Saturday Morning of Theoretical Physics

The Physics of “Flat” Electrons

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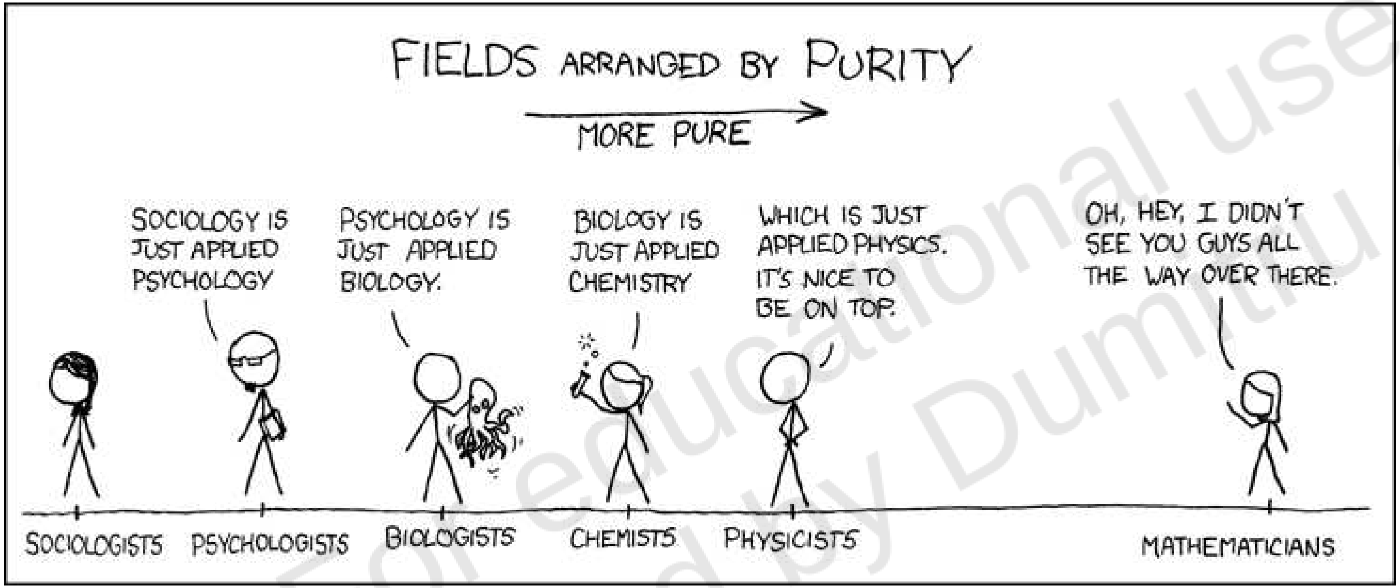
UNIVERSITY OF OXFORD

What are “flat electrons”?

More is different!

NOT a fundamental new particle...



Comic: "Purity" (xkcd #435), © Randall Munroe — https://xkcd.com/435

Philip W. Anderson

… but electrons in certain “materials” behave as they have no kinetic energy.

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Part 0

Introduction to band theory

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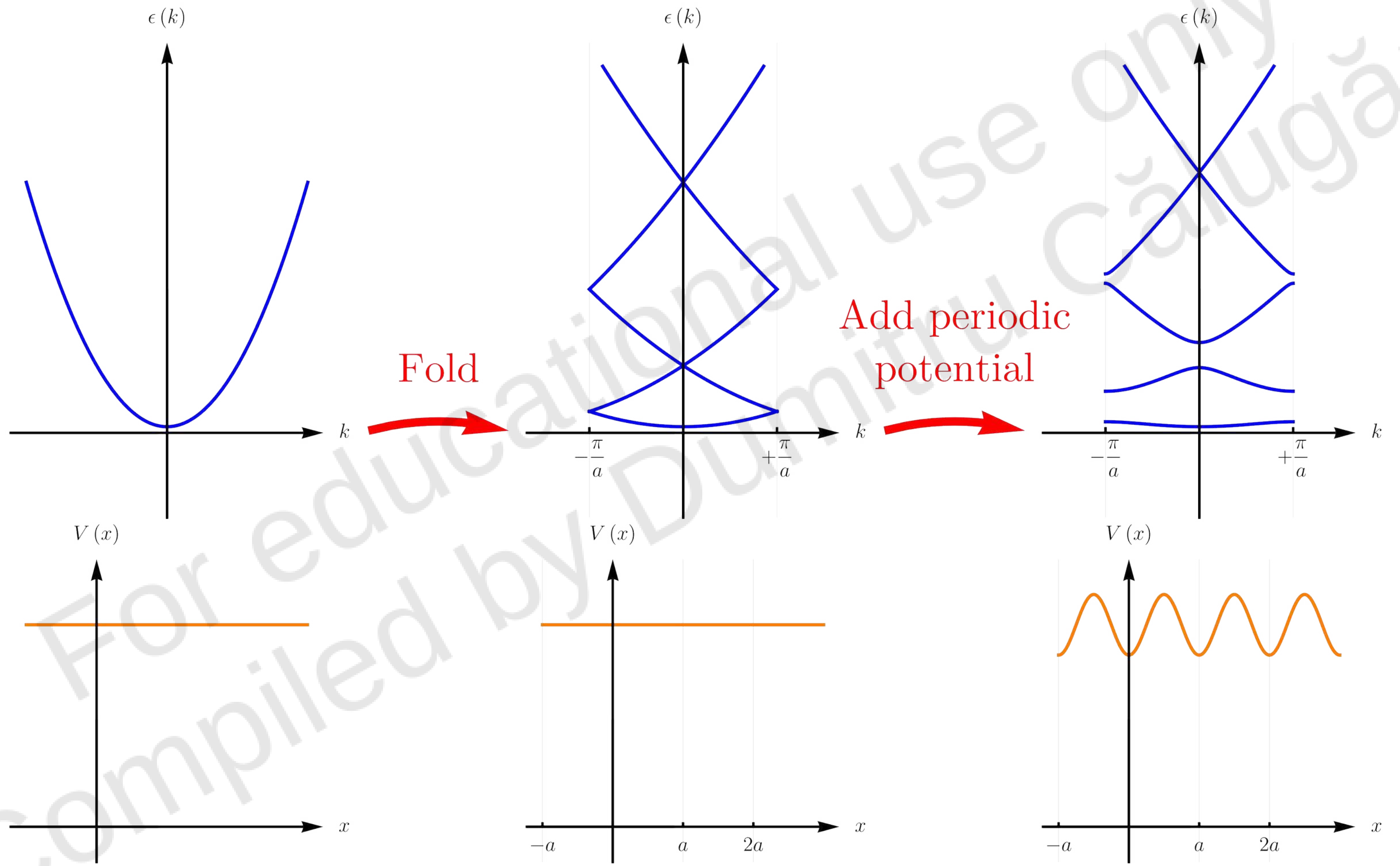
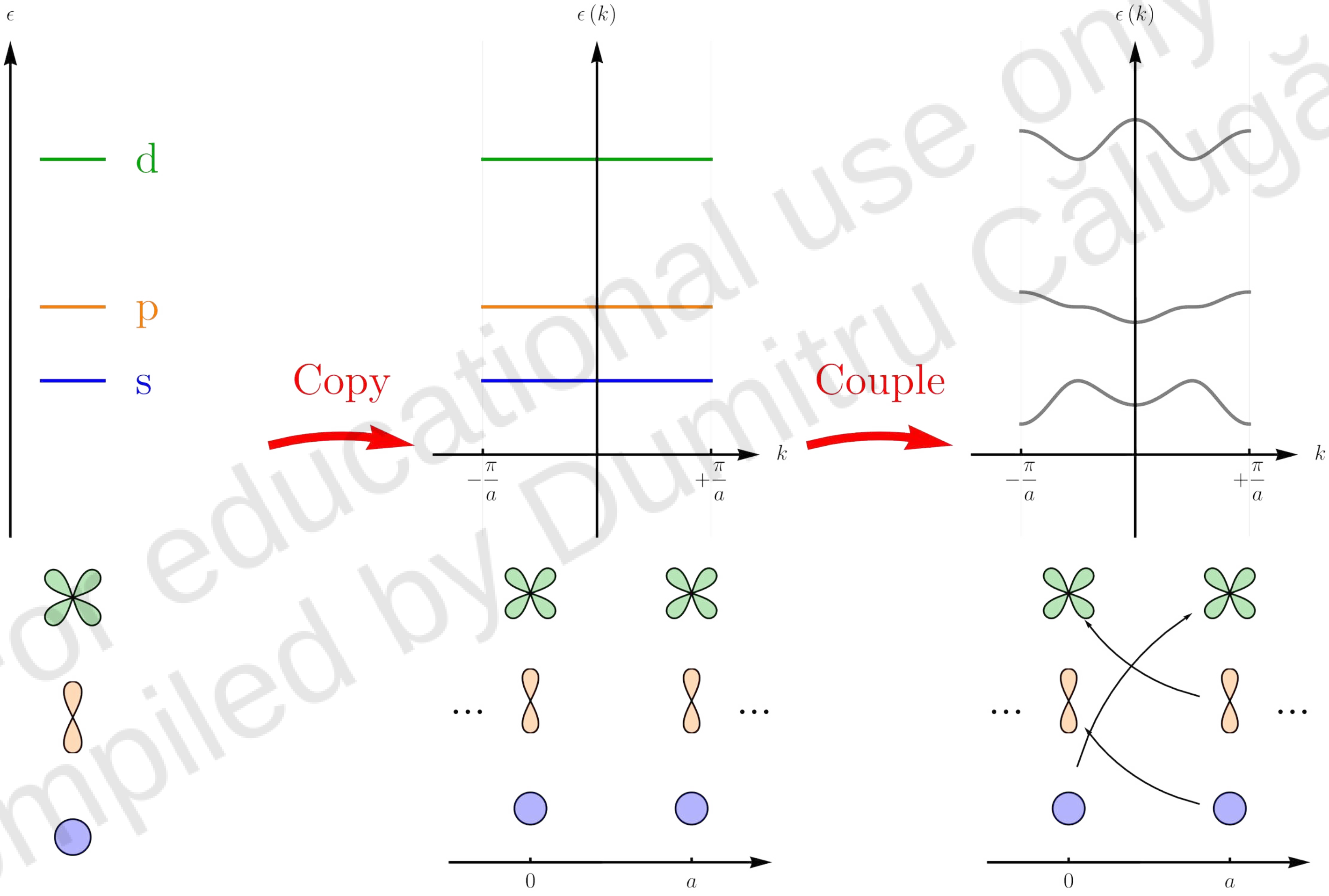
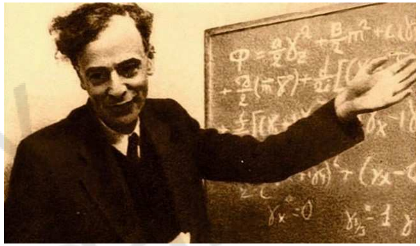
Band structures from free electrons

