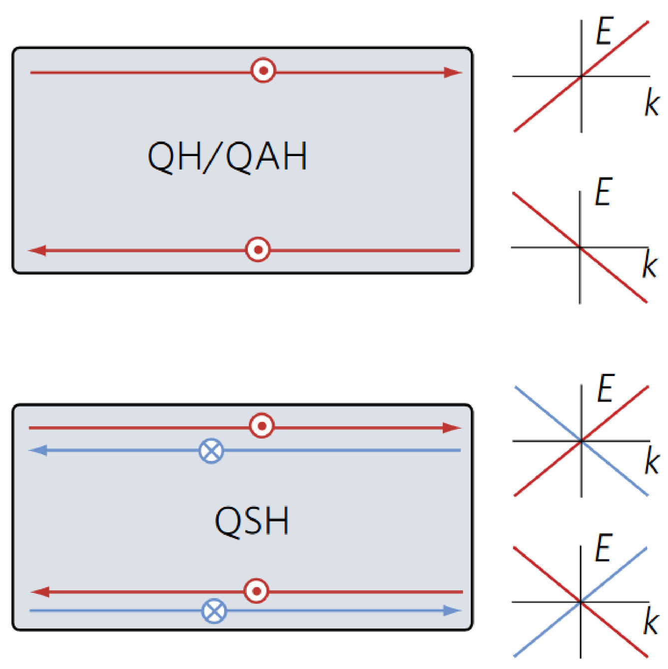
Topological bands in two-dimensional orbital-active bipartite lattices

Huan Wang[1] and Jing Wang[1, 2]

[1]State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China
[2]Institute for Nanoelectronic Devices and Quantum Computing, Fudan University, Shanghai 200433, China

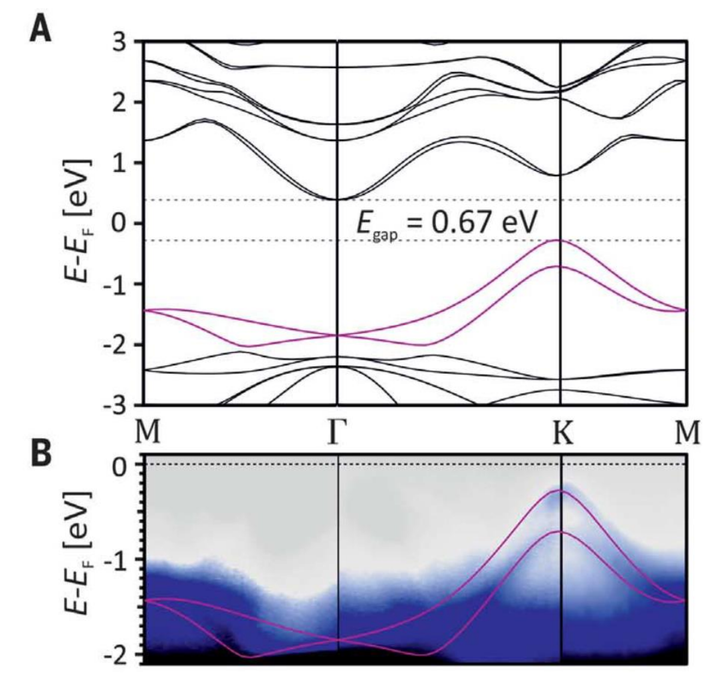
Motivation

The search for large gap quantum spin Hall (QSH) and quantum anomalous Hall (QAH) insulators is important both for fundamental and practical interests.



Wang, J., Zhang, SC. *Nature Mater* **16**, 1062–1067

The degenerate multi-orbitals p_x, p_y in honeycomb lattice provides a paradigm for QSH state with a boosted topological gap of the first order in atomic spin-orbit coupling.



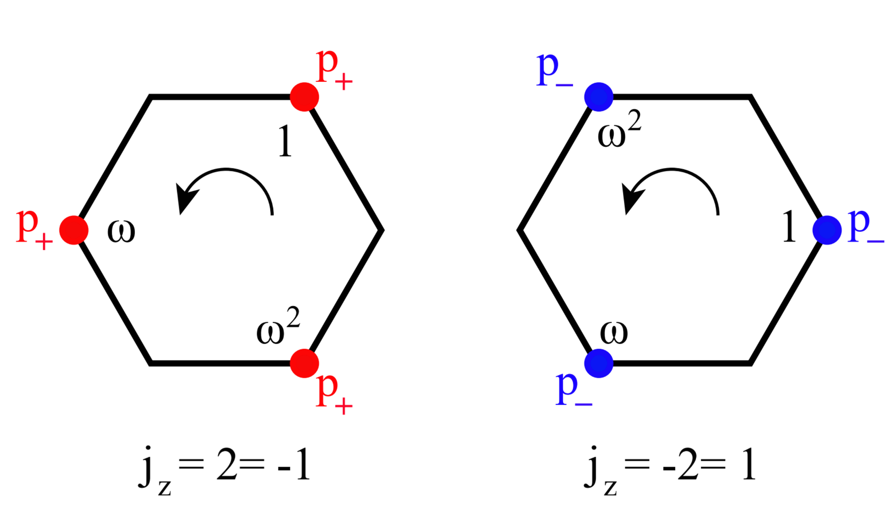
F. Reis, G. Li, et al, Science357,287–290 (2017)

