# Coexistance of Quantum Anomalous Hall and Anomalous Valley Hall Effects in Metal-Organic Frameworks

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**Abstract** Metal-organic frameworks(MOFs) constructed with special symmetries are emerging as new type of nontrivial two-dimensional (2D) topological structures [1]. We here design a plane layer MOF $C_6H_3N_3$-Au which captures $C_{3v}$ symmetry, breaking inversion symmetry, and spontaneous magnetic moment induced by N atoms. Using first-principles calculations, we find the spin polarized energy bands exactly exhibit different features in dispersion around the Fermi level, and consequently lead to different topological properties when SOC is taken into consideration: At Γ point in Brillouin zone(BZ) a non-trivial gap opens while in corners of BZ K/K' valley splitting occurs, both collaborate to a novel quantum anomalous Hall (QAH) and anomalous valley Hall effects coexisting system. Phases appearing with contributions from different orbitals of atoms, including $C_{3v}$ symmetry protected energy degeneration at Γ from $p_x/p_y$ orbitals of N(and $d_{xy}/d_{x^2-y^2}$ of Au), and breaking of inversion symmetry leading valley splitting of $p_z$ orbitals from N(and C). Different from previous work about this phenomenon which mainly concentrated on K/K' points through theoretically tuning spin-orbital coupling (SOC)[2], our work demonstrate that QAH effect and valleytronics can be realized separately at different momenta.

## Geometry and electronic structures of $C_6H_3N_3$-Au

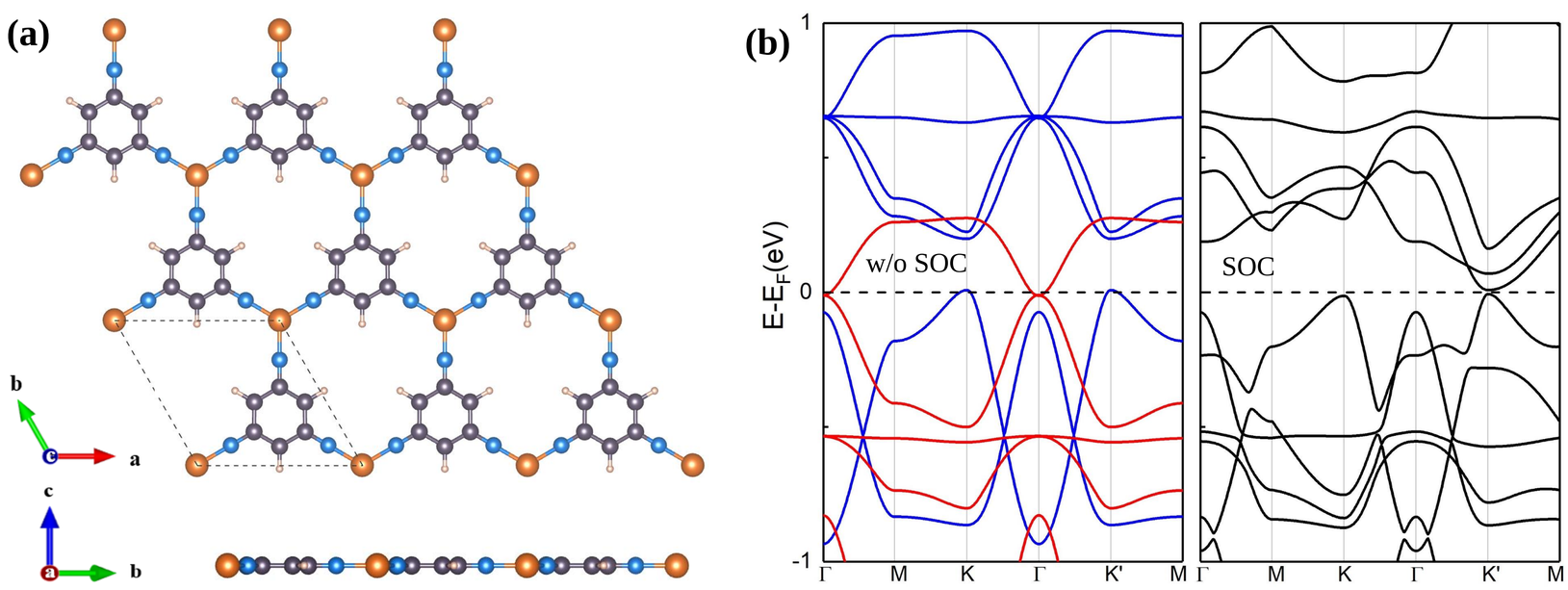


Fig.1 (**a**) The lattice structure of $C_6H_3N_3$-Au with planer triangular lattice that confirms $C_{3v}$ symmetry. N atoms serve as bridges connecting C and Au, and form a nearly hexagonal shape. There is one unpaired electron left for each N which is found to be spin polarized and hence originates spontaneous magnetic momentum large as 3 $\mu_B$ along z direction for a unit cell, a ferromagnetic ordering MOF is obtained. (**b**) Band structures calculated without SOC(left panel) and with SOC(right panel). When SOC is not taken into consideration, on Fermi level, bands of spin up have a degeneration at Γ while of spin down gapped globally. After SOC added, a nontrivial gap is induced at Γ for the spin up subspace, but the two gaps at K and K' points of spin down polarized bands show opposite variations which give rise to a possible valleytronics.