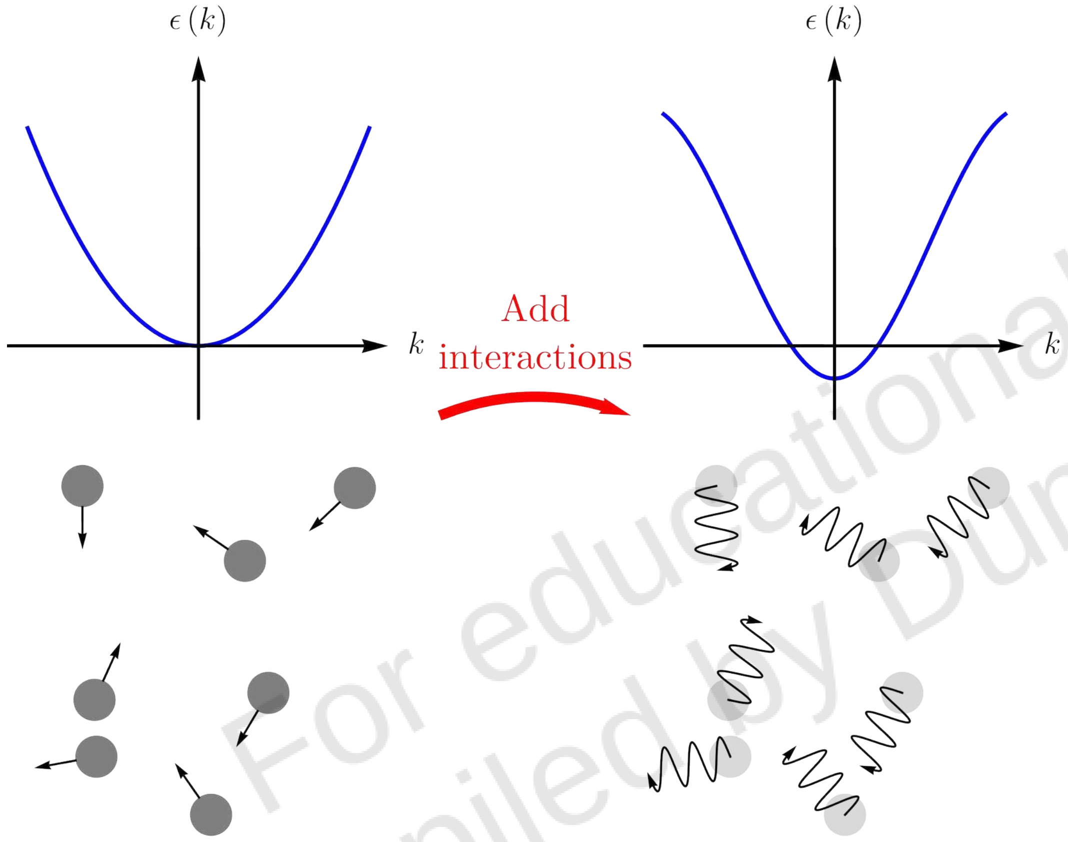


Band structures from orbitals



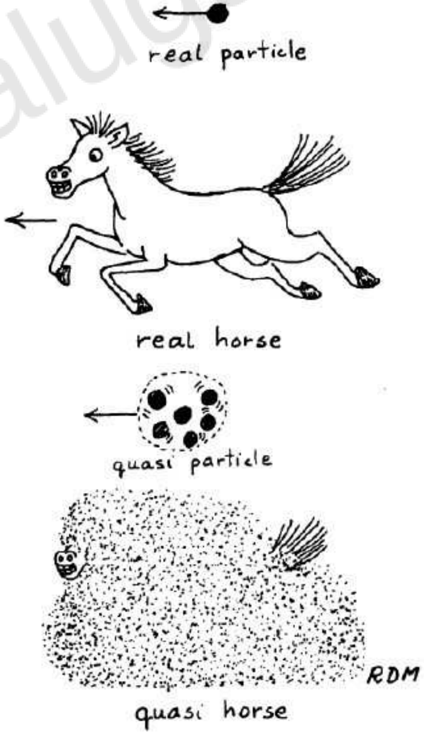
Landau Fermi liquid theory





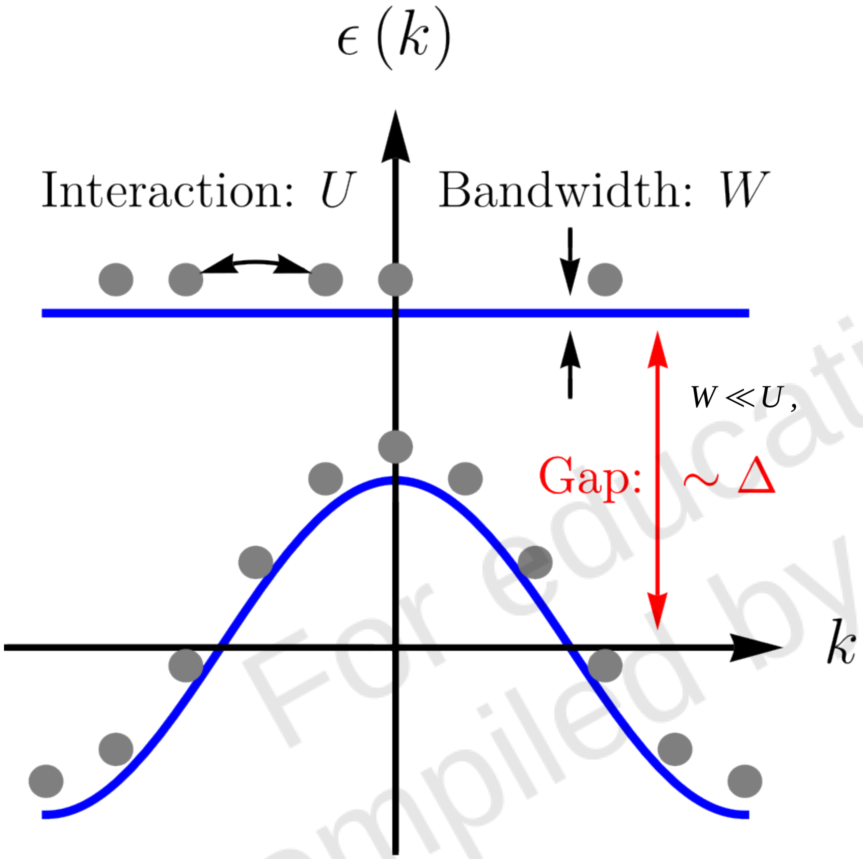
Non–interacting Fermi gas

Interacting quasi–particles



R. D. Mattuck, A Guide to Feynman Diagrams in the Many-Body Problem

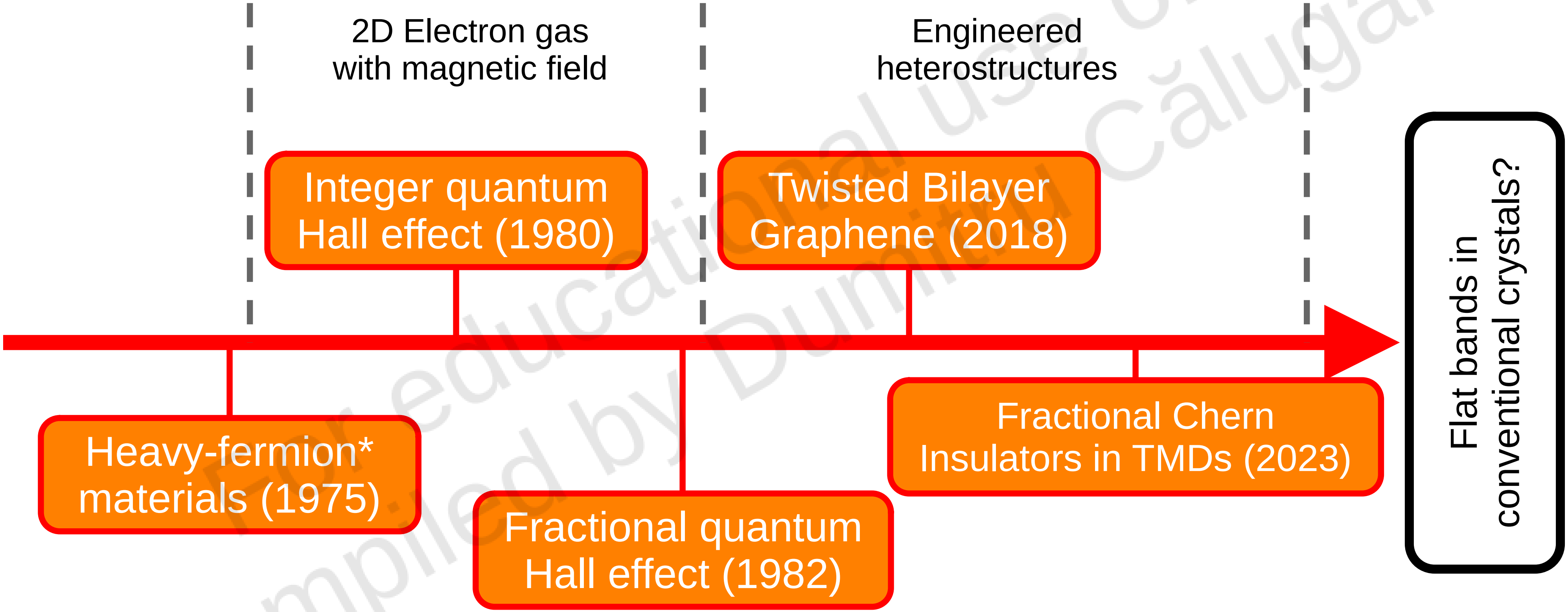
What about flat bands?



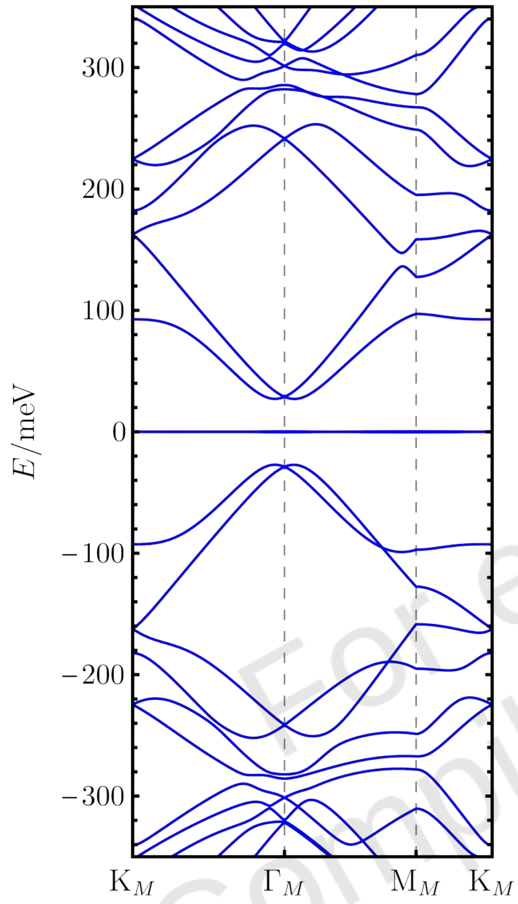
$$W \ll U \,(\text{sometimes: } W \ll \Delta)$$

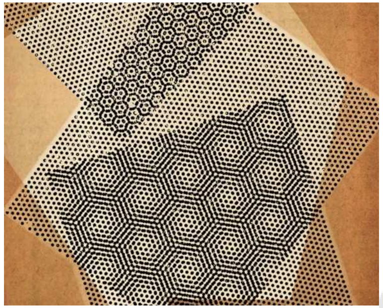
Cannot perturb away from the non-interacting problem!