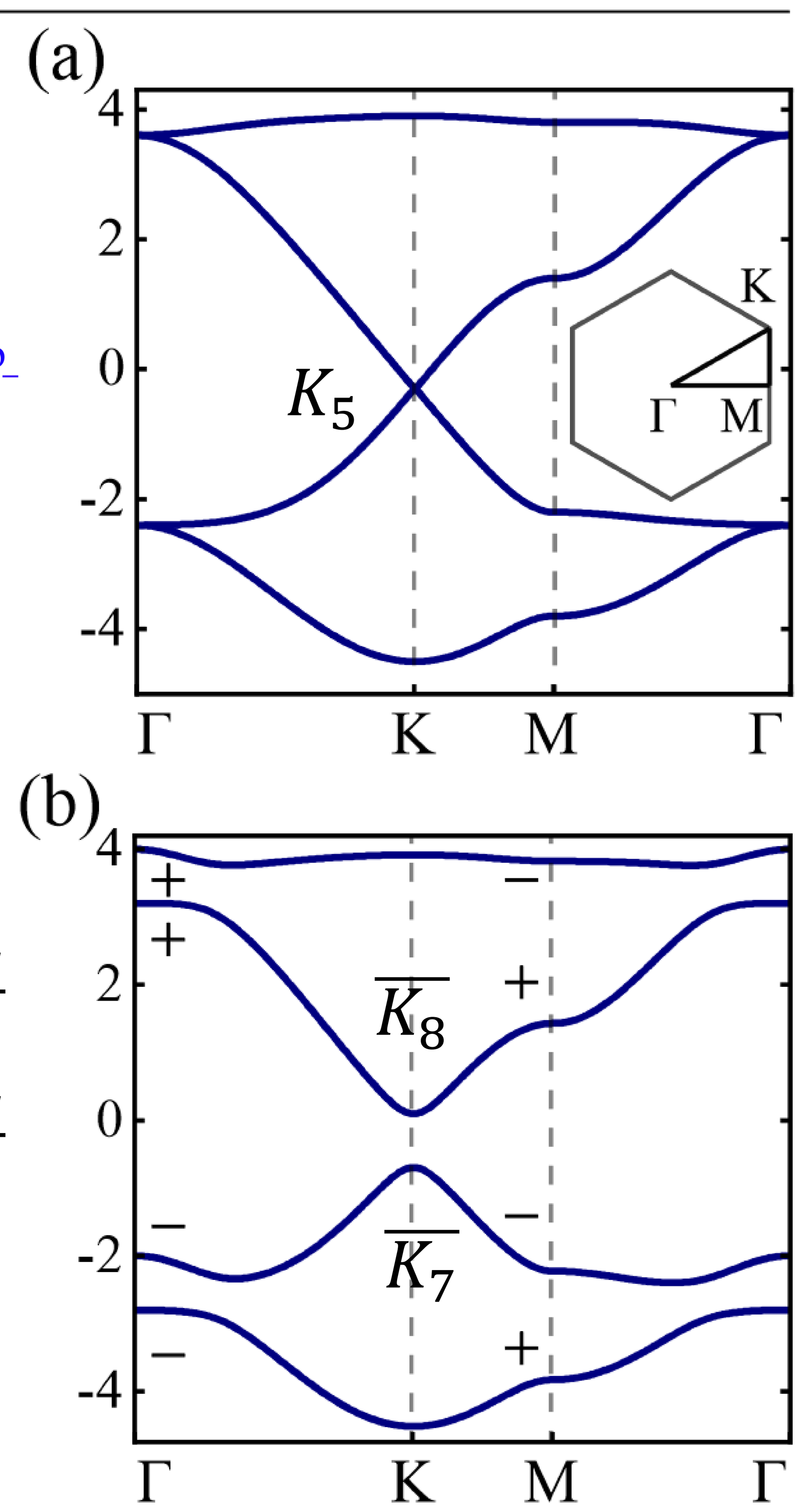
This motive us to explore the relation between symmetry and such large gap mechanism

