Intrinsic Topological Dice Flat Band in monolayer YCl

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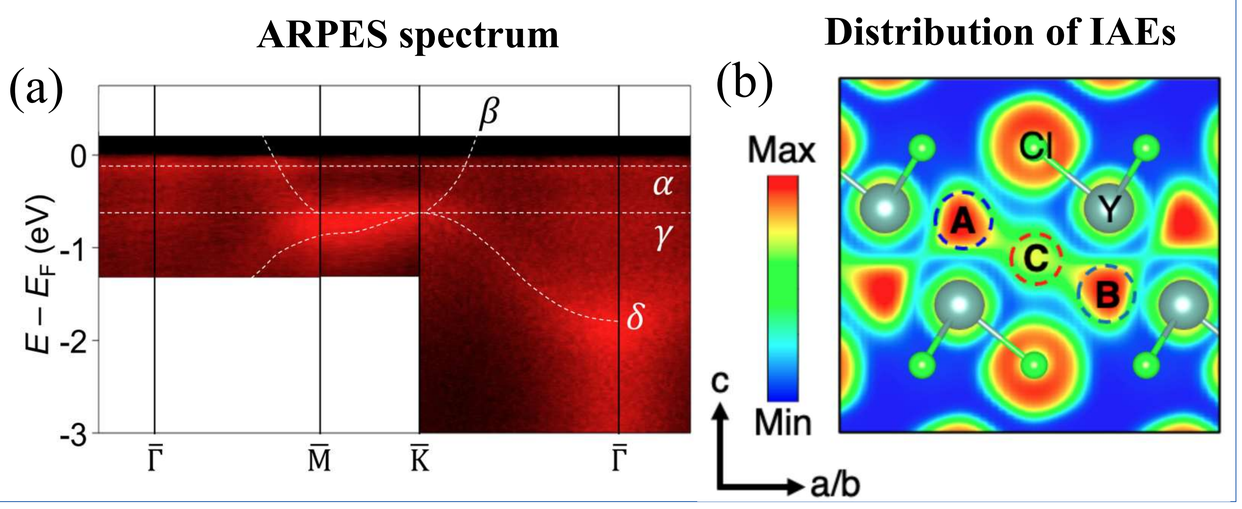
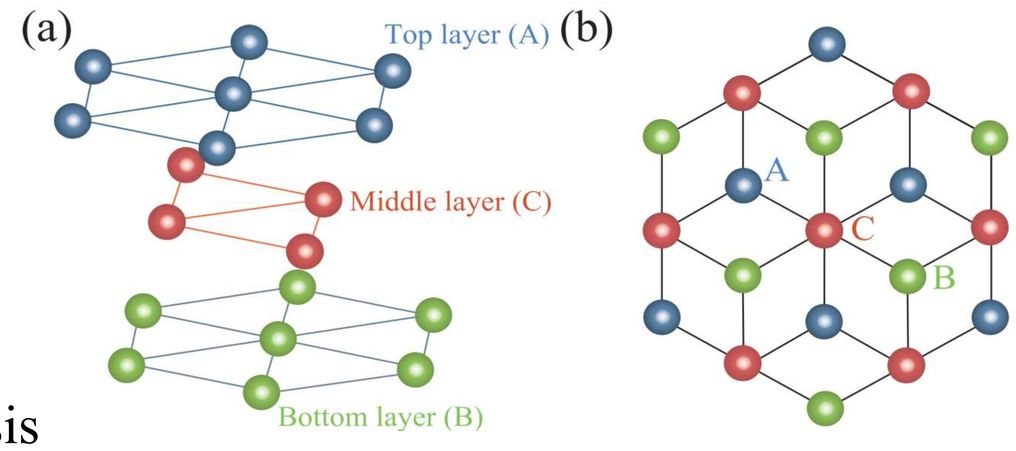
Background

The dice lattice known for its non-dispersive (flat) band was recently realized in ARPES of YCl, which shows layered electride YCl hosts a dice geometry formed by displaced interstitial-anionic-electrons (IAEs) Wannier centers (A,B,C sublattices) and ARPES measurements unambiguously identify two sets of dice-lattice bands in YCl, including a nearly dispersionless band at the Fermi level [1].