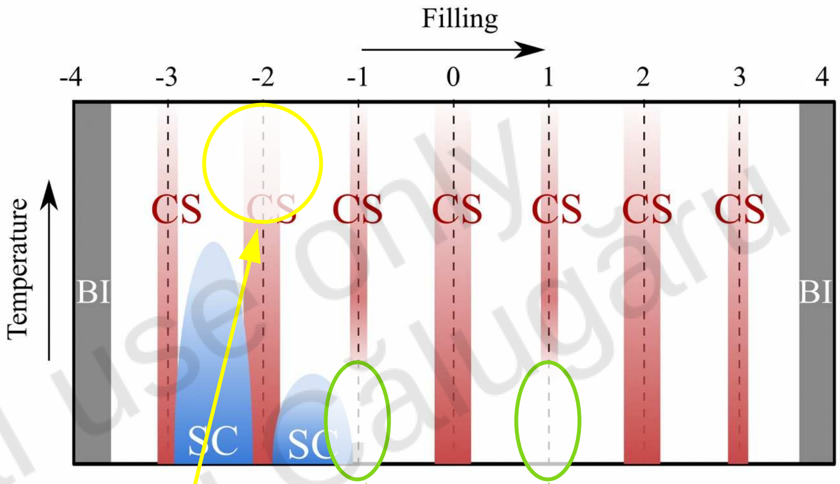
Brief history of flat bands*



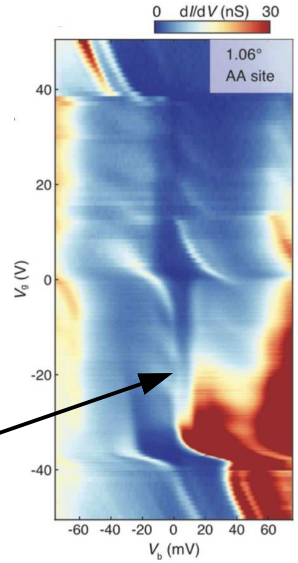
Twisted bilayer graphene







- Correlated insulator or correlated states (CS): Cao et al. 2018, Lu et al. 2019, Sharpe et al. 2019, Saito et al. 2020, Stepanov et al. 2020, Wong et al. 2020, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019
- Chern insulator: Serlin et al. 2019, Nuckolls et al. 2020, Choi et al. 2020, Saito et al. 2021, Das et al. 2021, Park et al. 2021, Wu et al. 2021
- Superconductivity (SC): Cao et al. 2018, Lu et al. 2019, Yankowitz et al. 2019, Saito et al. 2020, Stepanov et al. 2020
- Strange metal: Cao et al. 2020, Polshyn et al. 2019
- Pomeranchuk effect: Saito et al. 2021, Rozen et al. 2021
- Dirac-like behavior: Zondiner et al. 2020, Saito et al. 2021, Rozen et al. 2021
- Quantum-dot-like behavior: Wong et al. 2020, Xie et al. 2019, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019
- Zero-energy peak: Oh et al. 2021, Choi et al. 2021, Nuckolls et al. 2020



Not all flat bands are created equal

$$\hat{c}^\dagger |0\rangle = |1\rangle$$
$$\hat{c} |1\rangle = |0\rangle$$
$$\hat{n} \equiv \hat{c}^\dagger \hat{c}$$
$$\hat{n} |0\rangle = 0$$
$$\hat{n} |1\rangle = |1\rangle$$

The Hubbard model: interactions in a single band*

$$H = t \sum_s \sum_{\langle R, R' \rangle} \hat{c}^\dagger_{R,s} \hat{c}_{R',s} + U \sum_R \hat{n}_{R,\uparrow} \hat{n}_{R,\downarrow} - \mu \sum_{R,s} \hat{n}_{R,s}$$

Nearest-neighbor hopping

Onsite repulsion
$U \geq 0$

$|t| = 1, U = 0$ $t = 0, U = 1$

Perturbative

$U/|t|$

Non-interacting Exact flat-band limit

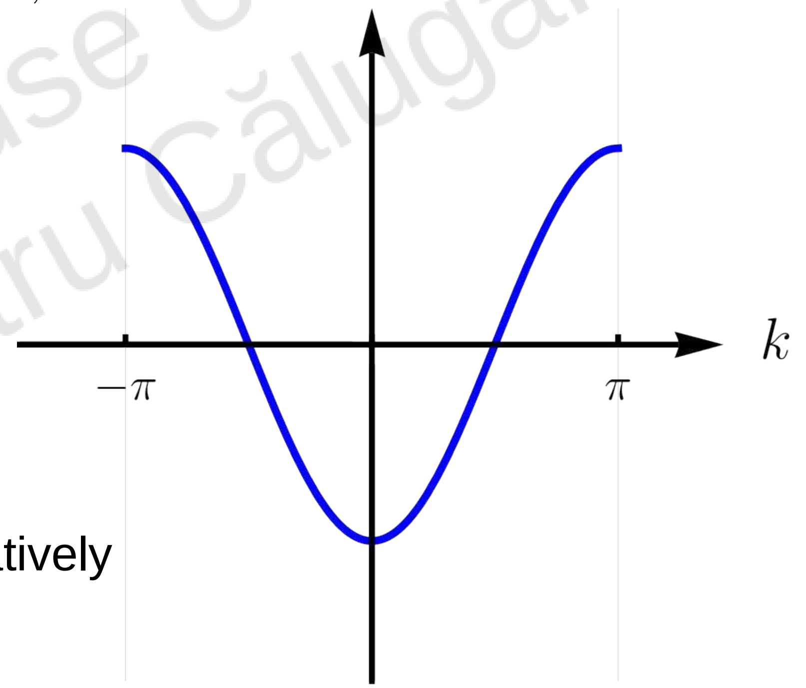
Non-interacting limit

$$H = t\sum_{s}\sum_{\langle R,R'\rangle}\hat{c}^{\dagger}_{R,s}\hat{c}_{R',s} = \sum_{s}\sum_{k}2t\cos(k)\hat{c}^{\dagger}_{k,s}\hat{c}_{k,s}$$

$$\hat{c}^{\dagger}_{k,s} = \sum_{R}\hat{c}^{\dagger}_{R,s}e^{ikR}$$

Work in momentum space

$\epsilon(k)\,,\ t<0$



$U \ll |t|$

Add interactions perturbatively

$|t| = 1, U = 0$

Perturbative

Non-interacting

$U/|t|$

Flat-band limit of the Hubbard model

Sites are independent (focus on a single site)

$$H_{\text{single site}} = U\hat{n}_\uparrow \hat{n}_\downarrow - \mu\left(\hat{n}_\uparrow + \hat{n}_\downarrow\right)$$

$$|\psi\rangle = |0\rangle \quad : \quad H_{\text{single site}}|\psi\rangle = 0$$

$$|\psi\rangle = |\uparrow\rangle, |\downarrow\rangle \quad : \quad H_{\text{single site}}|\psi\rangle = -\mu|\psi\rangle$$

$$|\psi\rangle = |\downarrow\uparrow\rangle \quad : \quad H_{\text{single site}}|\psi\rangle = (U - 2\mu)|\psi\rangle$$

Cannot explain the richness of twisted bilayer graphene…
Missing ingredient: Topology

$t = 0, U = 1$

$U/|t|$

Exact flat-band limit

Saturday Morning of Theoretical Physics

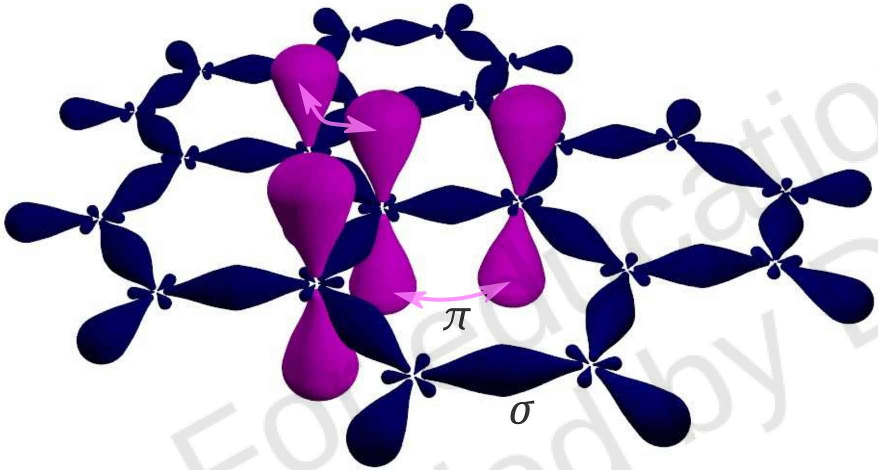
Part I

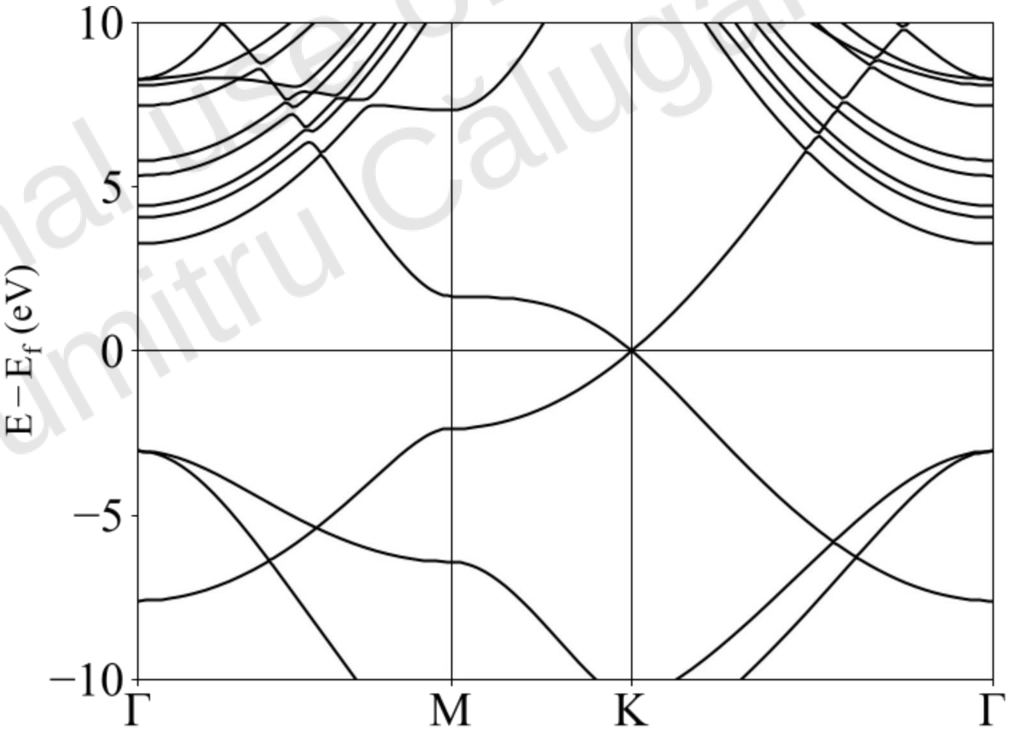
Topological Quantum Chemistry

B. Bradlyn, L. Elcoro, J. Cano, *et al.*, Nature 547, 298–305 (2017)

Electronic spectra

Graphene





Real space (Chemistry) ←?→ Reciprocal space (Physics)

Band structures *without* Hamiltonians

Space Group (SG): set of **symmetries** that define a crystal:

- Discrete lattice translations.
- Point group operations (rotations, reflections).
- Non-symmorphic operations (screw, glide).