Method

Topological Quantum Chemistry(TQC)

spinless	Γ	K	M
p_z	$\Gamma_2^- \oplus \Gamma_3^+$	K_6	$M_2^- \oplus M_3^+$
$p_x p_y$	$\Gamma_5^+ \oplus \Gamma_6^-$	$K_5 \oplus K_1 \oplus K_4$	$M_1^+ \oplus M_2^+ \oplus M_3^- \oplus M_4^-$
spinful	Γ	K	M
$p_+^\downarrow p_-^\uparrow$	$\overline{\Gamma}_8^+ \oplus \overline{\Gamma}_{12}^-$	$\overline{K}_7 \oplus \overline{K}_9$	$\overline{M}_5^+ \oplus \overline{M}_6^-$
$p_+^\uparrow p_-^\downarrow$	$\overline{\Gamma}_7^+ \oplus \overline{\Gamma}_{10}^-$	$\overline{K}_8 \oplus \overline{K}_9$	$\overline{M}_5^+ \oplus \overline{M}_6^-$





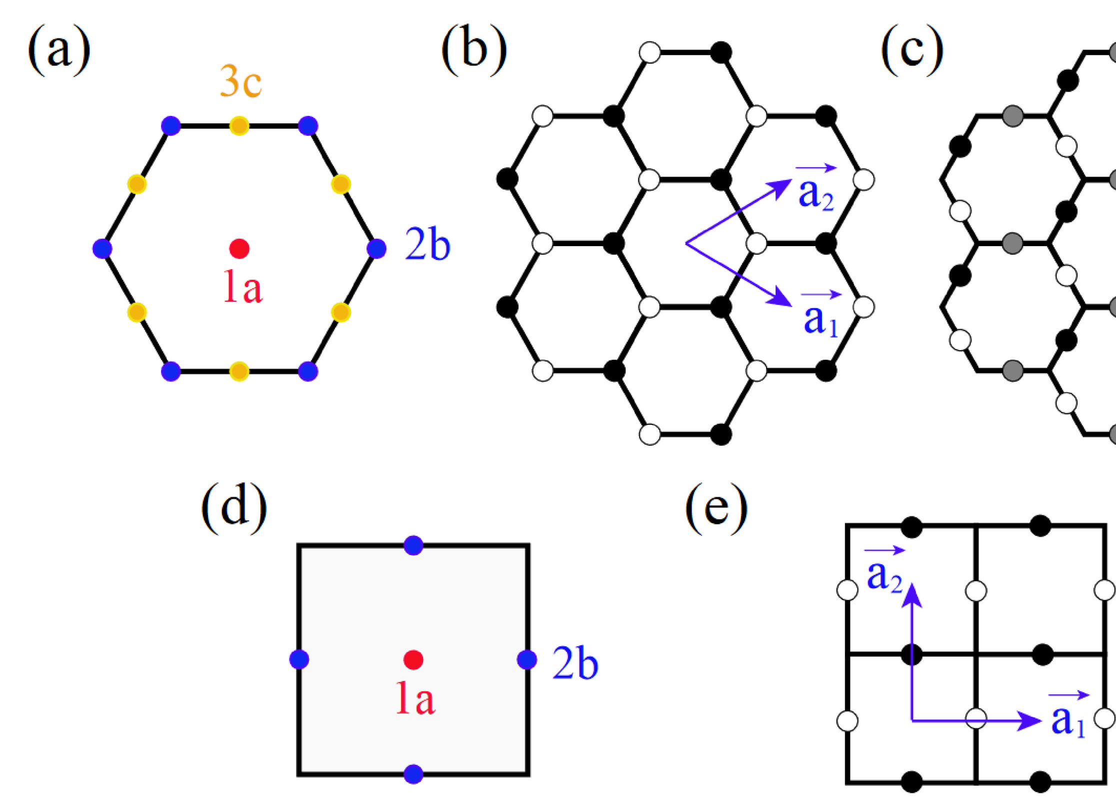
$$\vec{s}\cdot\vec{l}$$

$$p_+\uparrow \Rightarrow \frac{\lambda_{soc}}{2} \qquad p_+\downarrow \Rightarrow -\frac{\lambda_{soc}}{2}$$