## Orbital projections

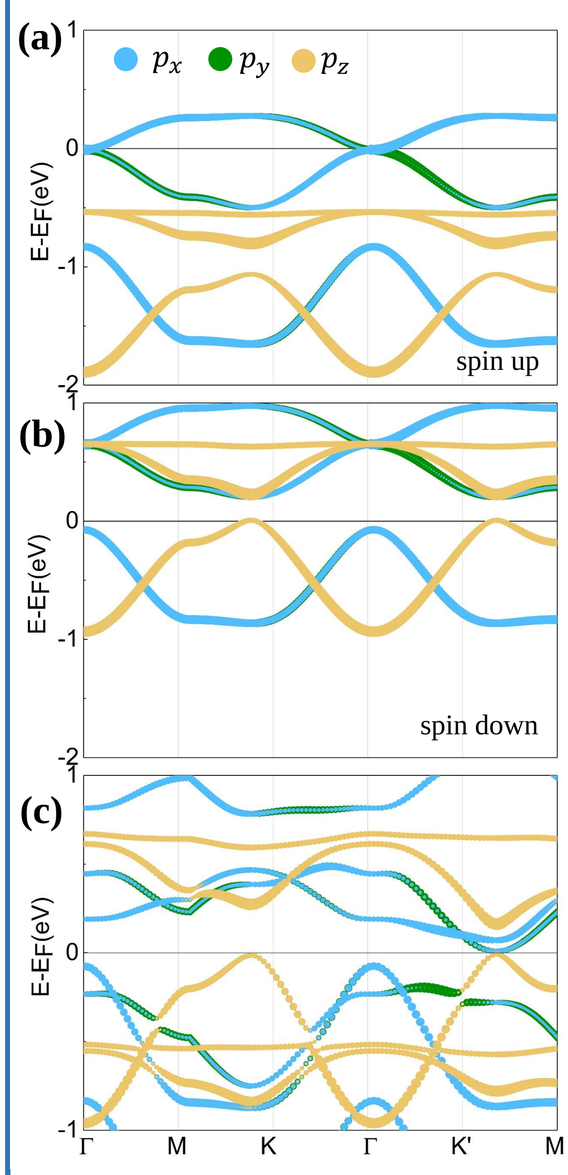


Fig.2 The orbitals $p_x$, $p_y$, and $p_z$ of N element project on energy bands, which can basically represent the symmetry features. Without SOC: (**a**) the degeneration at Γ of spin up bands mainly comes from eigenstates of $C_{3v}$ symmetry $p_x$ and $p_y$, (**b**) the valley gaps around Fermi level are mainly form $p_z$ orbitals. After SOC added, (**c**) band inversions between $p_x/p_y$ with $p_z$ show up around Fermi level and contribute to nontrivial topological properties.