Ingredients:

- One of the 230 SGs.
- Atoms at some lattice positions.
- Orbitals (s, p, d, ...).

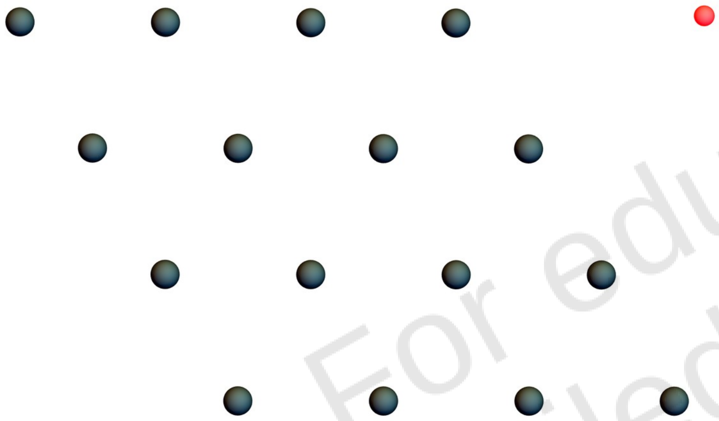
How do we go from real space orbitals sitting at lattice sites to any electronic band structure (without a Hamiltonian)?

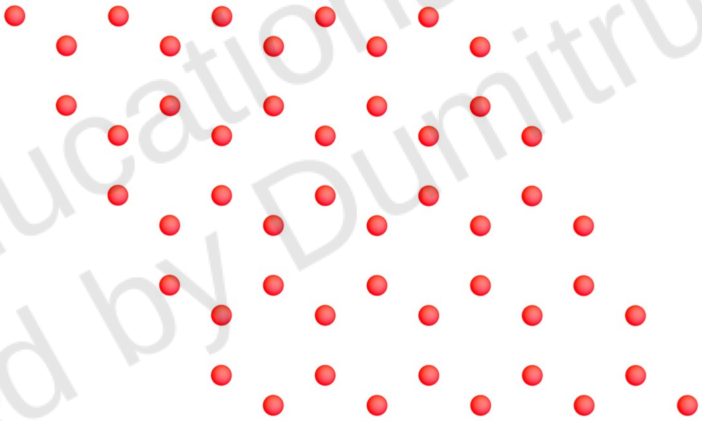
Elementary Band representations (EBRs)

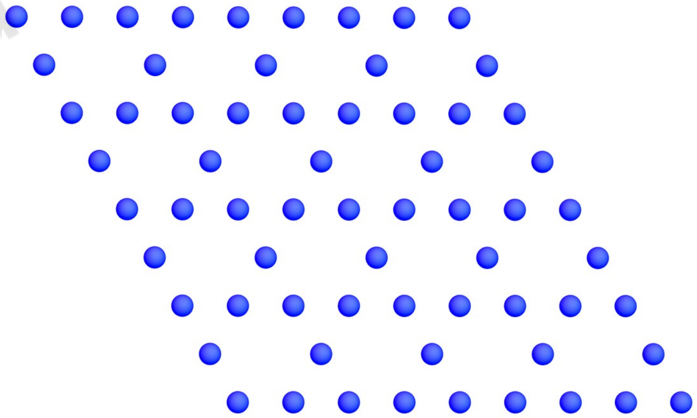
B. Bradlyn, L. Elcoro, J. Cano, *et al.*, Nature 547, 298–305 (2017)

Many lattice position choices

Several ways to arrange the atoms within the unit cell where all atoms are related by symmetry.







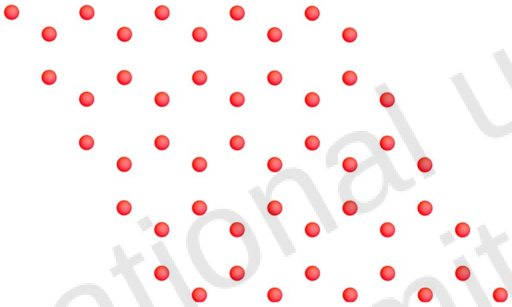
1 atom/unit cell (triangular)

2 atoms/unit cell (honeycomb)

3 atoms/unit cell (kagome)

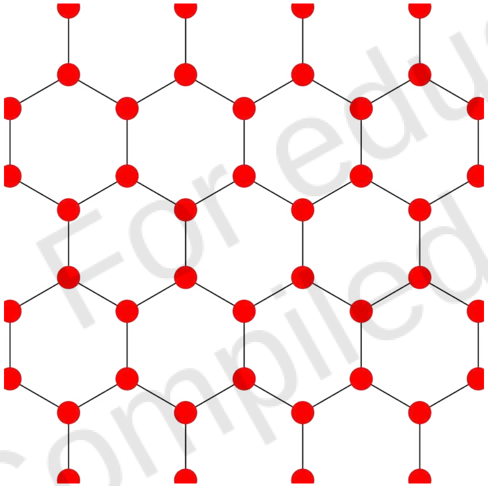
Many orbital choices

Several ways to choose electronic orbitals for a given arrangement (orbital arrangement must be consistent with SG symmetry).

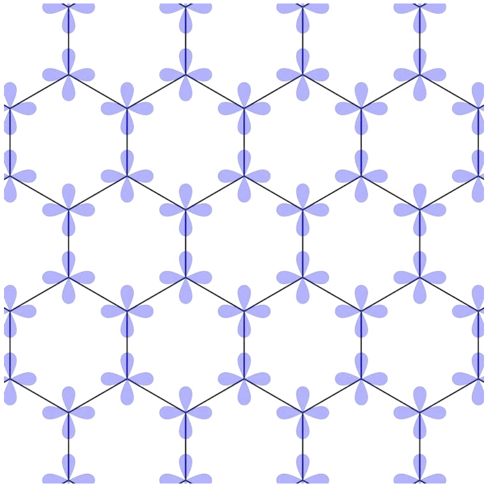


s (or p_z) orbitals

p_x and p_y orbtials



2 atoms/unit cell
(honeycomb)

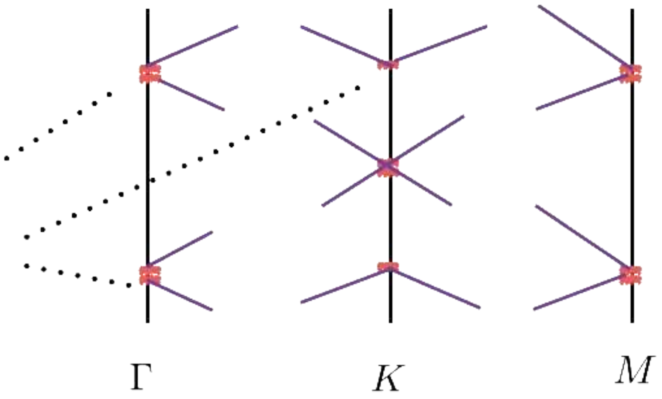


Elementary band representations (EBRs)

*Can we build all the possible band structure for these cases (i.e. all **atomic limits**)?*

- **Key insight**: Think of bands as representations! (J. Zak, H. Bacry, L. Michel)
- Then ask questions about *representation reducibility* (**Elementary bands**)
- Find all the irreps (**EBRs**)
- Single/double groups, w/wo time reversal, different orbitals, different Wyckoff positions: more than 10,000 irreps tabulated on the Bilbao Crystallographic server.
- Can also obtain the irreps of EBRs at momenta in the Brillouin zone.
- By construction, a band representation has an atomic limit, and all atomic limits yield a band representation.

$$(\rho \uparrow S) \downarrow G_{\mathbf{k}}$$



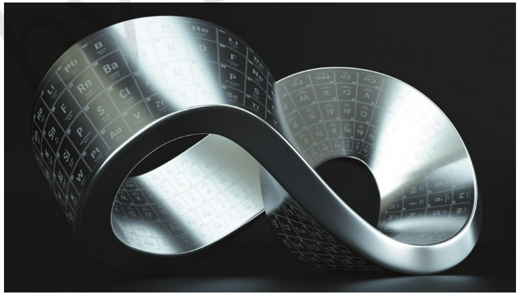
B. Bradlyn, L. Elcoro, J. Cano, *et al.*, Nature 547, 298–305 (2017)

Topological Quantum Chemistry (TQC)

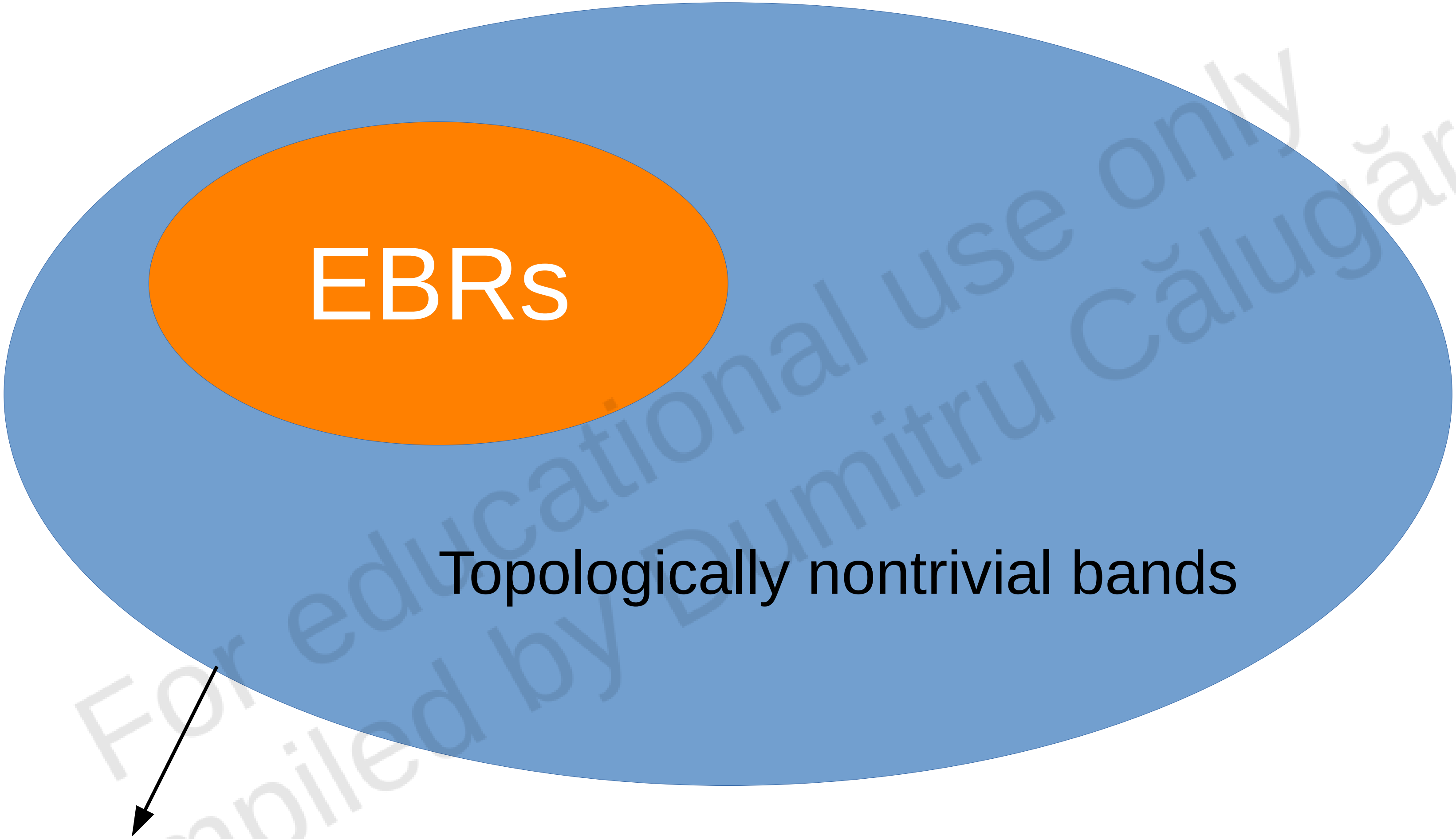
TQC provides a unified framework for the treatment of all topological phases arising from crystalline symmetries. It relies on:

