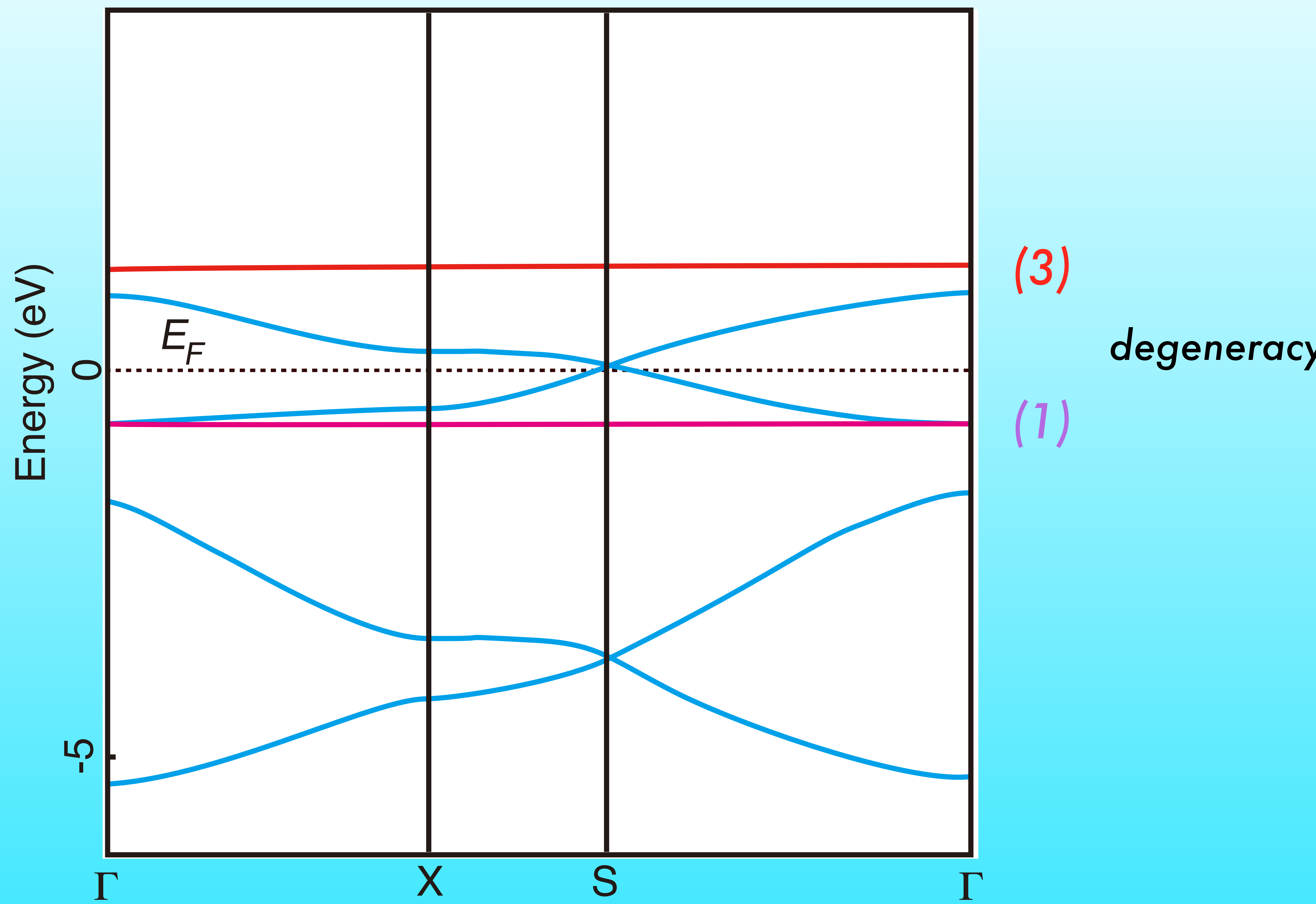
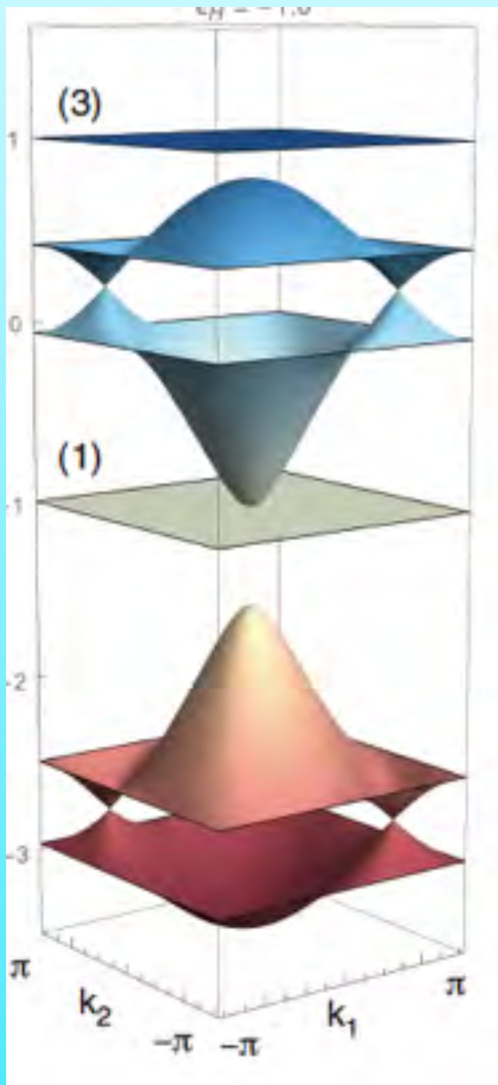
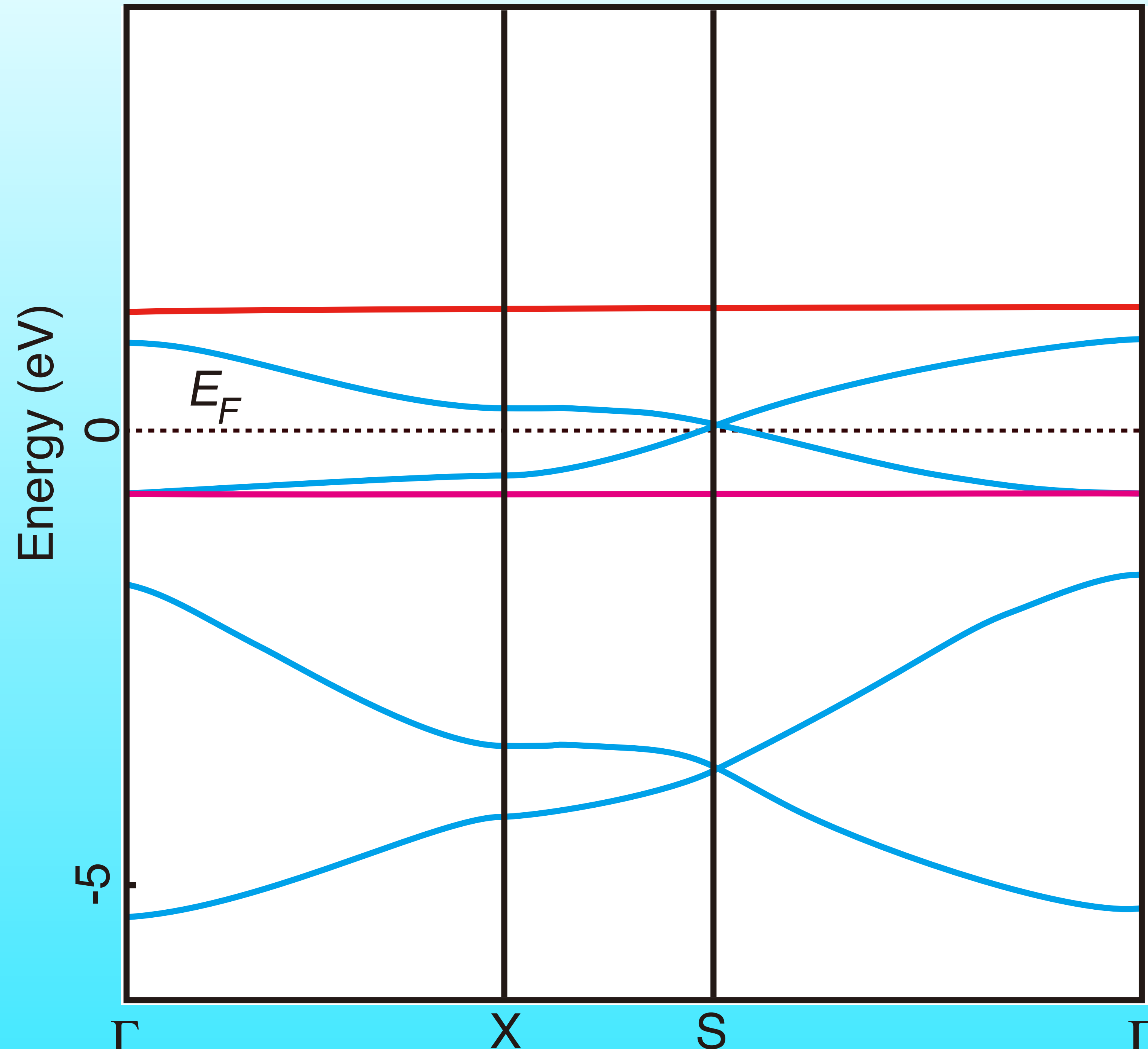


Classify into two: bands of Dirac fermions & else

☆ *Simplified silicene* : *Dirac cones & Flat bands*

"Topological" deformation of the bands





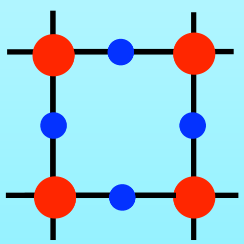
Dirac cones : Symmetry protected

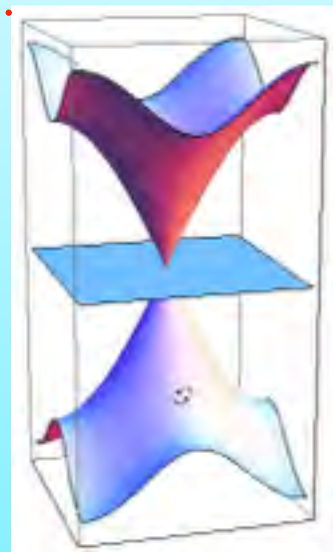
Flat bands : Due to multi-orbital character !!