## Valley splitting with SOC tuning

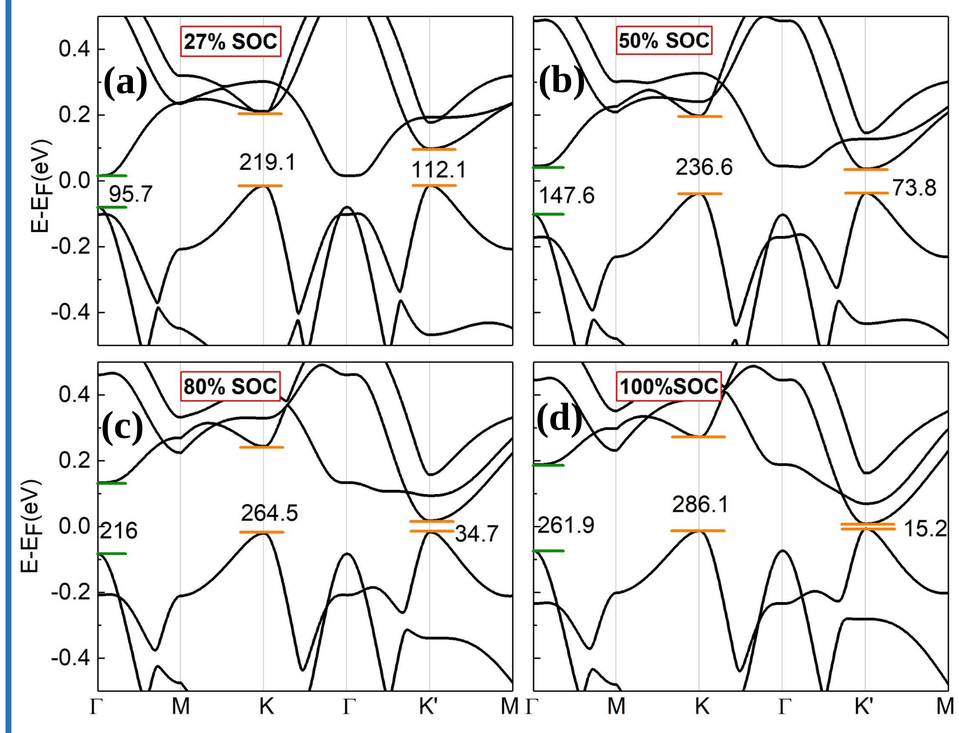


Fig.3 The band gaps variations are measured (in unit meV) under SOC tuning with respect to (**a**) 27%, (**b**) 50%, (**c**) 80%, (**d**) 100%. As SOC becoming stronger, the gap at Γ (green short lines) enlarges; nevertheless the gaps at valleys K and K' (orange short lines) exhibit opposite changings, and the valley splitting is as large as 271.1 meV. A valley polarization current may occurs at K' when electrons of valence bands are excited to conduction bands, once the gap induced by SOC at Γ is topological nontrivial, the metallic edge states will be valley polarized.

## Berry curvatures & edge states

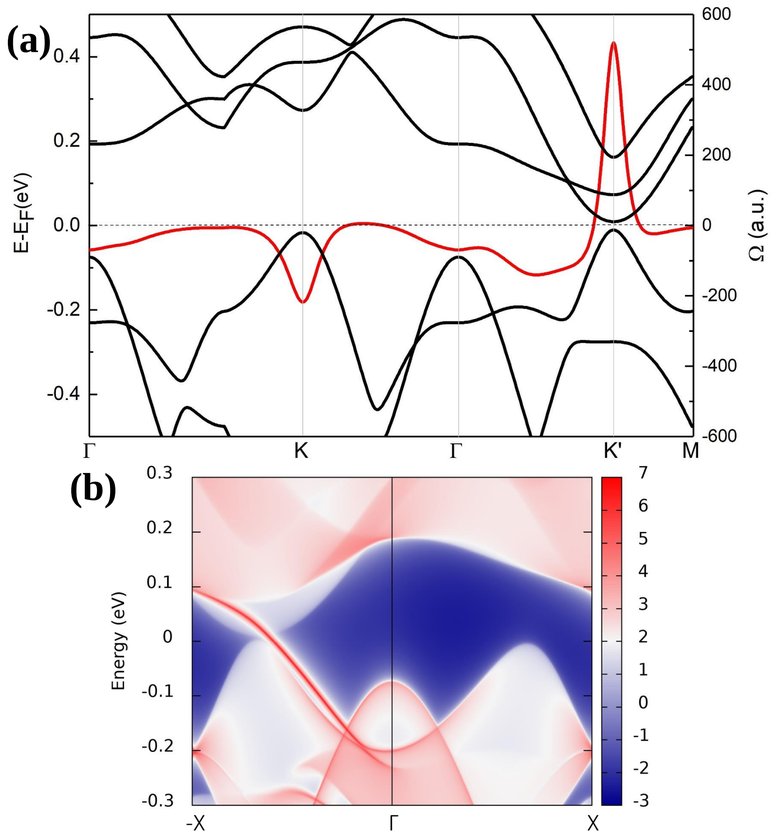


Fig.4 (**a**) The Berry curvatures (red solid line) of valence bands calculated by Wannier interpolation give opposite values at K/K', as well as non-trivial dispersion around Γ, of which the integral over whole BZ (Chern number) is -1. (**b**) Density of boundary states of semi-infinite structure, with metallic edge states connecting top valence band and bottom conduction band at K', convince the QAH and anomalous valley Hall effects coexisting features.

## Conclusions

- A special MOF with $C_{3v}$ symmetry protected QAH and anomalous valley Hall effects is constructed. The SOC induces topological non-trivial band gap opening at Γ point, and band splitting at valleys K/K' is large enough to lead the metallic edge states of QAH effect transferring to the valley.
- Such special edge states here originate from mechanism that quite different from previous theoretical researches, hence it inspires new type designs of MOFs with special symmetries to realize novel topological phases.

**References:** 1. Wang, Z. F. *et al.*, *Phys. Rev. Lett.* **110,** 196801 (2013). 2. Pan, H. *et al.*, *Phys. Rev. Lett.* **112**, 106802 (2014). 3. Xiao, D. *et al.*, *Phys. Rev. Lett.* **99**, 236809 (2007).

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