- **EBRs** which enumerate a basis for all electronic bands induced from atomic orbital (**atomic limits**).
- **compatibility relations**, constraining how bands can connect across the Brillouin zone.

"All sets of bands not induced from symmetric, localized orbitals, are topologically non-trivial by design."



B. Bradlyn, L. Elcoro, J. Cano, *et al.*, Nature 547, 298–305 (2017)



All possible bands (i.e. satisfying
the compatibility relations)

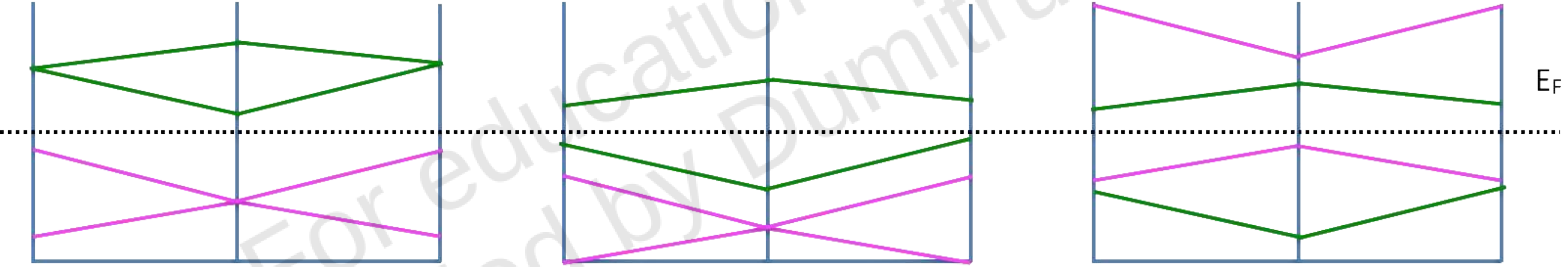
Example

$$\mathcal{B} = \sum_i a_i \mathrm{EBR}_i$$

Linear Combination of EBRs
Atomic (Trivial)

Split EBRs
(Topological)

General Linear Combination with at least a non-positive and/or non-integer coefficients*
(Topological)



$$\mathcal{B} = \mathrm{EBR}_1$$

$$\mathcal{B} = \mathrm{EBR}_1 + \frac{1}{2}\mathrm{EBR}_2$$

$$^*\text{Fragile: } \mathcal{B}_F = \mathrm{EBR}_1 - \mathrm{EBR}_2$$

$$\mathcal{B}_F + \mathrm{EBR}_2 = \mathrm{EBR}_1 = \text{Trivial}$$

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Part II
(Topological)
Flat Bands in Crystalline Materials

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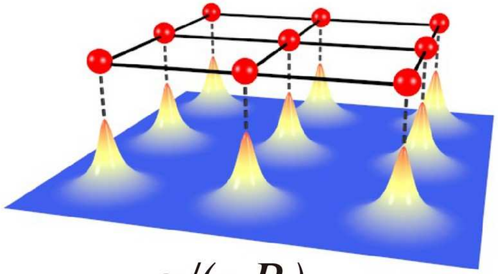
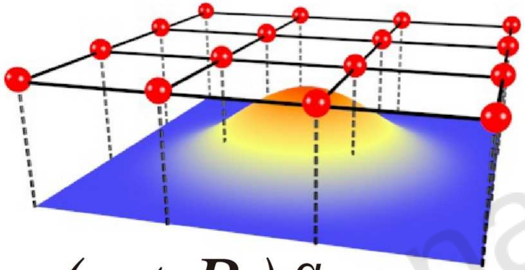
Why *topological* flat bands?



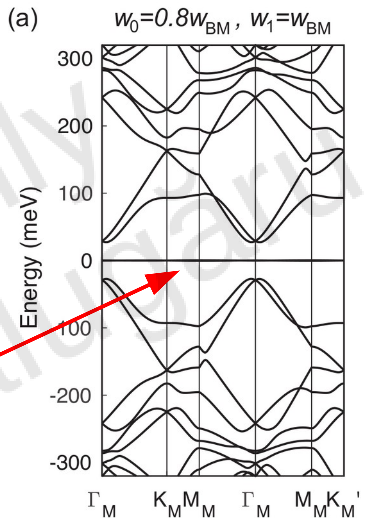
$e^{-\alpha/(r-R_i)}$

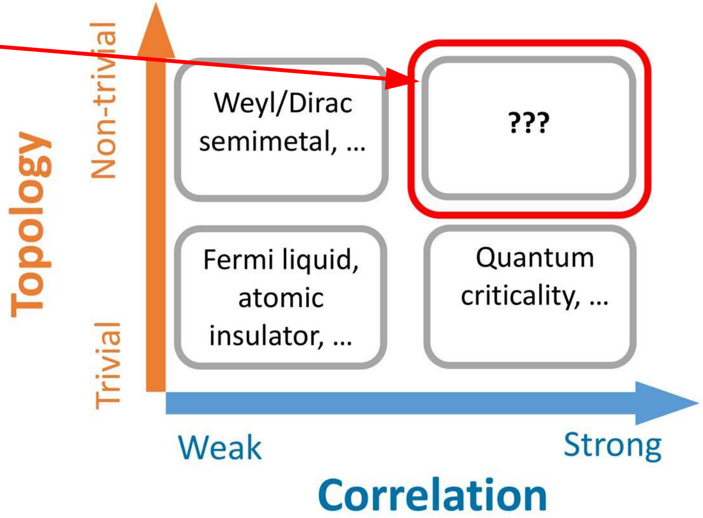
Trivial atomic flat band



$(r\text{-}t\text{-}R_i)^{-\alpha}$

Topological flat bands

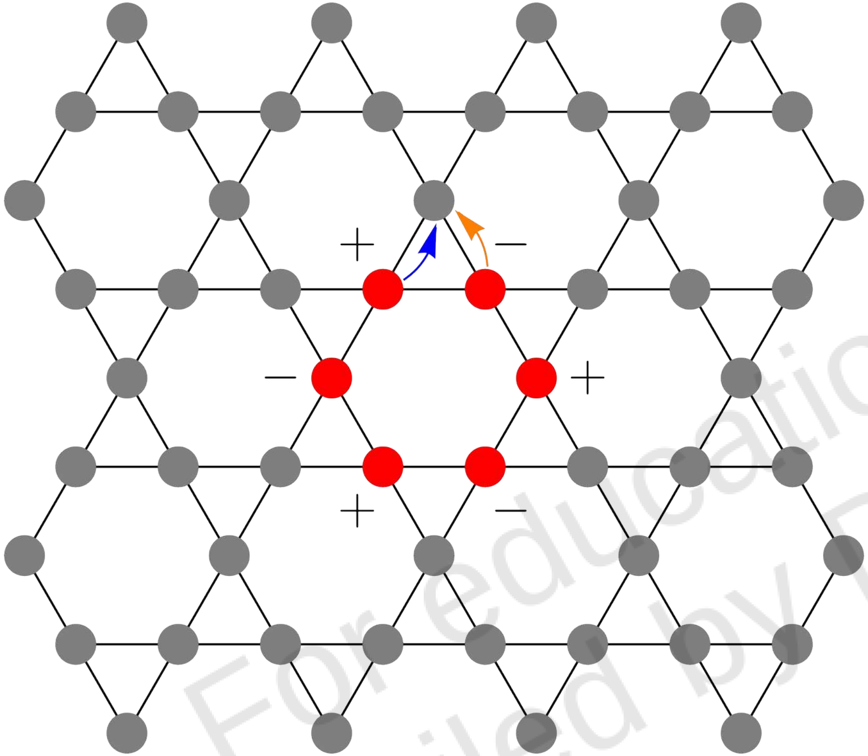


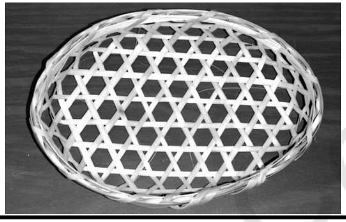


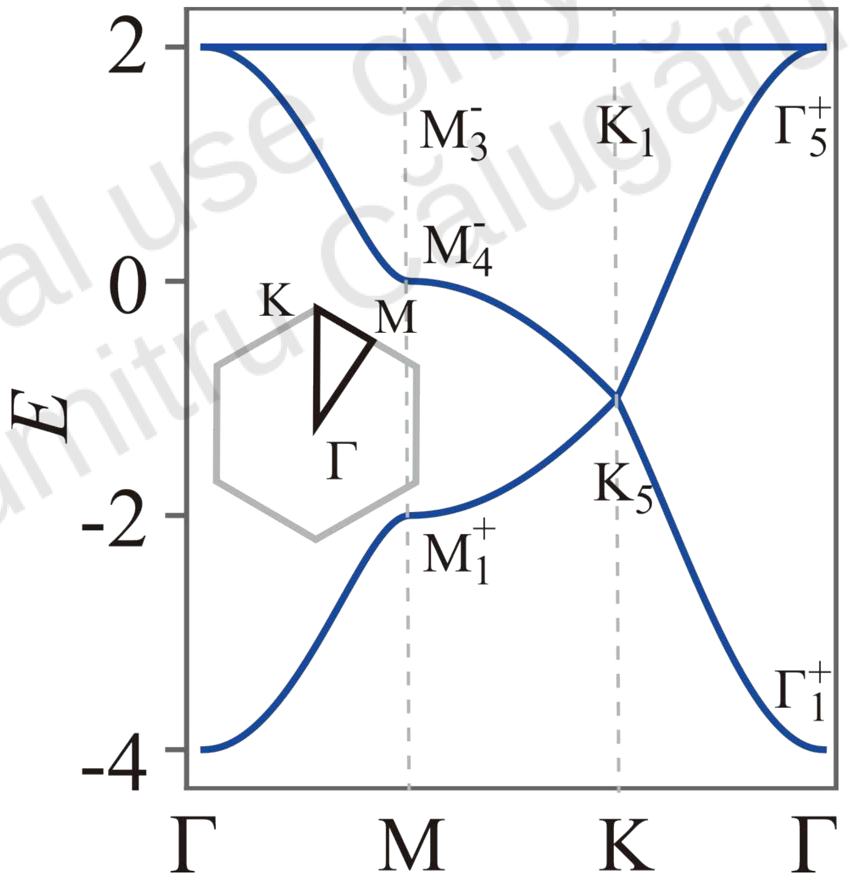
$$H = \cancel{t\sum_{s}\sum_{\langle \mathbf{R},\mathbf{R}'\rangle} \hat{c}^\dagger_{\mathbf{R},s}\hat{c}_{\mathbf{R}',s}} + U\sum_{\mathbf{R}} \hat{c}^\dagger_{\mathbf{R},\uparrow}\hat{c}_{\mathbf{R},\uparrow}\hat{c}^\dagger_{\mathbf{R},\downarrow}\hat{c}_{\mathbf{R},\downarrow},$$

N. Regnault, Y. Xu, MR. Li, *et al.*, Nature 603, 824–828 (2022)

How to design a (nontrivial) flat band?

