Monolayer V_2MX_4: A new family of quantum anomalous Hall insulators

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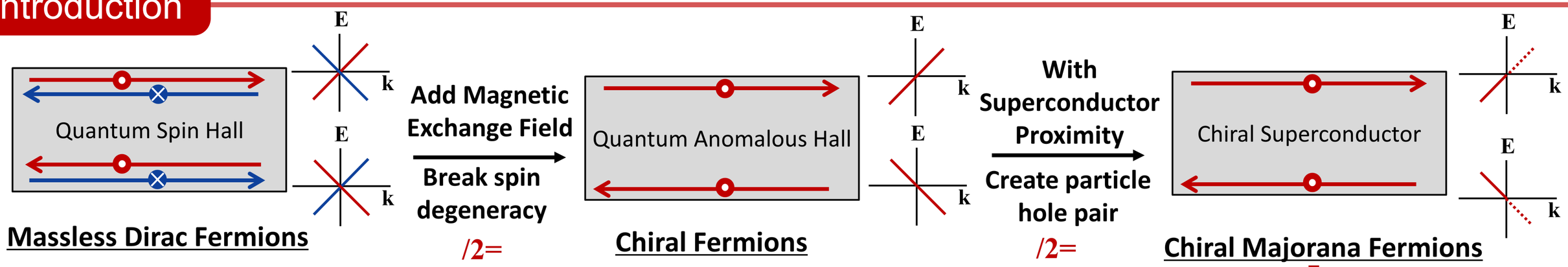
Introduction



How do we achieve this step?

Candidates for quantum computing!

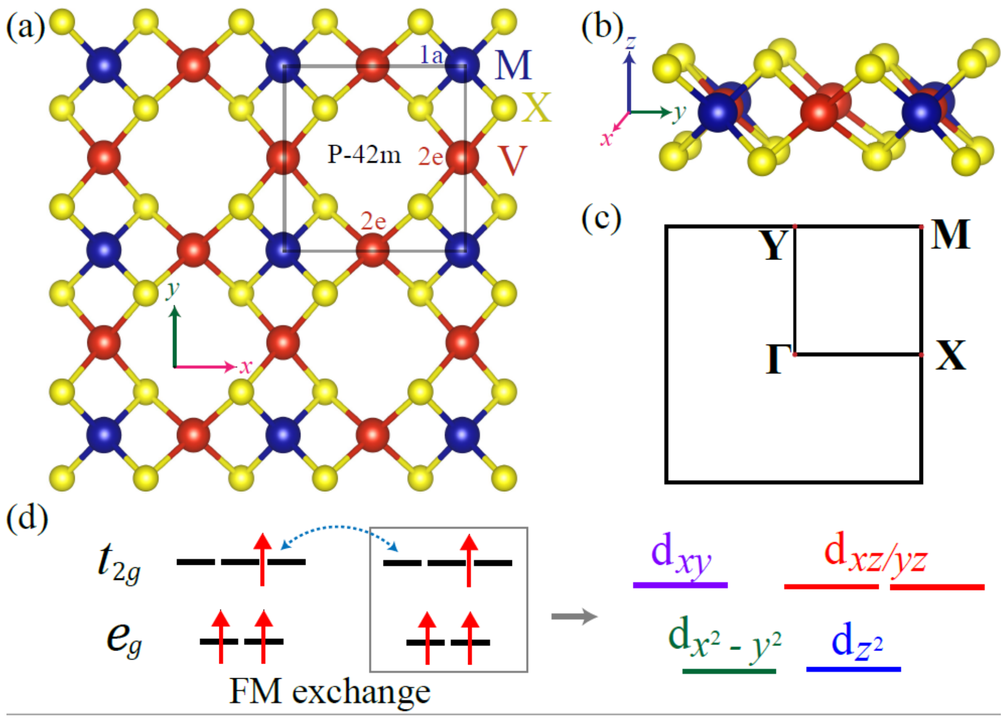
1.Doped **T**opological **I**nsulator(TI)
Mature technology and lots of results
Dirty Always small exchange gap

2.TI/Magnetic Insulator Heterojunction
Cleaner than doping
Technically difficult

3.Intrinsic Magnetic Topological Material
Ideal material for QAH Rare and hard to find
Only MnBi2Te4 realized in experiment