☆ "Flat" bands in 1,2,3 dimensions

dp (Lieb) model

Mielke-Tasaki, Comm.Math.Phys. 158, 341 (1993)





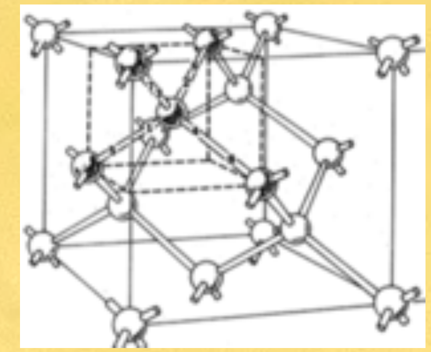
d=2 Kagome
d=3 Pyrochlore

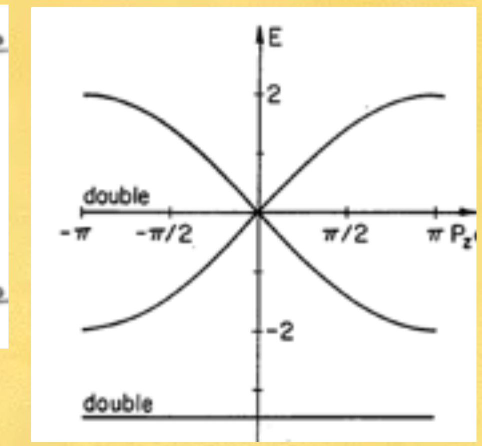
Y. Hatsugai, I. Maruyama, EPL 95, 20003 (2011)

d=3, Weaire-Thorpe model

Weaire-Thorpe, Phys. Rev. B4, 2508 (1971)

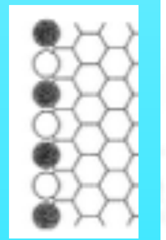
Dagotto, Fradkin, Moreo, Phys. Lett.B 172, 383 (1986)

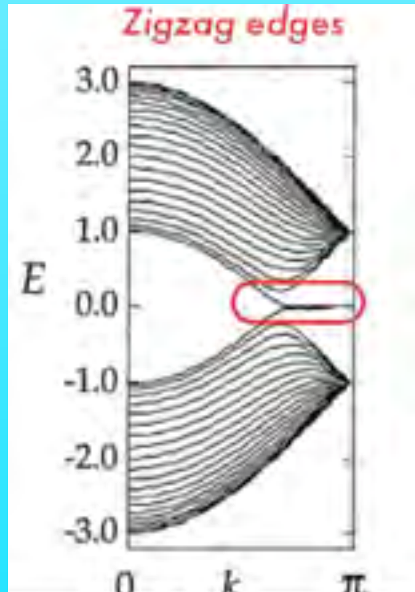




Fujita states 1D

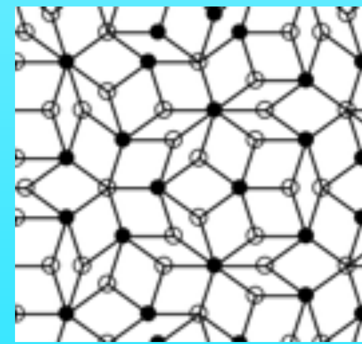
JPSJ 65, 1920 (1996)

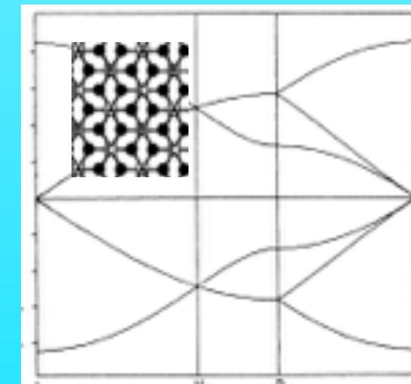




Ring states on Penrose tiling

Kohmoto-Sutherland, Phys. Rev. Lett. 56, 2740(1986)

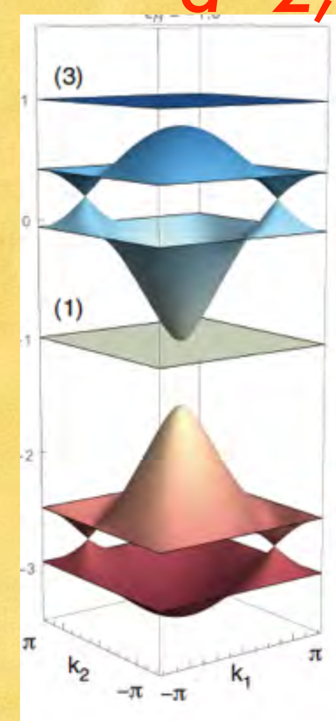


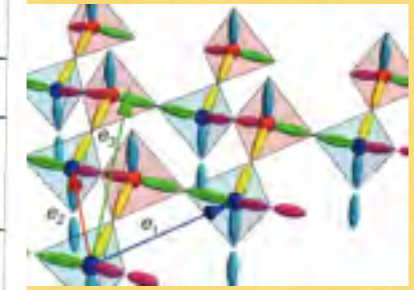


dice lattice

B.Sutherland, Phys. Rev. B34, 5208(1986)

d=2, Silicene





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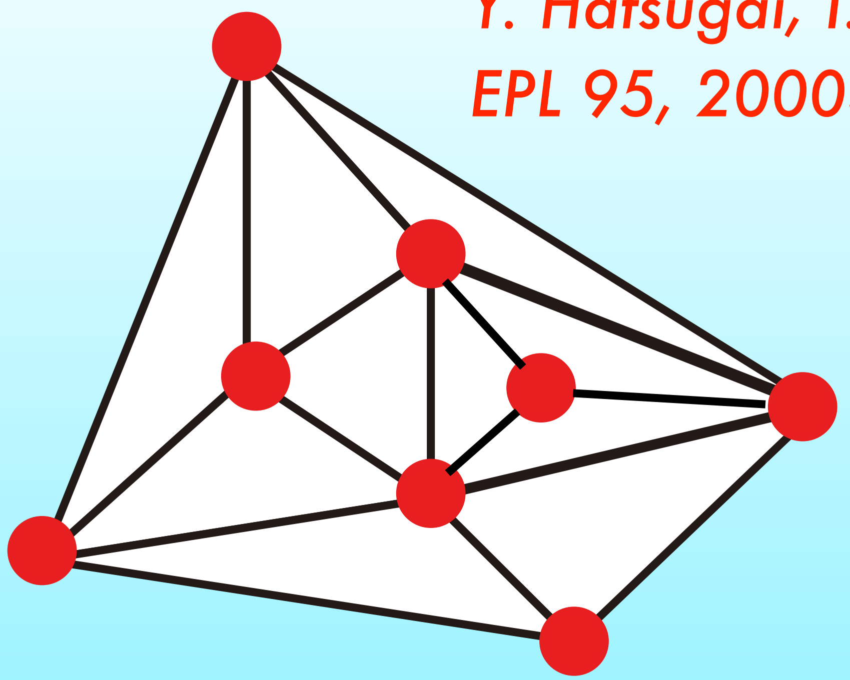
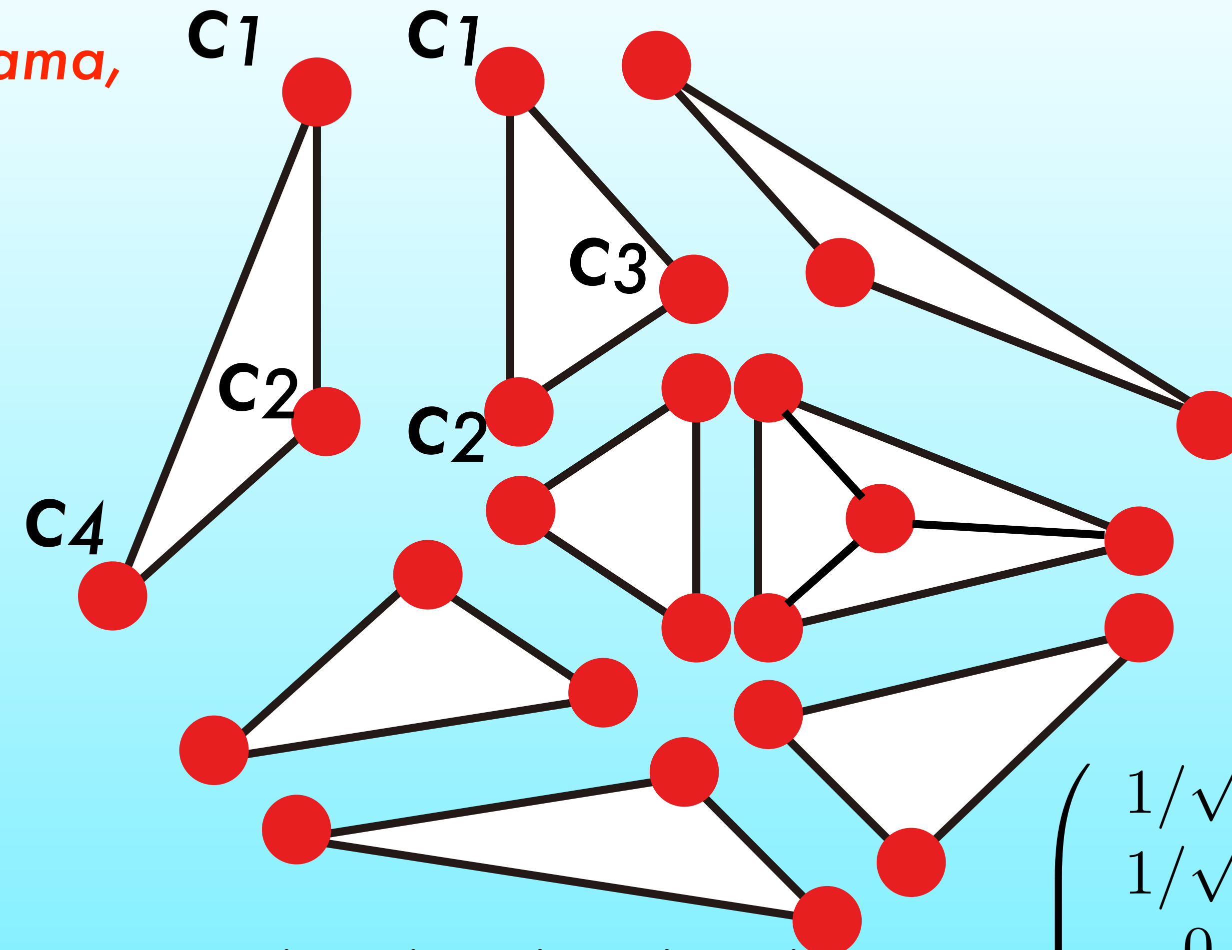
Overlapping MO's