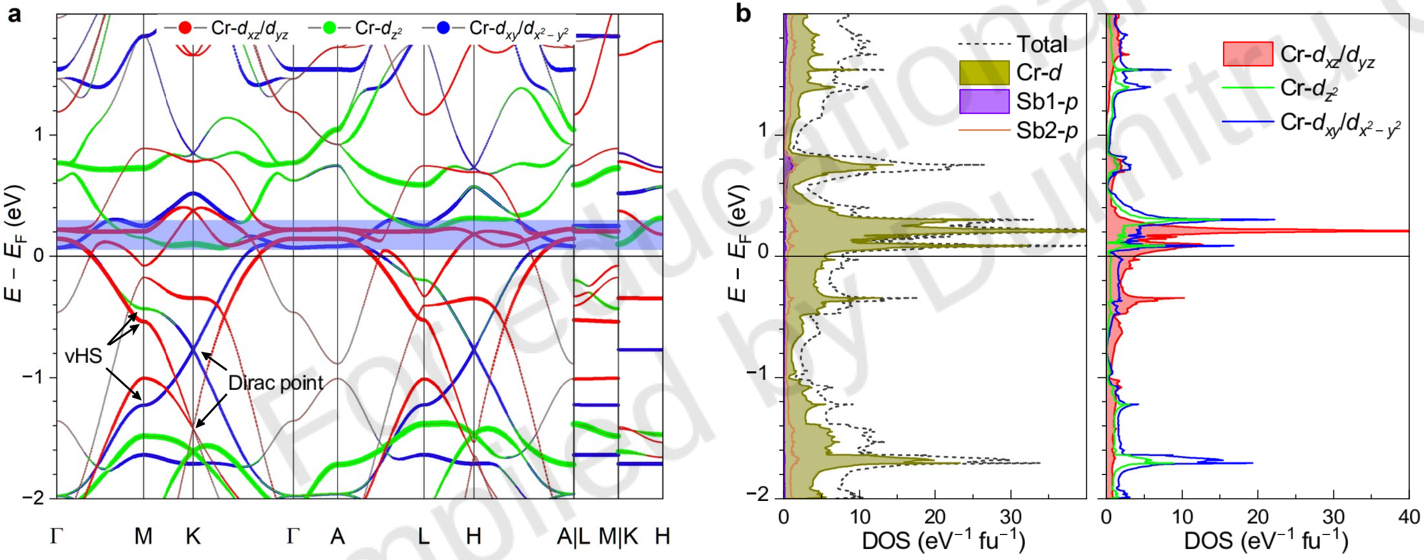


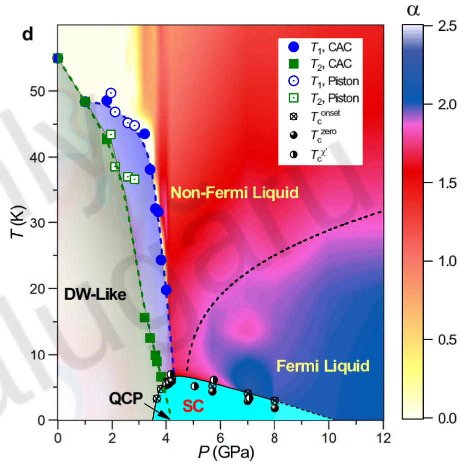


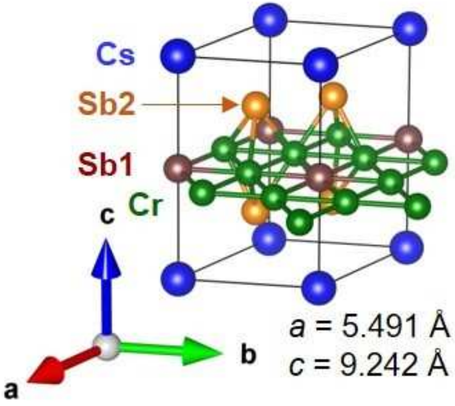


Kagome metals

Recent example: $CsCr_3Sb_5$

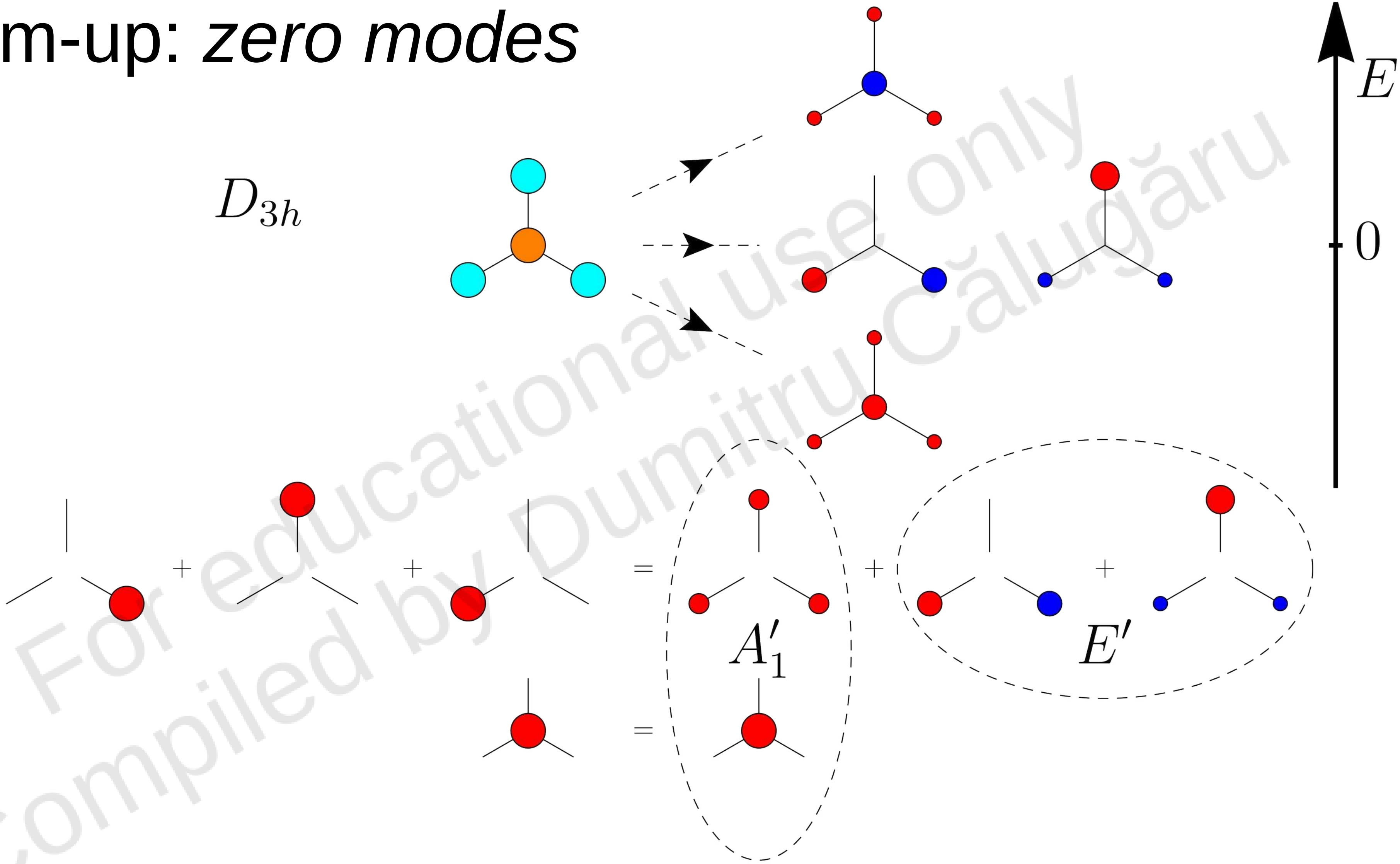




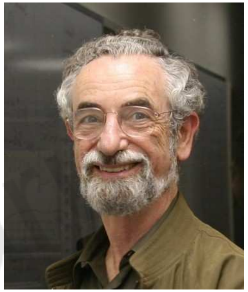


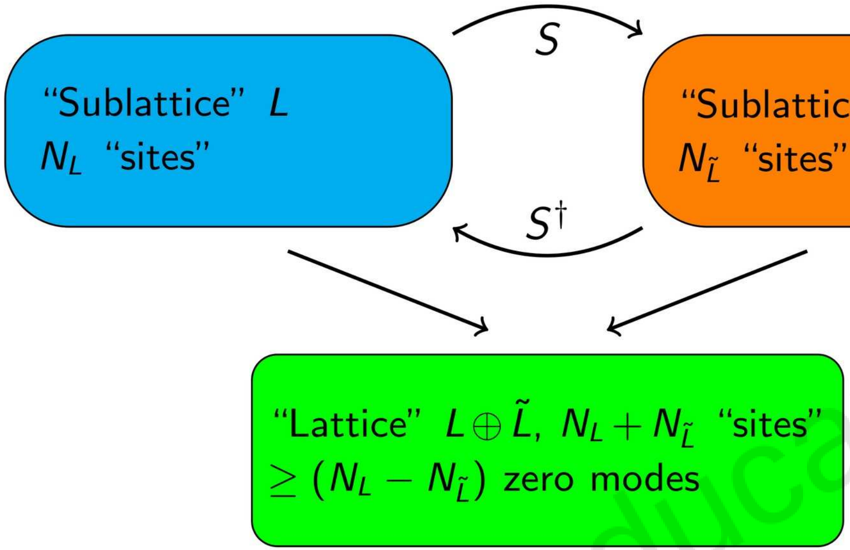
Y. Liu, ZY. Liu, JK. Bao, *et al.*, Nature 632, 1032–1037 (2024)