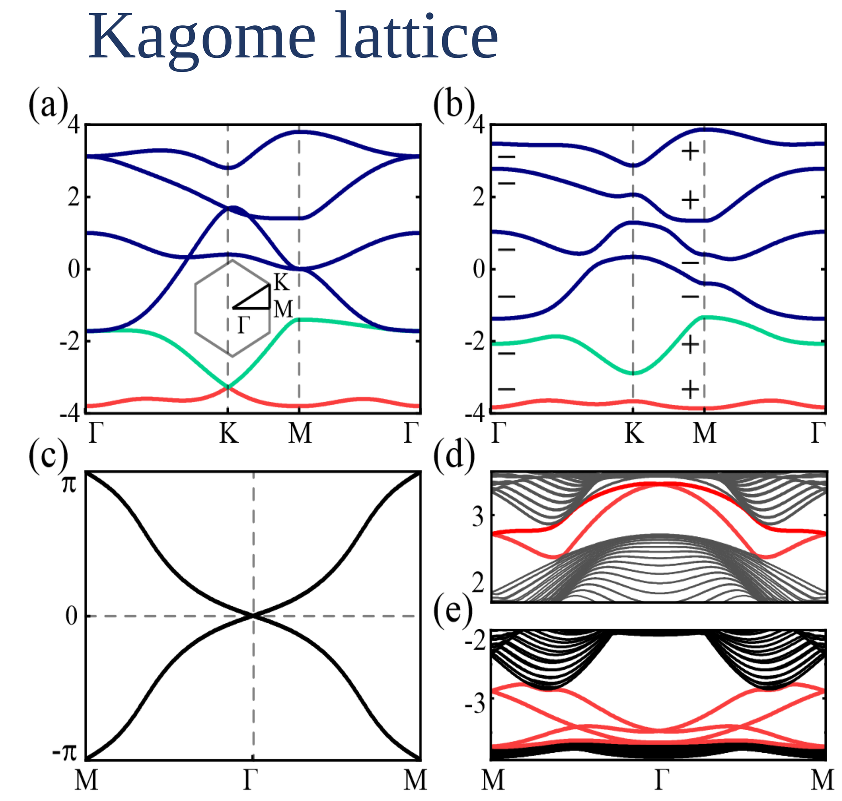
$$p_-\downarrow \Rightarrow \frac{\lambda_{soc}}{2} \qquad p_-\uparrow \Rightarrow -\frac{\lambda_{soc}}{2}$$