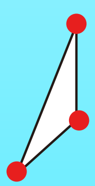
Y. Hatsugai, I. Maruyama, EPL 95, 20003 (2011)



MO's



MO annihilation op.



$$C^\dagger = (c_1^\dagger + c_2^\dagger + c_4^\dagger)/\sqrt{3} = (c_1^\dagger, c_2^\dagger, c_3^\dagger, c_4^\dagger, c_5^\dagger, \cdots) \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \\ 0 \\ \vdots \end{pmatrix}$$

$$= \boldsymbol{c}^\dagger \psi \qquad \psi^\dagger \psi = 1$$ normalized

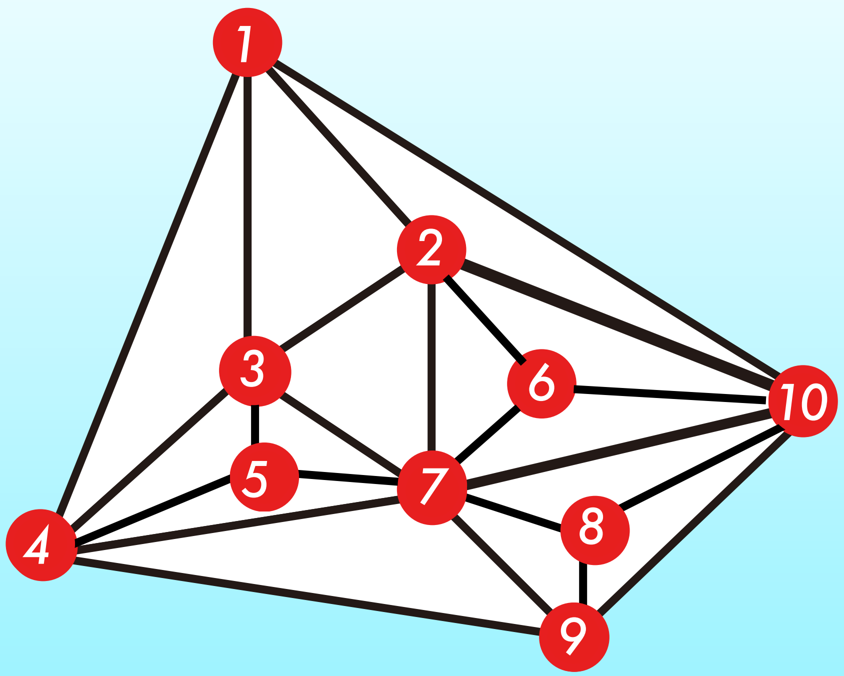
$$C^\dagger C = (c_1^\dagger c_2 + \cdots)/3 = \boldsymbol{c}^\dagger P \boldsymbol{c}, \ P = \psi\psi^\dagger = P^2$$ projection

$$H - \mu \mathcal{N} = \sum_{m=1}^{M} \mathcal{E}_m C_m^\dagger C_m = \boldsymbol{c}^\dagger h \boldsymbol{c}, \qquad h = \sum_{m=1}^{M} \mathcal{E}_m P_m$$

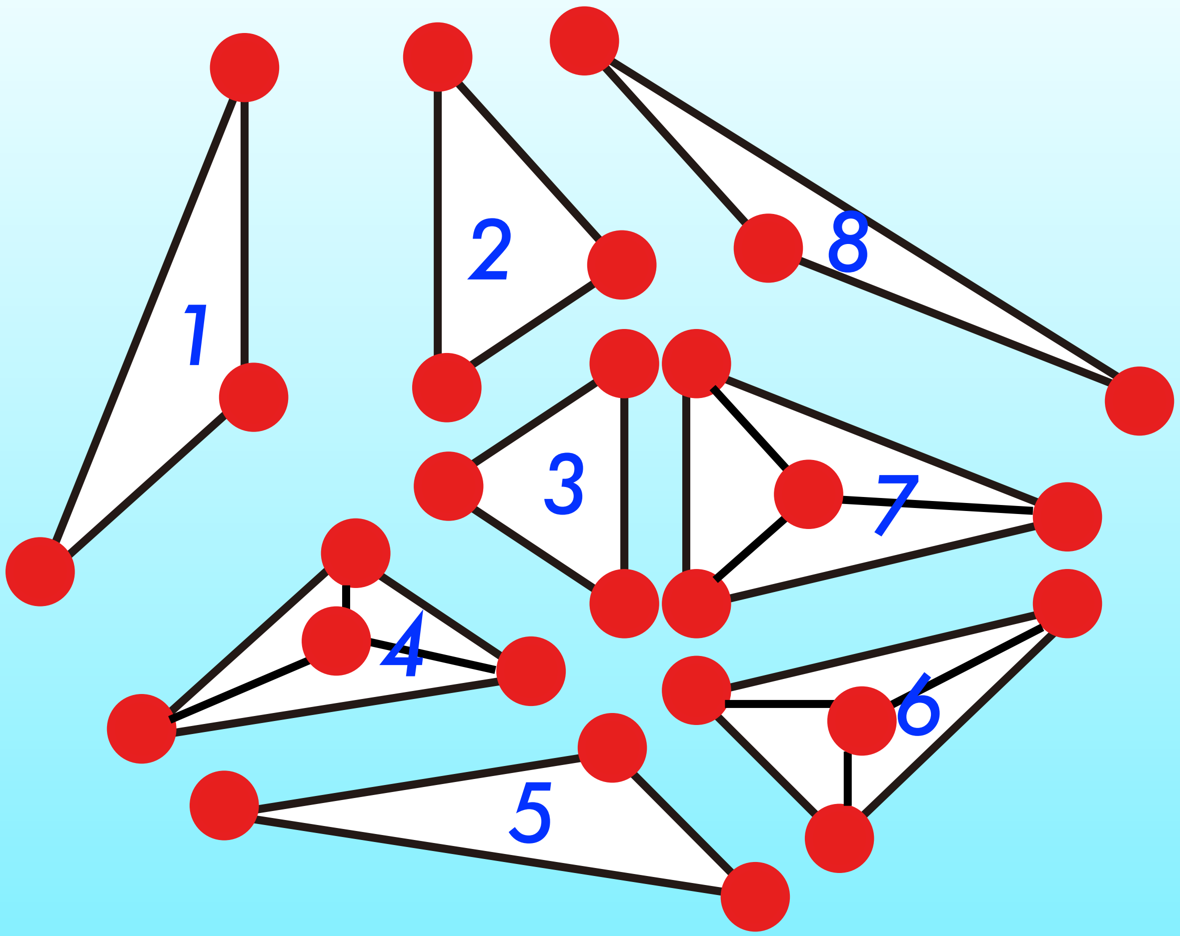
Sum of projections

$$P_m P_n \neq 0, \ (m \neq n)$$ Itinerancy : NON orthogonality of MO's

Overlapping MO's



MO's



$$Z \geq 10 - 8 = 2$$ At least 2 zero energies !