Monolayer V_2MX_4 family: FM ground state, $C = -1$ QAH, large gap

Structure and Magnetic Properties



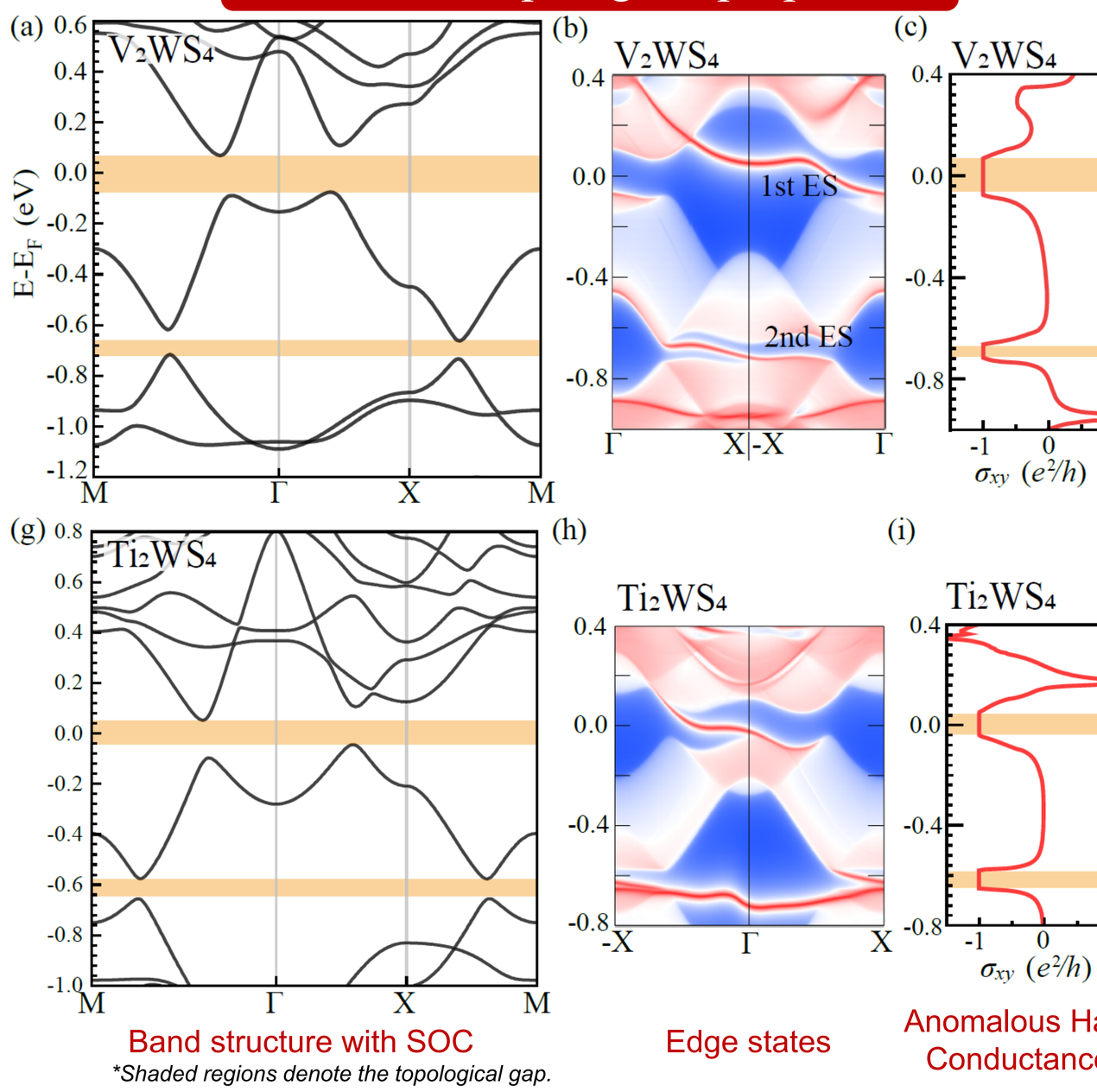
The magnetic ground state of the 2D materials class is FM along z direction
Spin magnetic moment ~2.6 (1.3) μ_B per V (Ti) atom.
FM From :