Warm-up: *zero modes*



Lieb's construction





$$H_{\mathbf{k}} = \begin{array}{cc} \begin{array}{cc} N_L & N_{\tilde{L}} \end{array} & \\ \begin{pmatrix} \mathbb{0} & S_{\mathbf{k}} \\ S_{\mathbf{k}}^\dagger & \mathbb{0} \end{pmatrix} & \begin{array}{c} N_L \\ N_{\tilde{L}} \end{array} \end{array}$$

$$\operatorname{rank}(H_{\mathbf{k}}) = \operatorname{rank}(S_{\mathbf{k}}) + \operatorname{rank}\left(S_{\mathbf{k}}^\dagger\right) = 2\operatorname{rank}(S_{\mathbf{k}}) \leq 2N_{\tilde{L}}$$

$$\operatorname{nulity}(H_{\mathbf{k}}) = \dim(H_{\mathbf{k}}) - \operatorname{rank}(H_{\mathbf{k}}) \geq (N_L - N_{\tilde{L}})$$

Generalized bipartite construction

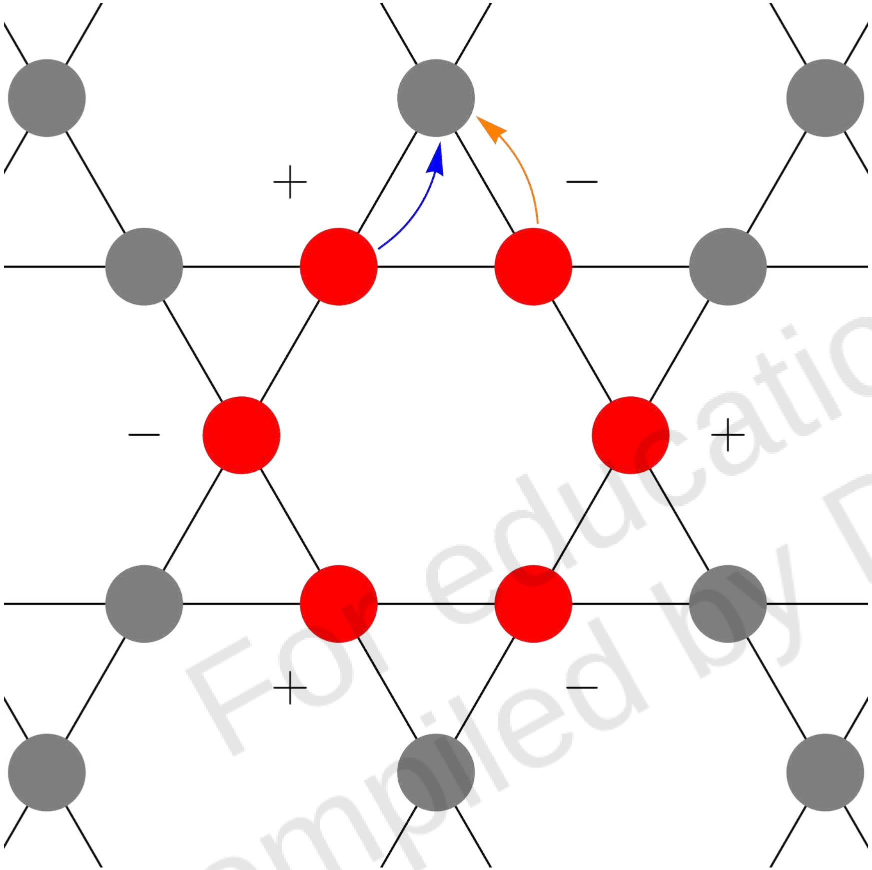
- Generalization of Lieb's construction without strict chiral symmetry: **onsite degenerate** terms on the big sublattice and **arbitrary hoppings** in the small sublattice:

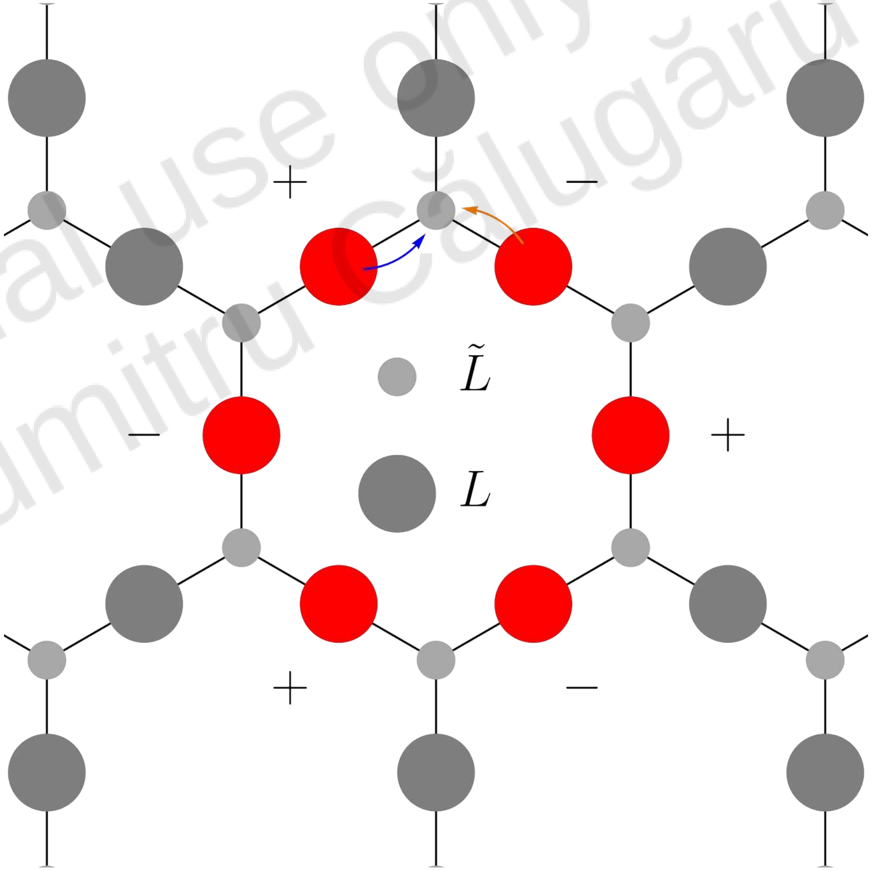
$$H_{\mathbf{k}} = \begin{array}{cc} & \begin{array}{cc} N_L & N_{\tilde{L}} \end{array} \\ & \left(\begin{array}{cc} a\mathbb{1} & S_{\mathbf{k}} \\ S_{\mathbf{k}}^{\dagger} & B_{\mathbf{k}} \end{array}\right) \begin{array}{c} N_L \\ N_{\tilde{L}} \end{array} \end{array}$$

- The two "sublattices": sites, orbitals, spins, etc.
- Any "coupling" between the two "sublattices".
- **Topological properties of flat bands depend only on the orbitals.**
- 7000 **materials** catalogued.

D. Călugăru, A. Chew, L. Elcoro, *et al.*, Nat. Phys. 18, 185–189 (2022)

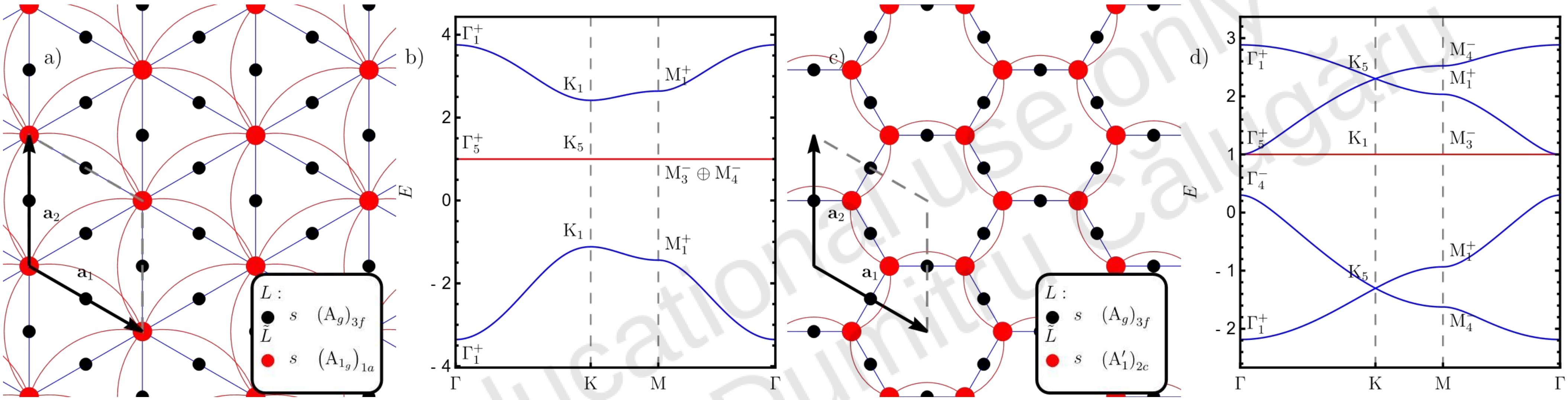
Bipartite lattices are all-encompassing





D. Călugăru, A. Chew, L. Elcoro, *et al.*, Nat. Phys. 18, 185–189 (2022)

Example of various flat bands



Flat bands are **gapped** and **topological** (fragile).

$$\mathcal{B}_{\mathrm{FB}} = (\mathrm{A}_g)_{3f} \uparrow \mathcal{G} \boxminus (\mathrm{A}_{1_g})_{3f} \uparrow \mathcal{G}$$
$$= (\Gamma_5^+) + (\mathrm{K}_5) + (\mathrm{M}_3^- \oplus \mathrm{M}_4^-)$$

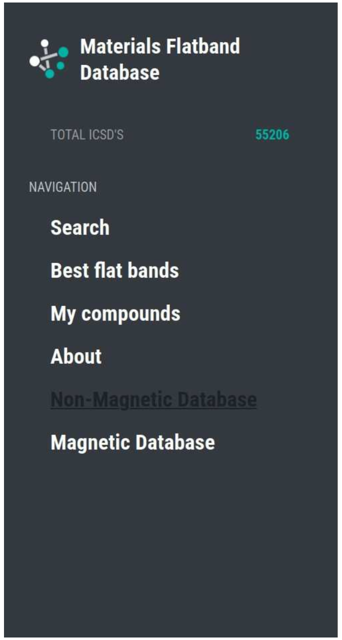
Flat bands have a symmetry-enforced **gapless point**.

$$\mathcal{B}_{\mathrm{FB}} = (\mathrm{A}_g)_{3f} \uparrow \mathcal{G} \boxminus (\mathrm{A}'_1)_{2c} \uparrow \mathcal{G}$$
$$= (\Gamma_5^+ \boxminus \Gamma_4^-) + (\mathrm{K}_1) + (\mathrm{M}_3^-)$$

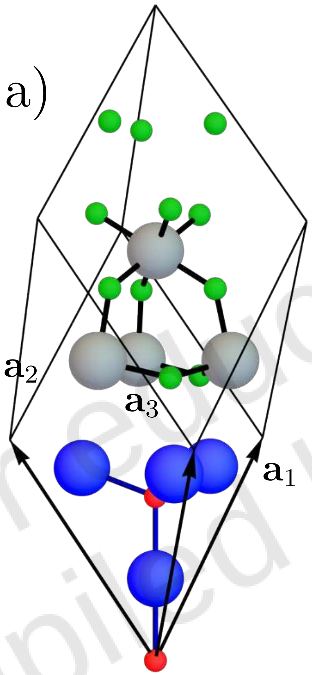
Can **diagnose** non-trivial flat band **topology** and understand the emergence of **gapless** points.