Seven band tight-binding model



Basis

$|\boldsymbol{k}, t, 0\rangle, |\boldsymbol{k}, t, +2\rangle, |\boldsymbol{k}, t, -2\rangle, |\boldsymbol{k}, s, 0\rangle, |\boldsymbol{k}, b, 0\rangle, |\boldsymbol{k}, b, +2\rangle, |\boldsymbol{k}, b, -2\rangle$

$$H_{TB}(\boldsymbol{k}) = \begin{pmatrix} h_t(\boldsymbol{k}) & h_{ts}(\boldsymbol{k}) & h_{tb}(\boldsymbol{k}) \\ h_{ts}^{\dagger}(\boldsymbol{k}) & h_s(\boldsymbol{k}) & h_{sb}(\boldsymbol{k}) \\ h_{tb}^{\dagger}(\boldsymbol{k}) & h_{sb}^{\dagger}(\boldsymbol{k}) & h_b(\boldsymbol{k}) \end{pmatrix}$$

Considering three distinct generators: C_{3z}, M_x, P by symmetry constraint:

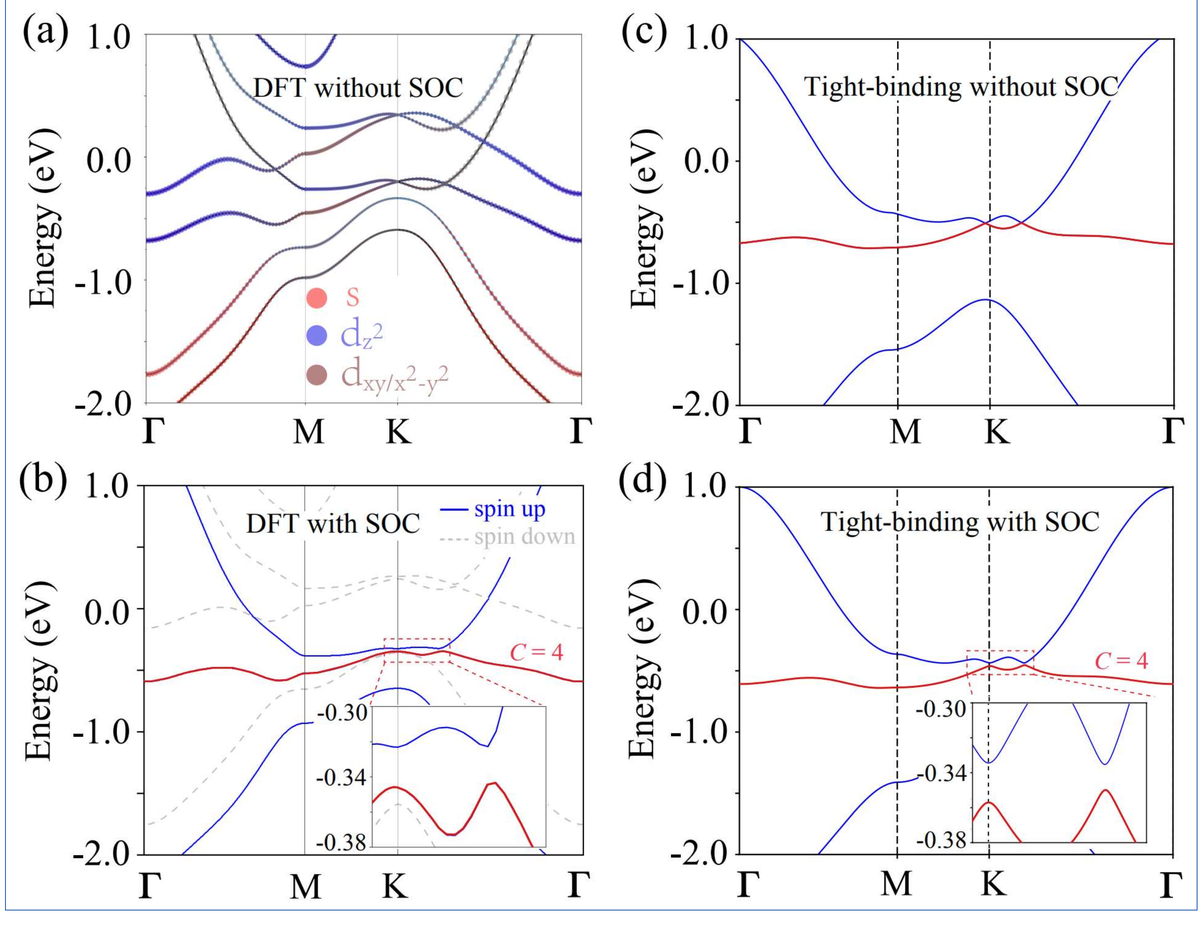
$$H_{ij} = t_{ij}(\boldsymbol{R_m}) e^{i\boldsymbol{k}\cdot(\boldsymbol{R_m})}$$

$$t^{ij}(\boldsymbol{R_m}) = \boldsymbol{D^j}(R)\, t^{ij}(\boldsymbol{R_m})\, \boldsymbol{D^{i\,\dagger}}(R)$$