Theorem

$$Z \geq N - M$$

Z: # of zero eigen states

N: # of sites

M: # of MO's

Do NOT need translational invariance

If translationally invariant, use in momentum space

PROOF

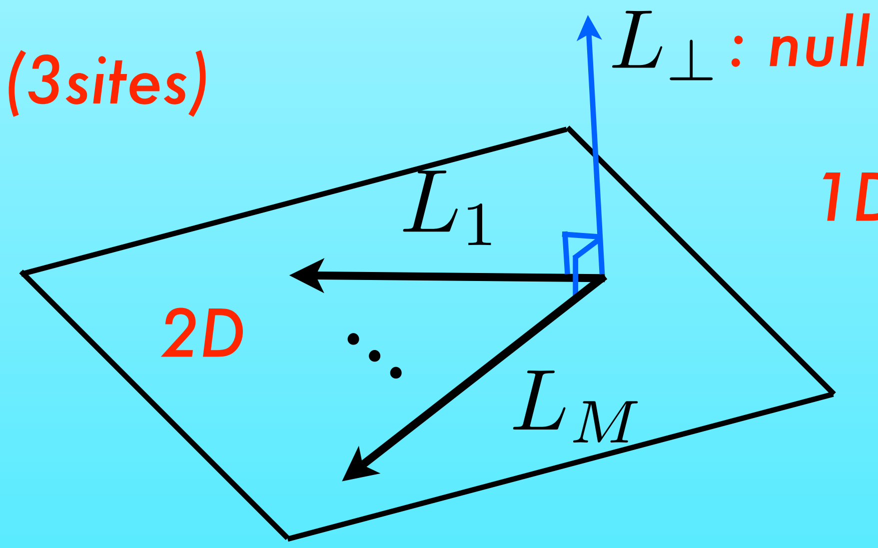
N dimensional Hamiltonian = Sum of **M** projections

Diagonalizable within M dimensional linear space

⇒ Non zero energy bands are at most M

Rest is null, N-M zero energy "flat" bands in N-dim.

ex: 3D (3sites)



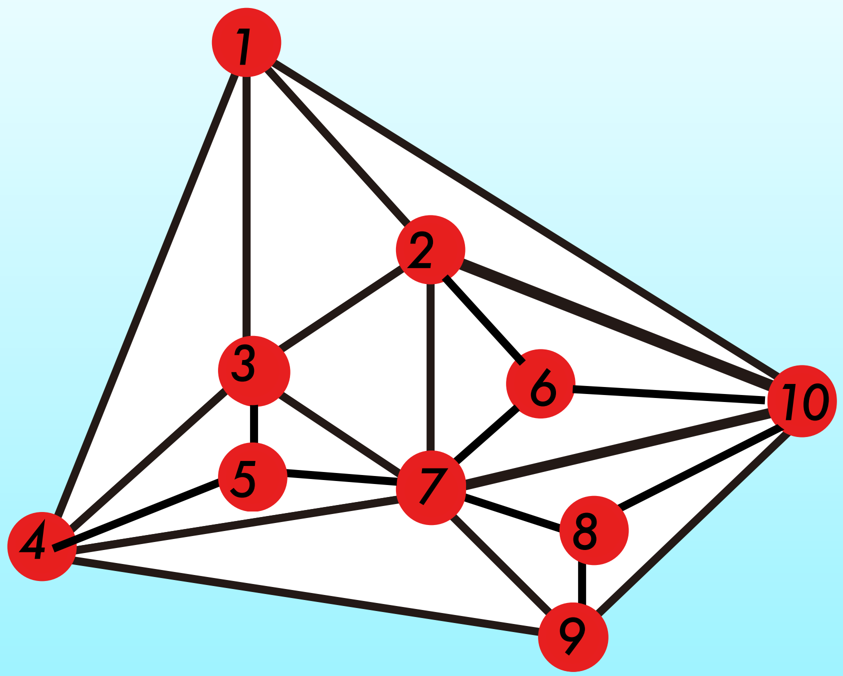
1D is null (1 zero energy)

Flat bands are stable for perturbation

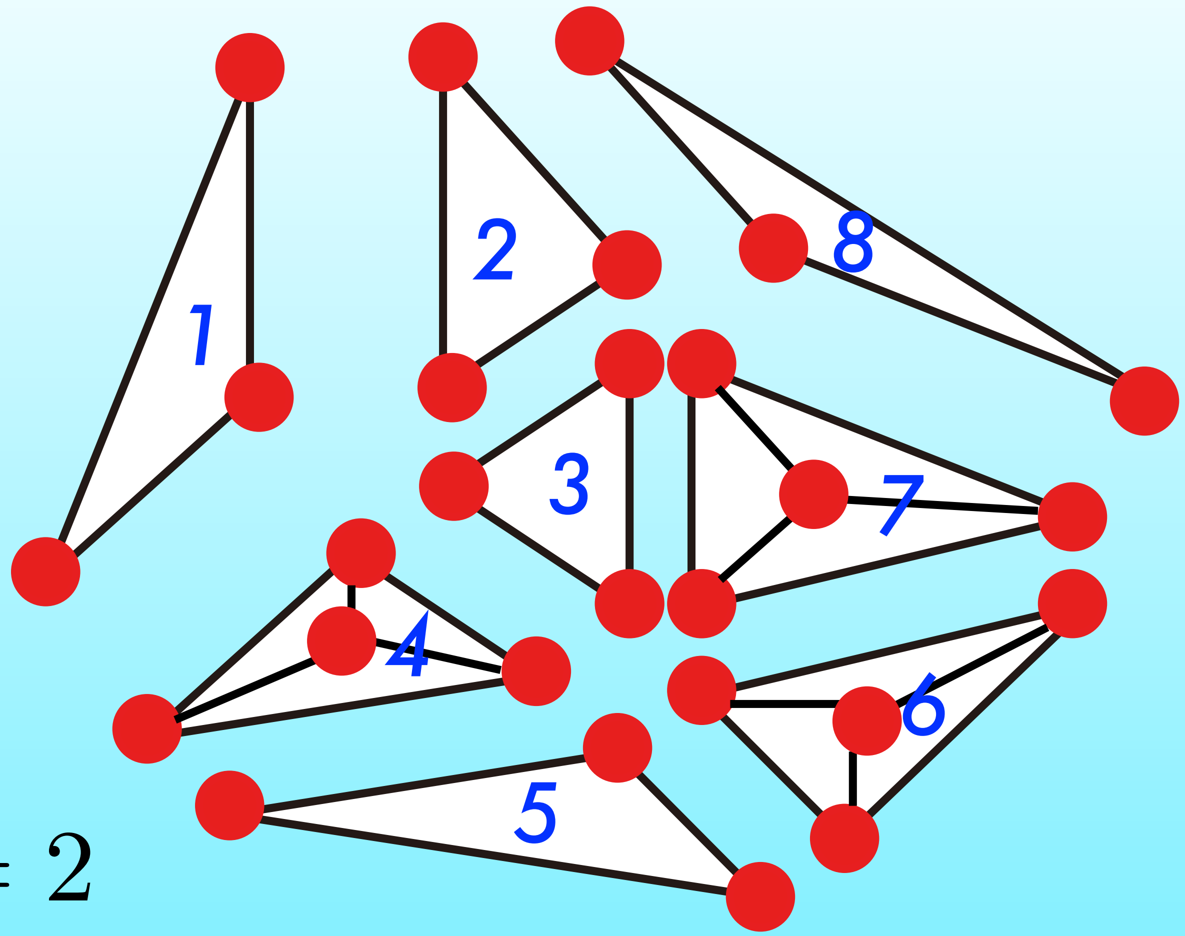
(deformation of MO's)

$$C_{\triangle} = (c_1 + c_2 + c_3)/\sqrt{3} \quad \to (*c_1 + *c_2 + *c_3)/\sqrt{*}$$

Overlapping MO's



MO's



$$Z \geq 10 - 8 = 2$$

$$Z \geq N - M$$

N : *number of sites (degree of freedom)*

M : *number of MO's (itinerancy by overlapping)*

Slightly extended theorem $M = \sum_m \dim P_m$ **ex.** $P = \psi_1 \psi_1^\dagger + \psi_2 \psi_2^\dagger, \ \dim P = 2$

If the itinerancy is not enough, some states are localized

Physical meaning of flat bands

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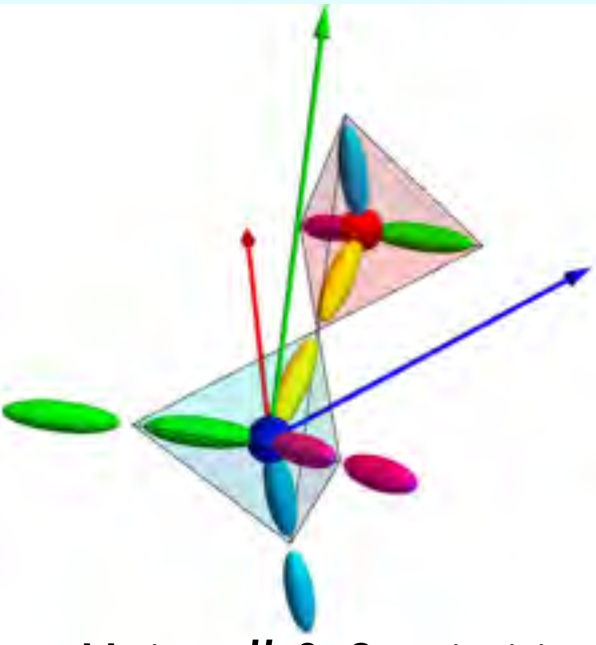
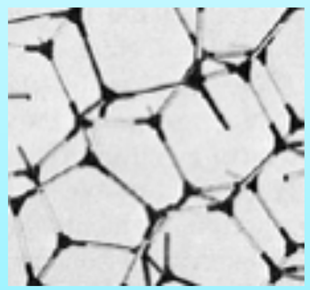
☆ Weaire-Thorpe model