D. Călugăru, A. Chew, L. Elcoro, *et al.*, Nat. Phys. 18, 185–189 (2022)

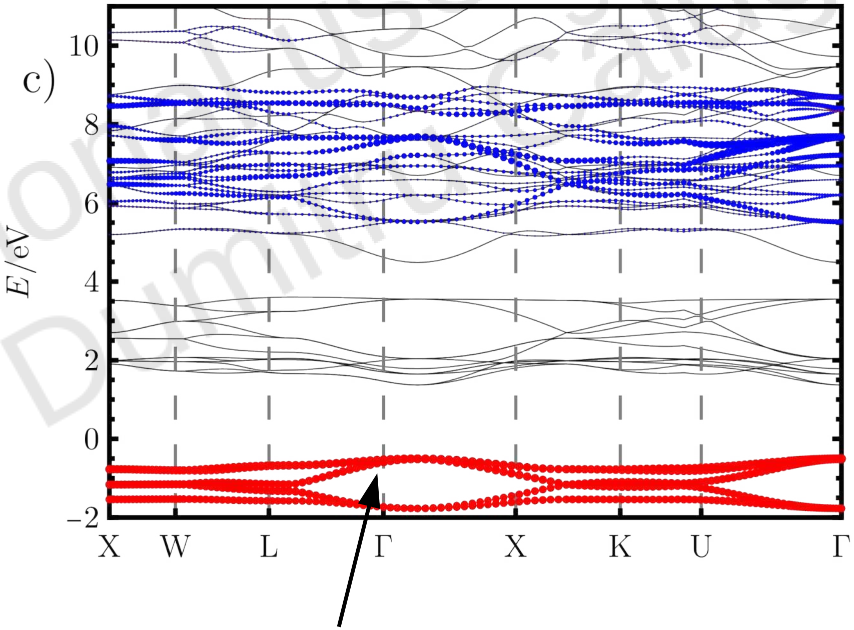
Flat band online database



$Ca_2Ta_2O_7$



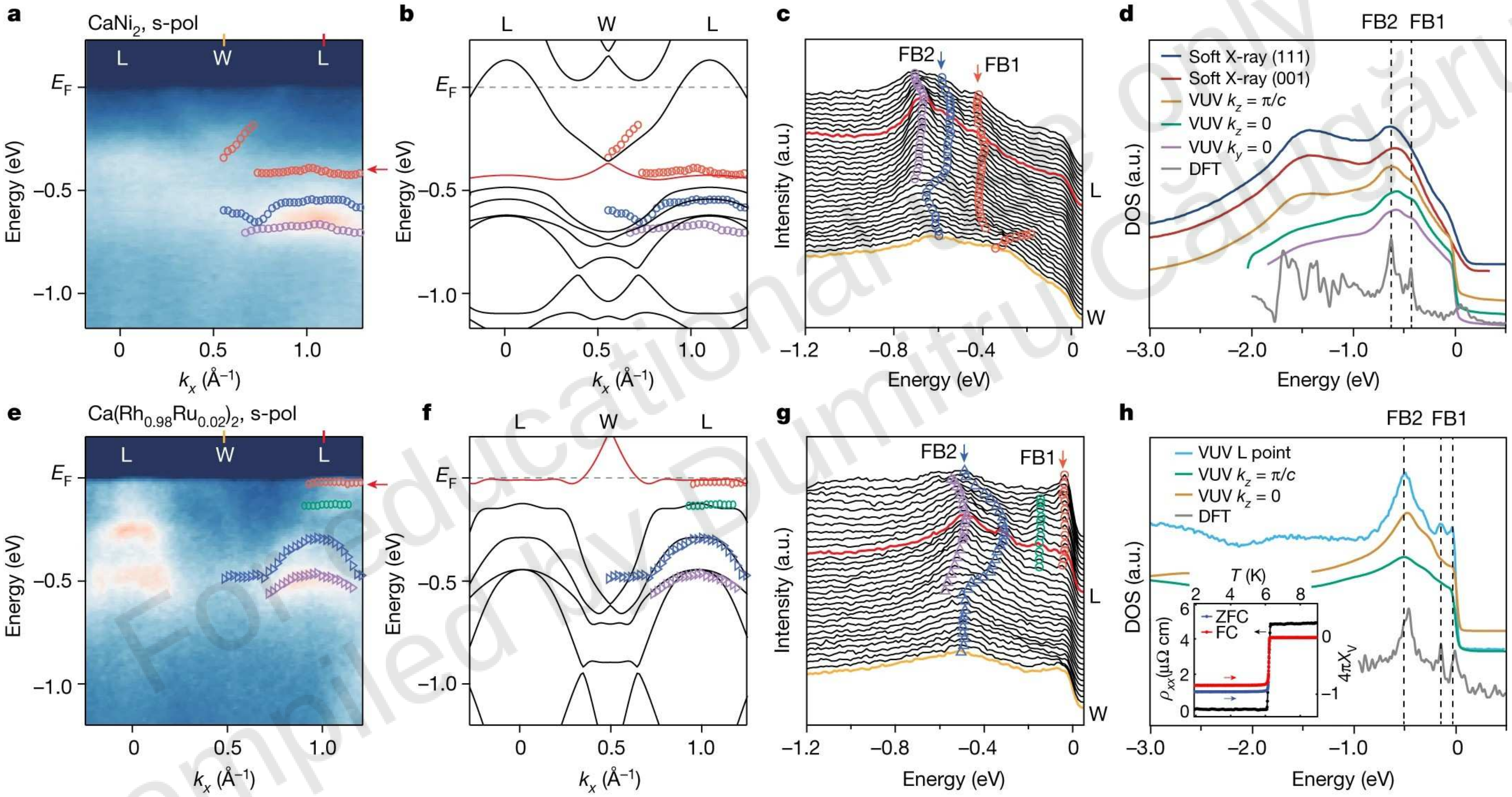
Flat bands of $Ca_2Ta_2O_7$



Band touching point

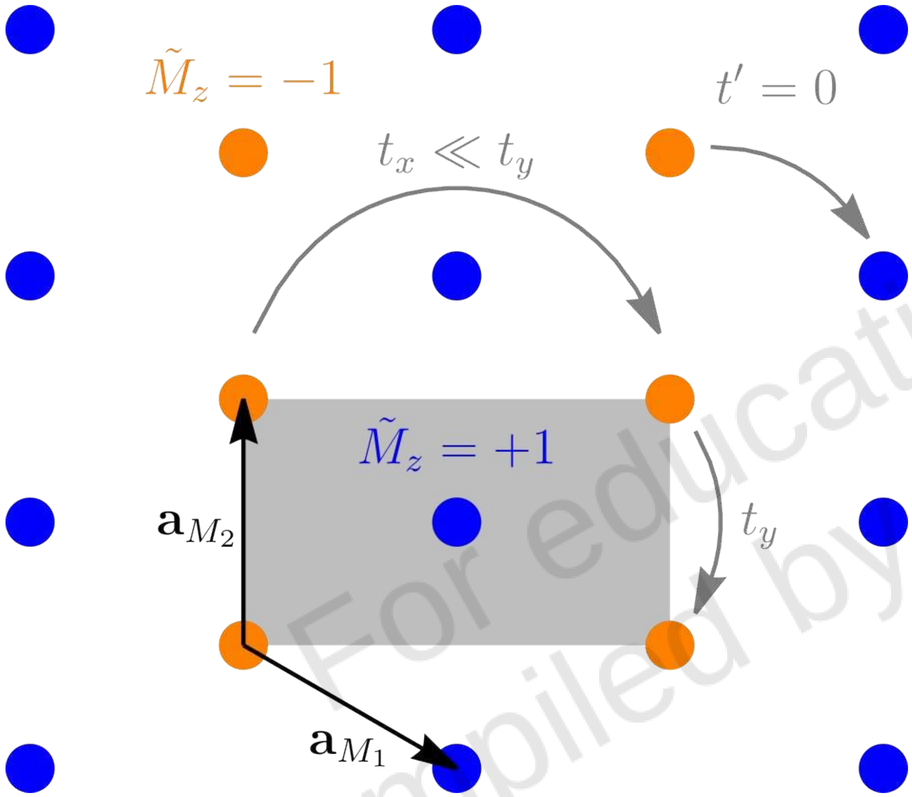
N. Regnault, Y. Xu, MR. Li, *et al.*, Nature 603, 824–828 (2022)

Flat bands and superconductivity



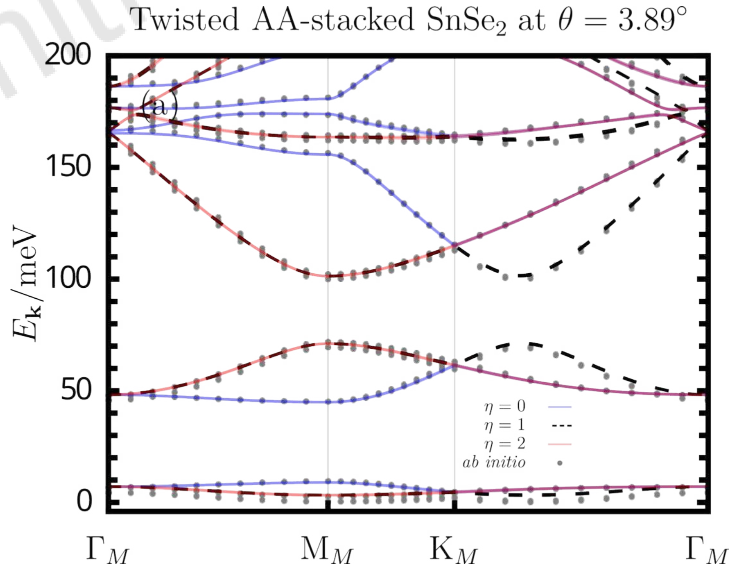
J.P. Wakefield, M. Kang, P.M. Neves, *et al.*, Nature 623, 301–306 (2023)

Trivial flat(ish) bands revisited



$$\left[T'_{\mathbf{a}_{M_2}}, \tilde{M}_z\right] = \left\{T'_{\mathbf{a}_{M_1}}, \tilde{M}_z\right\} = 0$$

Quasi-1D chains uncoupled at the single-particle level



D. Călugăru, Y. Jiang, H. Hu, H. Pi, *et al.*, Nature (2025, *in press*)

Conclusions

- Flat bands are a versatile platform for engineering exotic phases of matter **beyond Fermi liquids**.
- Not all flat bands are created equally (**topology is important**).
- A **simple and universal** construction prescription for crystalline flat bands exists.
- The construction leads to a **real material database**.
- Doping into crystalline flat bands can be linked to emerging superconductivity.
- Modeling these new platforms requires new tools! **Dominik's talk**.