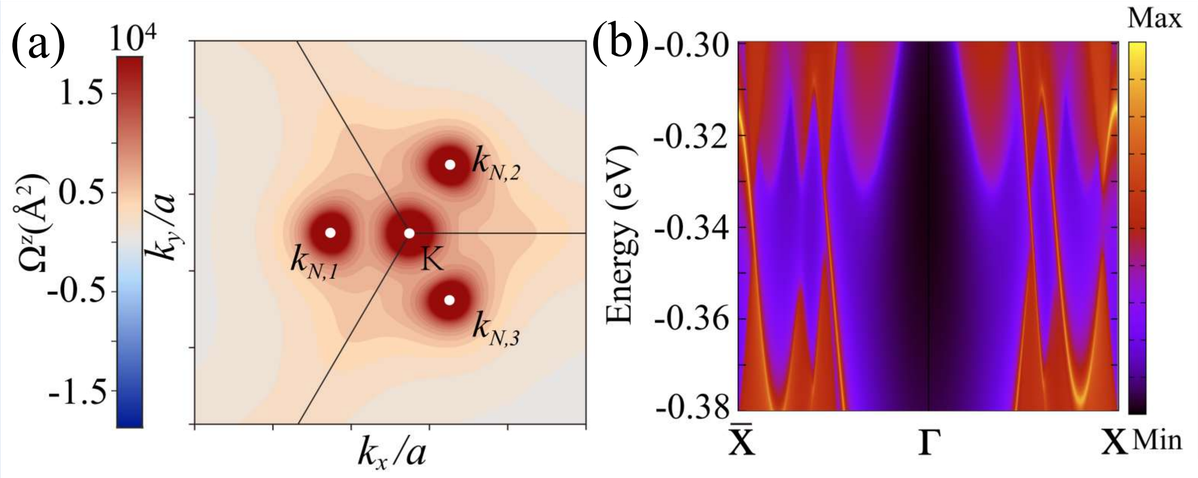
Span the basis $|d_{+2}, \uparrow\rangle, |d_{-2}, \uparrow\rangle, |d_{+2}, \downarrow\rangle, |d_{-2}, \downarrow\rangle$ with the atomic SOC :

$$H_{soc} = \lambda s_z \tau_z$$

Flat band topology

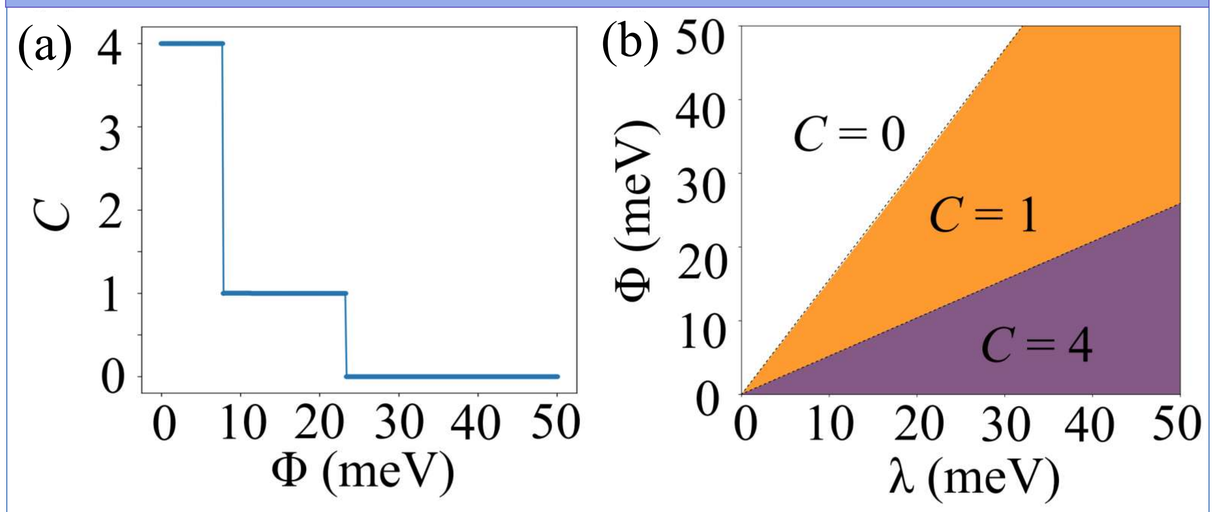


Berry curvature and edge states



Four Berry curvature hot positive spots are found per valley at $+K$ and its neighborhoods and four branches of chiral edge states in an infinite strip geometry.

Role of displacement field and phase diagram



H_D=diag(Φ, Φ, Φ, 0, -Φ, -Φ, -Φ)

Conclusions

- Combining symmetry analysis, fully relativistic DFT and realistic tight-binding, we find Y-4d orbital SOC gaps Dirac crossings at $\pm k$ and endows the dice flat band with $C = \pm 4$.
- The flat Chern band is intrinsic (no moiré) and its global topology and valley Berry curvature are tunable by a vertical displacement field [2].

References

[1]arXiv:2508.21311, [2] arXiv:2509.05958.