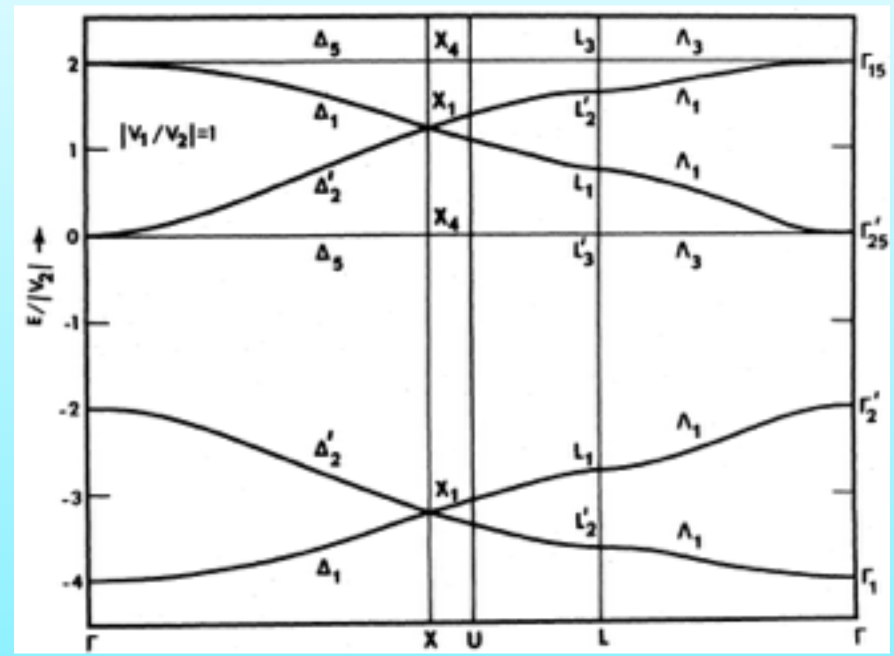
Weaire-Thorpe, Phys. Rev. B4, 2508 (1971)

3D Multiorbital (sp^3) tight binding hamiltonian





Unit cell & 3 primitive translations



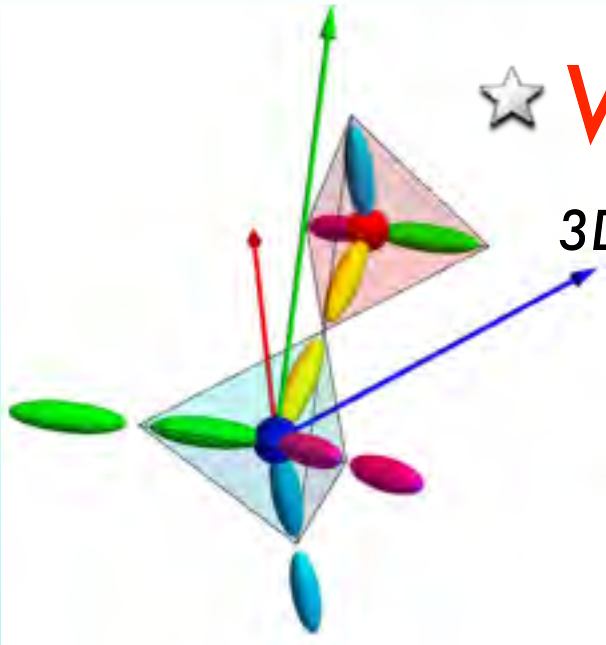
Gapless points !

flat bands !

$H_{WT}(k) =$

Simple but 8×8 : need some work to diagonalize

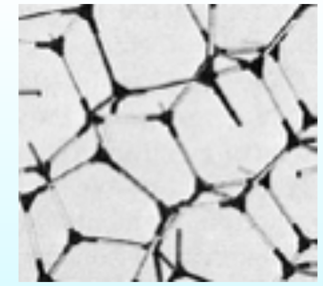
$$
\begin{bmatrix}
V_1 & V_1 & V_1 & V_1 & V_2 & 0 & 0 & 0 \\
V_1 & V_1 & V_1 & V_1 & 0 & V_2 & 0 & 0 \\
V_1 & V_1 & V_1 & V_1 & 0 & 0 & V_2 & 0 \\
V_1 & V_1 & V_1 & V_1 & 0 & 0 & 0 & V_2 \\
V_2 & 0 & 0 & 0 & V_1 & V_1 e^{i(k_y+k_z)} & V_1 e^{i(k_z+k_x)} & V_1 e^{i(k_x+k_y)} \\
0 & V_2 & 0 & 0 & V_1 e^{-i(k_y+k_z)} & V_1 & V_1 e^{i(k_x-k_y)} & V_1 e^{-i(k_z-k_x)} \\
0 & 0 & V_2 & 0 & V_1 e^{-i(k_z+k_x)} & V_1 e^{-i(k_x-k_y)} & V_1 & V_1 e^{i(k_y-k_z)} \\
0 & 0 & 0 & V_2 & V_1 e^{-i(k_x+k_y)} & V_1 e^{i(k_z-k_x)} & V_1 e^{-i(k_y-k_z)} & V_1
\end{bmatrix}
$$



Unit cell & 3 primitive translations

☆ Weaire-Thorpe model

3D Multiorbital (sp^3) tight binding hamiltonian



Weaire-Thorpe, Phys. Rev. B4, 2508 (1971)

$$H_{WT}(k) = \begin{bmatrix} V_1 & V_1 & V_1 & V_1 & V_2 & 0 & 0 & 0 \\ \cdots & V_1 & V_1 & V_1 & 0 & V_2 & 0 & 0 \\ \cdots & \cdots & V_1 & V_1 & 0 & 0 & V_2 & 0 \\ \cdots & \cdots & \cdots & \cdots & 0 & 0 & 0 & V_2 \\ \cdots & \cdots & \cdots & \cdots & V_1 & V_1 e^{i(k_y+k_z)} & V_1 e^{i(k_z+k_x)} & V_1 e^{i(k_x+k_y)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & V_1 & V_1 e^{i(k_x-k_y)} & V_1 e^{-i(k_z-k_x)} \\ 0 & \cdots & \cdots & \cdots & \cdots & V_1 e^{-i(k_x-k_y)} & V_1 & V_1 e^{i(k_y-k_z)} \\ 0 & 0 & \cdots & \cdots & \cdots & \cdots & V_1 e^{-i(k_y-k_z)} & V_1 \end{bmatrix}$$

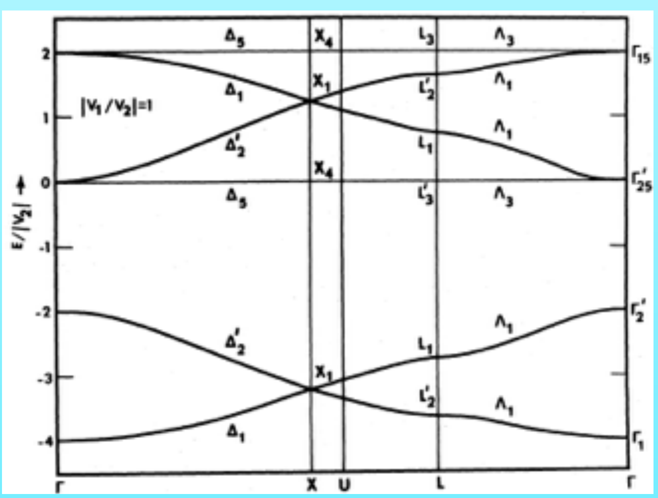
Counting dimensions !

$$= 4V_1 \begin{bmatrix} \psi_0\psi_0^\dagger & 0 \\ 0 & \psi_k\psi_k^\dagger \end{bmatrix} + \cdots \qquad \psi_k = \frac{1}{2}\begin{bmatrix} 1 \\ e^{-ik_1} \\ e^{-ik_2} \\ e^{-ik_3} \end{bmatrix}$$

$$= -2V_2 E_8 + 4V_1 P_1 + 4V_1 P_2 + 2 \cdots$$

$$= +2V_2 E_8 + 4V_1 P_1 + 4V_1 P_2 - 2V_2 P_{3-}$$

written by 2 ways



flat bands !

$$P_i = \Psi_i \Psi_i^\dagger \qquad \Psi_1 = \begin{bmatrix} \psi_0 \\ 0 \end{bmatrix}, \Psi_2 = \begin{bmatrix} 0 \\ \psi_k \end{bmatrix}, \Psi_{3\pm} = \frac{1}{\sqrt{2}} \begin{bmatrix} E_4 \\ \pm E_4 \end{bmatrix}$$

projections $P_i^2 = P_i \qquad P_1 P_2 = 0 \qquad P_1 P_{3\pm} \neq 0$ Non orthogonal

$$\dim P_1 = \dim P_2 = 1, \ \dim P_{3\pm} = 4$$

$1 + 1 + 4 = 6 \qquad 8 - 6 = 2$ Flat bands at $\pm 2V_2$!!