1. Direct exchange between V(Ti) pairs due to Hund's rule. (1NN)
2. Super-exchange from V(Ti)-M-V(Ti). (2NN)

Materials	a (Å)	T_c (K)	MAE (meV)	E_g (meV)
V_2WS_4	5.74	470	12.1	279
V_2WSe_4	5.82	440	13.2	258
V_2MoS_4	5.72	310	2.0	115
V_2MoSe_4	5.83	284	2.2	70
Ti_2WS_4	5.75	240	10.7	259
Ti_2WSe_4	5.79	210	13.7	275

TABLE I. Lattice constant, MAE per unit cell, Curie temperature T_c from Monte Carlo simulations, and band gap E_g from using the Heyd-Scuseria-Ernzerhof hybrid functional method [51] (Fig. S4).

Bands and topological properties



Band structure with SOC
**Shaded regions denote the topological gap.*

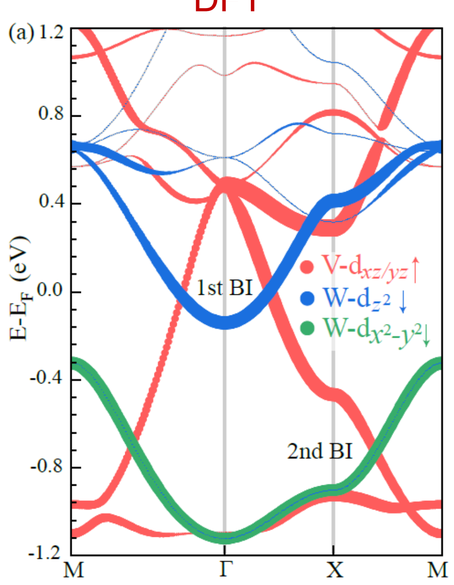
Edge states

Anomalous Hall Conductance

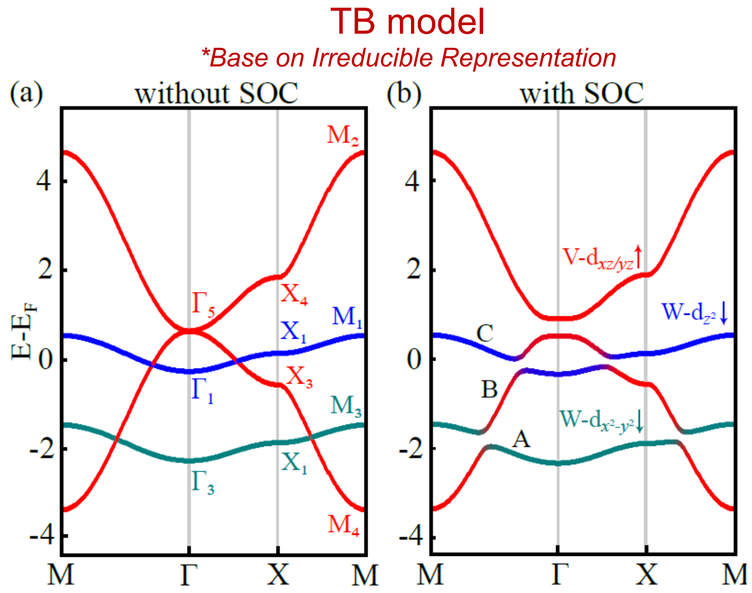
Other materials in TABLE I. have similar results

Origin of Topology

DFT



TB model
**Base on Irreducible Representation*



d −orbitals projection bands structure

1. Spin polarized quadratic band touching of degenerate V(Ti) − $d_{xz/yz}$
2. Band inversion between V(Ti) − $d_{xz/yz}$ and W(Mo) − $d_{z^2}/d_{x^2-y^2}$

Reference

1. arXiv: 2303.14685
(Old version, will be updated soon)

2. arXiv: 2211.08938
Monolayer *ATiX*, another QAH family we predicted.
3. Physics Review Letter.**102**,187001(2009)
QSH → QAH → Chiral Majorana Fermions.
4. Physics Review Letter.**122,** 206401(2019)
Science **23**,eaax8156 (2020) 1st intrinsic QAH MnBi2Te4.