$$j_z = \mp\frac{3}{2} \qquad j_z = \mp\frac{1}{2}$$

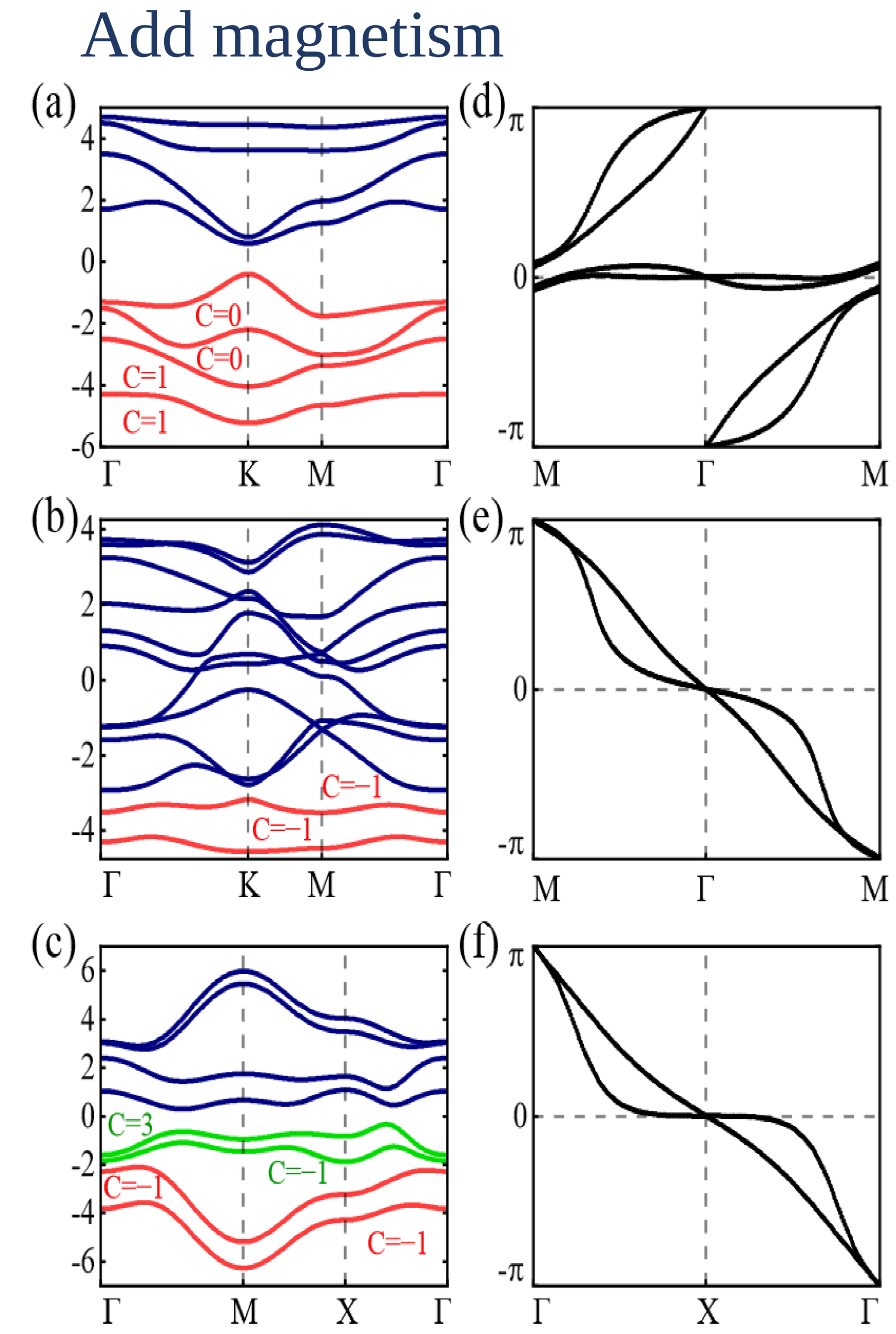
Result



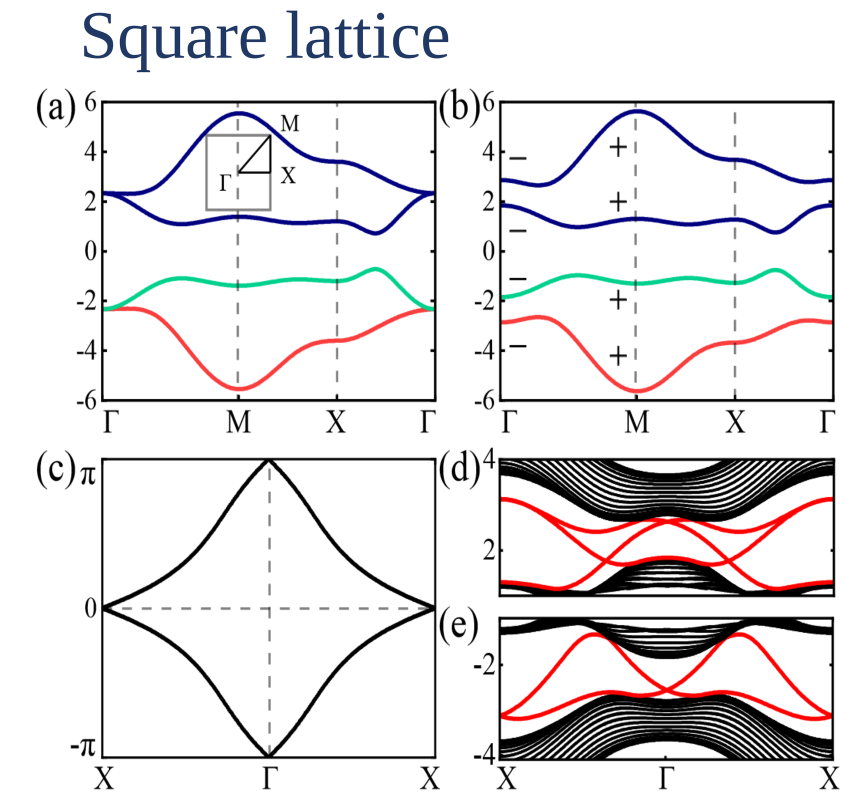
Kagome lattice



Add magnetism



Square lattice



Summary

We extend the large gap QSH state on honeycomb lattice to general 2D lattices, which is based on symmetry analysis and EBRs, though we find such phenomenon in many other lattice, if we further consider the filling, honeycomb lattice is still the best case. On the other hand, it also explain why honeycomb lattice is the first discovered system to hold such mechanism.

Reference

[1] B. Bradlyn, L. Elcoro, J. Cano, M. G. Vergniory,Z. Wang, C. Felser, M. I. Aroyo, and B. A. Bernevig,"Topological quantum chemistry," Nature (London)547,298–305 (2017)

[2] Gu-Feng Zhang, Yi Li,and Congjun Wu, "Honey-comb lattice with multiorbital structure: Topologicaland quantum anomalous hall insulators with large gaps,"Phys. Rev. B90, 075114 (2014)