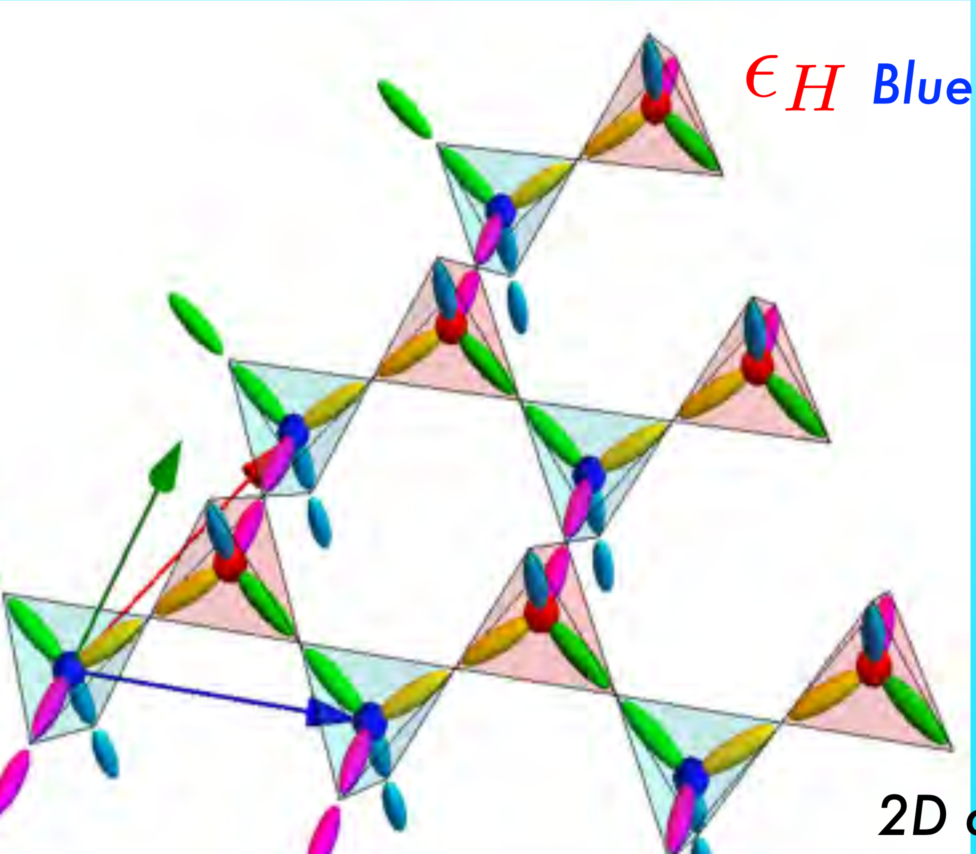
☆ *Extended* Weaire-Thorpe model for *silicene* with *hydrogen termination* (ϵ_H)

2D Multiorbital (sp^3) tight binding hamiltonian

$$H^{\epsilon_H}_{\text{Silicene}}(k) = \begin{bmatrix} H_V(0) - \epsilon_H \mathcal{E} & V_2 E_4^C \\ V_2 E_4^C & H_V(k) - \epsilon_H \mathcal{E} \end{bmatrix}$$

$$H^{\epsilon_H}_{\text{Silicene}} \pm V_2 E_8 = 4V_1 P_1 + 4V_1 P_2 \pm 2V_2 P^C_{3\pm} \pm (V_2 \mp \epsilon_H) P_5$$

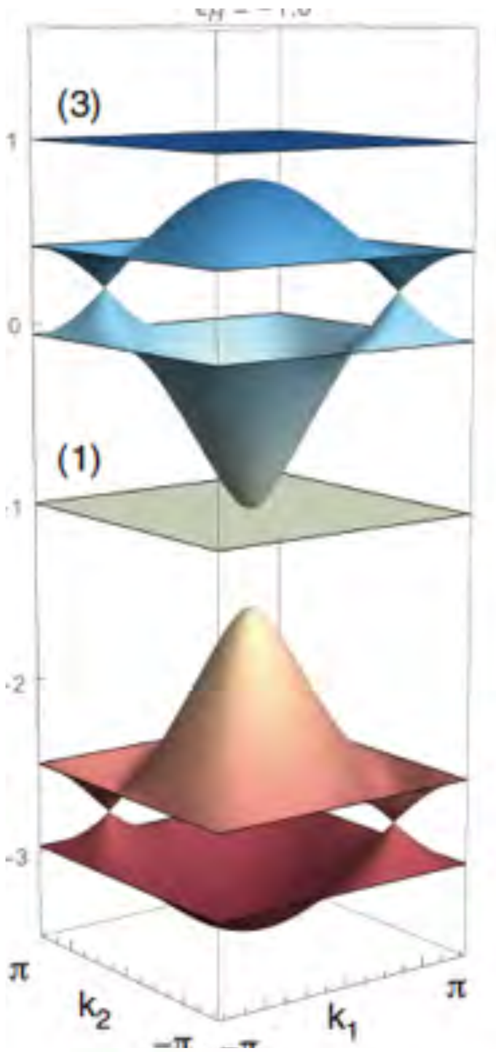
$$\dim P_1 + \dim P_2 + \dim P_{3\pm} + \dim P_5 = 1 + 1 + 3 + 2 = 7$$

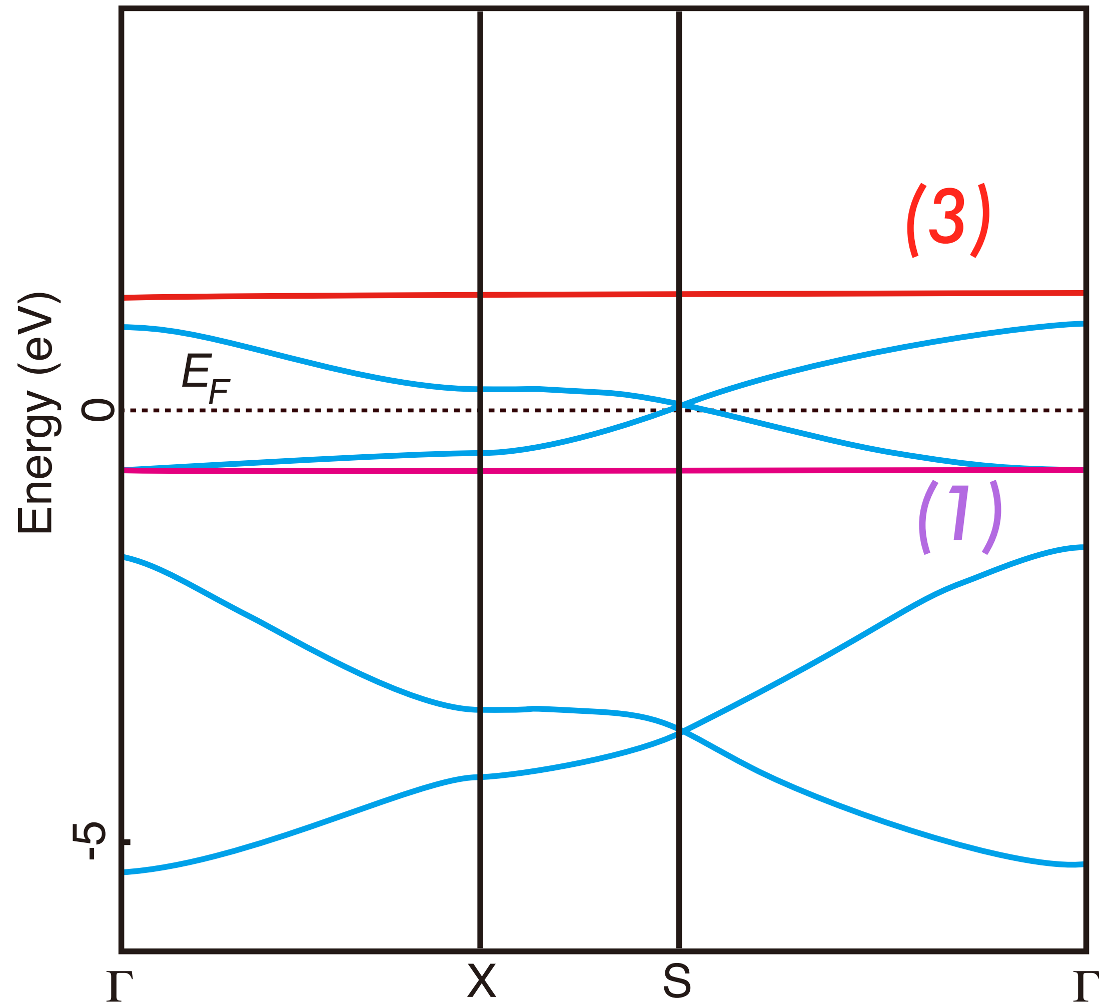


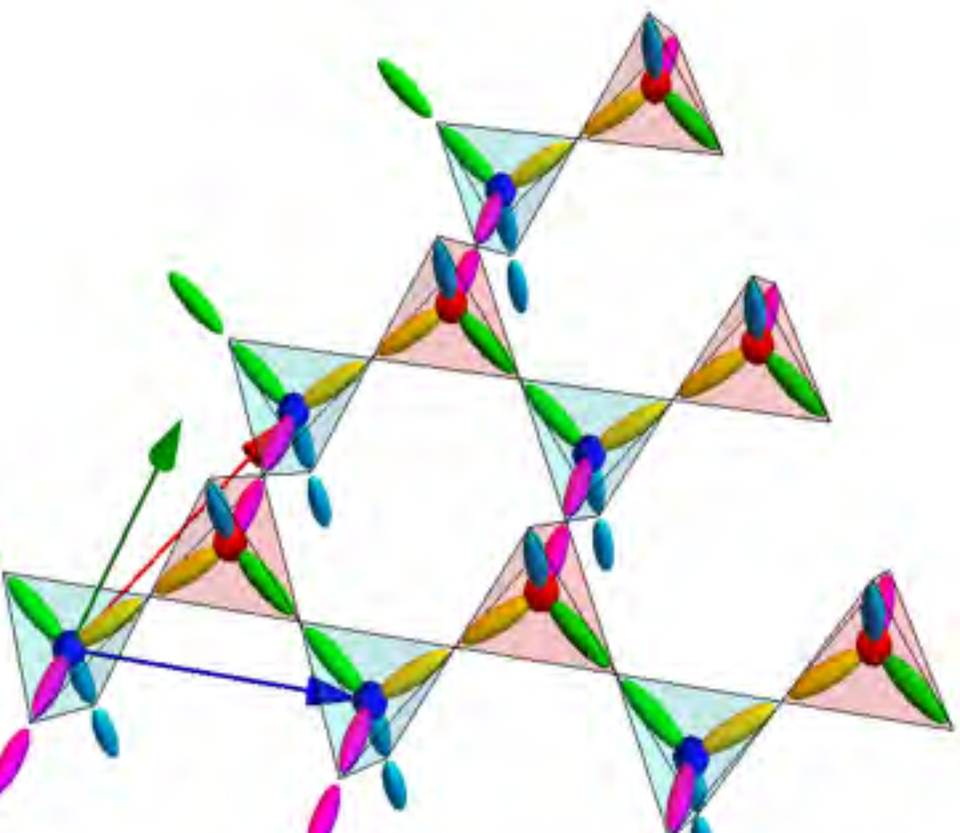
ϵ_H *Blue bonds are special*

8-7=1 flat band at $\pm V_2$

2D array of the unit cells







When $\epsilon_H = V_2 < 0$

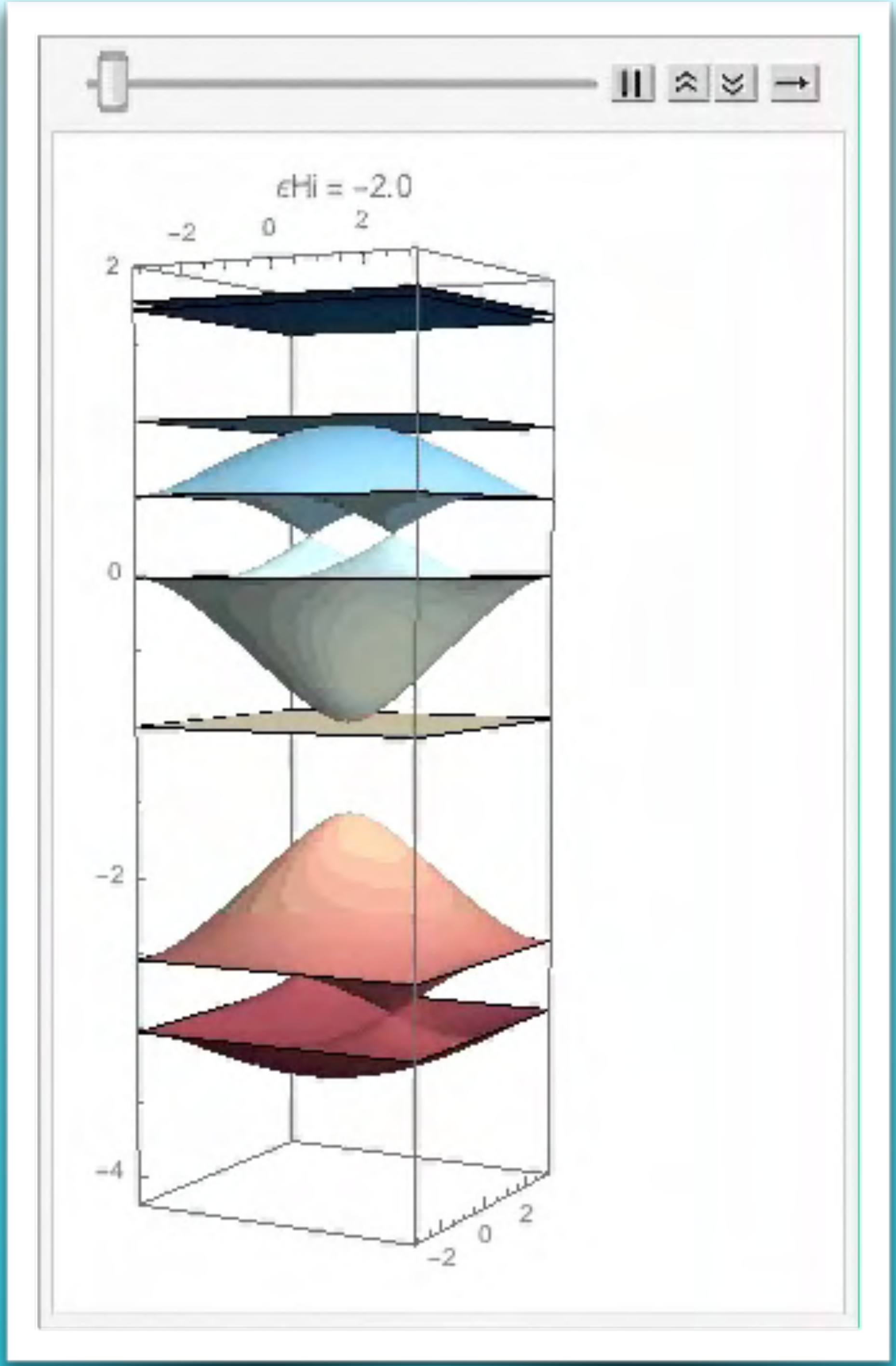
8-5=3 flat bands at $-V_2$

triply degenerate

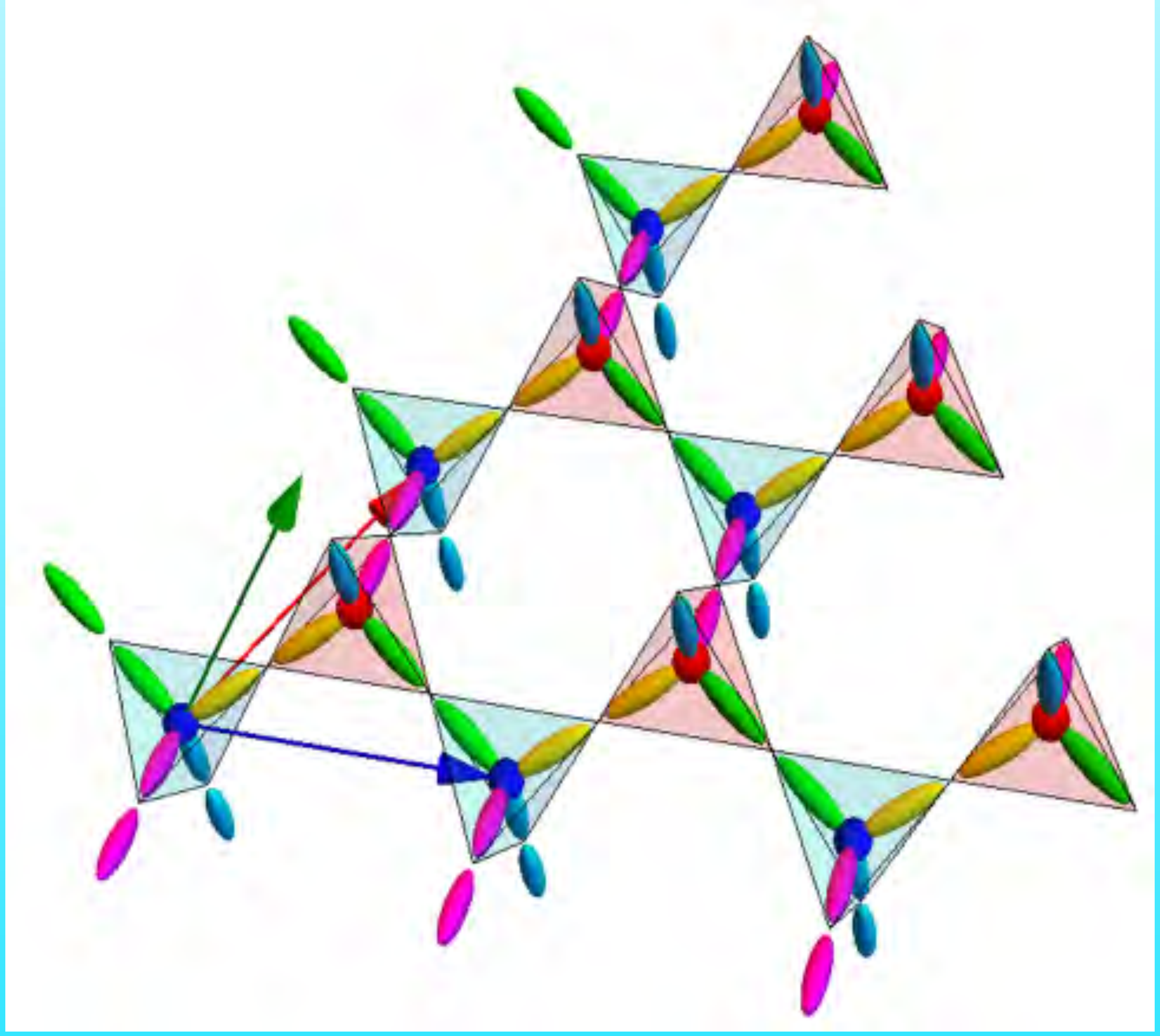
8-7=1 flat band at $+V_2$

it cells

☆ Various band ordering by changing ϵ_H (hydrogen termination)



"Blue bonds are special"



☆ *Buckling can be included partly*

$$h_{\mathrm{local}}(\theta) = \sum_{\langle i,j \rangle} V_{ij} c_i^\dagger c_j + \mathrm{h.c.},$$

$$V_{ij} = \begin{cases} V_1 & (\langle i,j \rangle = \langle 01 \rangle, \langle 12 \rangle, \langle 20 \rangle) \\ V_1' & (\langle i,j \rangle = \langle 03 \rangle, \langle 13 \rangle, \langle 23 \rangle) \end{cases}$$

$$\frac{V_1'}{V_1} = \frac{\cos\theta}{\cos\theta_0}, \ \cos\theta_0 = -\frac{1}{3}$$

$$H^{\epsilon_H, \cos\theta}_{\mathrm{Silicene}}(\boldsymbol{k}) = \begin{bmatrix} H_V^\theta(0) - \epsilon_H^\theta \mathcal{E} & V_2 E_4^C \\ V_2 E_4^C & H_V^\theta(\boldsymbol{k}) - \epsilon_H^\theta \mathcal{E} \end{bmatrix},$$

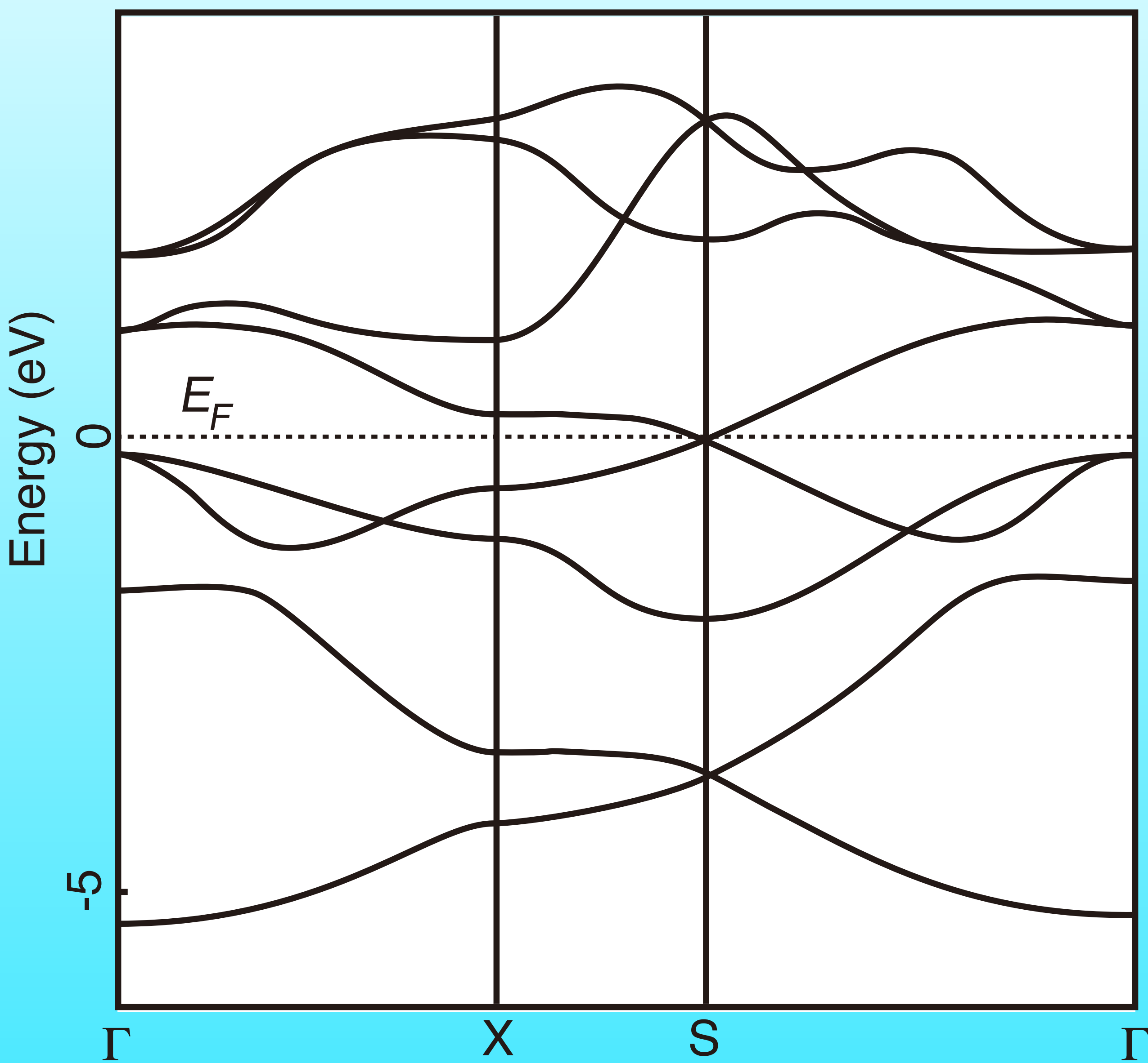
$$H_V^\theta(\boldsymbol{k}) = 4V_1 \psi_{\boldsymbol{k}}^\theta (\psi_{\boldsymbol{k}}^\theta)^\dagger,$$

$$\psi_{\boldsymbol{k}}^\theta = \mathrm{diag}\left(\frac{\cos\theta}{\cos\theta_0}, 1, 1, 1\right)\psi_{\boldsymbol{k}},$$

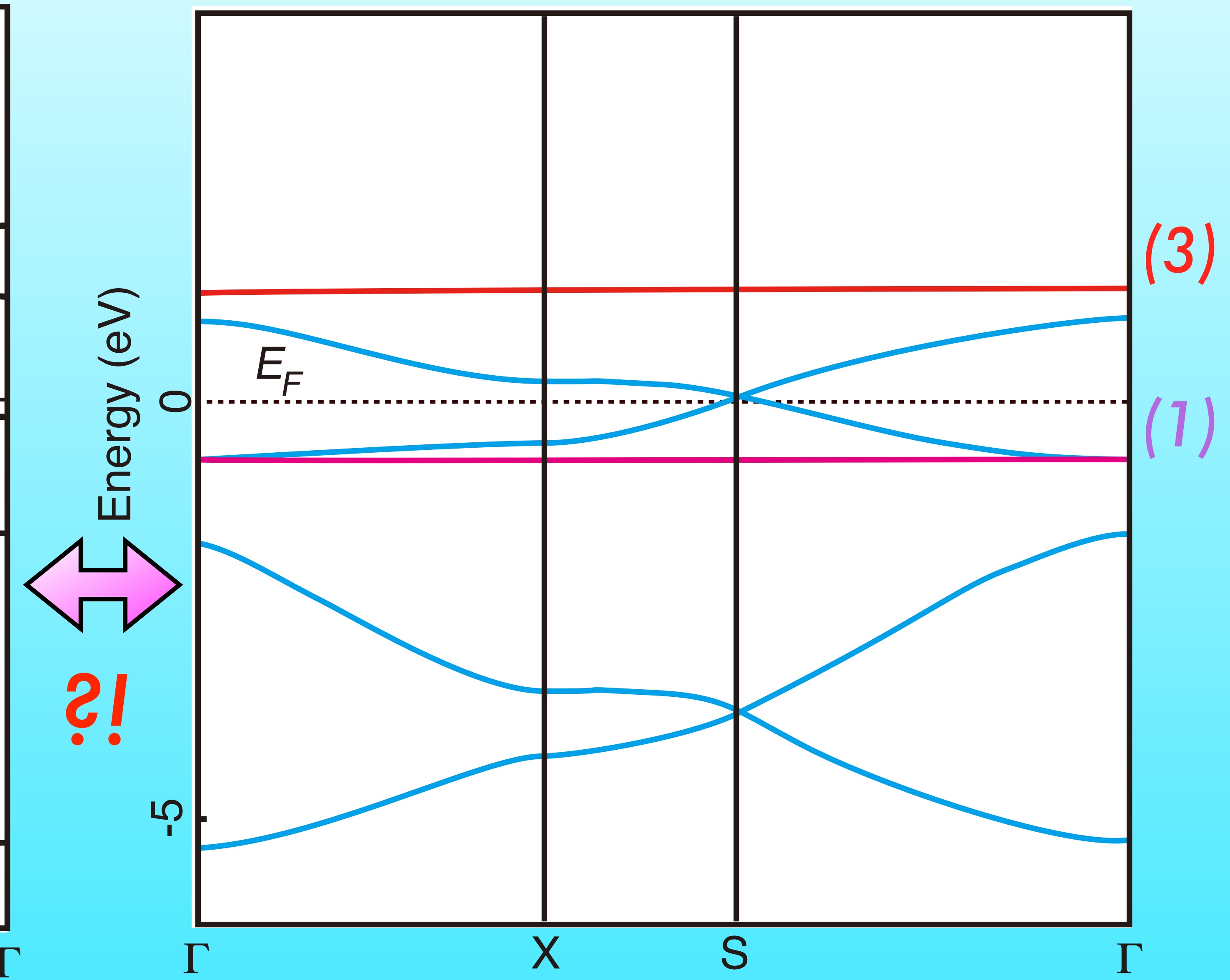
$$\epsilon_H^\theta = \left(\frac{\cos\theta}{\cos\theta_0}\right)^2 \epsilon_H$$

Summary

first principle



analytic



Less dispersive bands: due to multi-orbital character

Possible instability (ferromagnetic/structure)