Diverse quantum anomalous Hall effects with high Chern numbers in buckled honeycomb lattices

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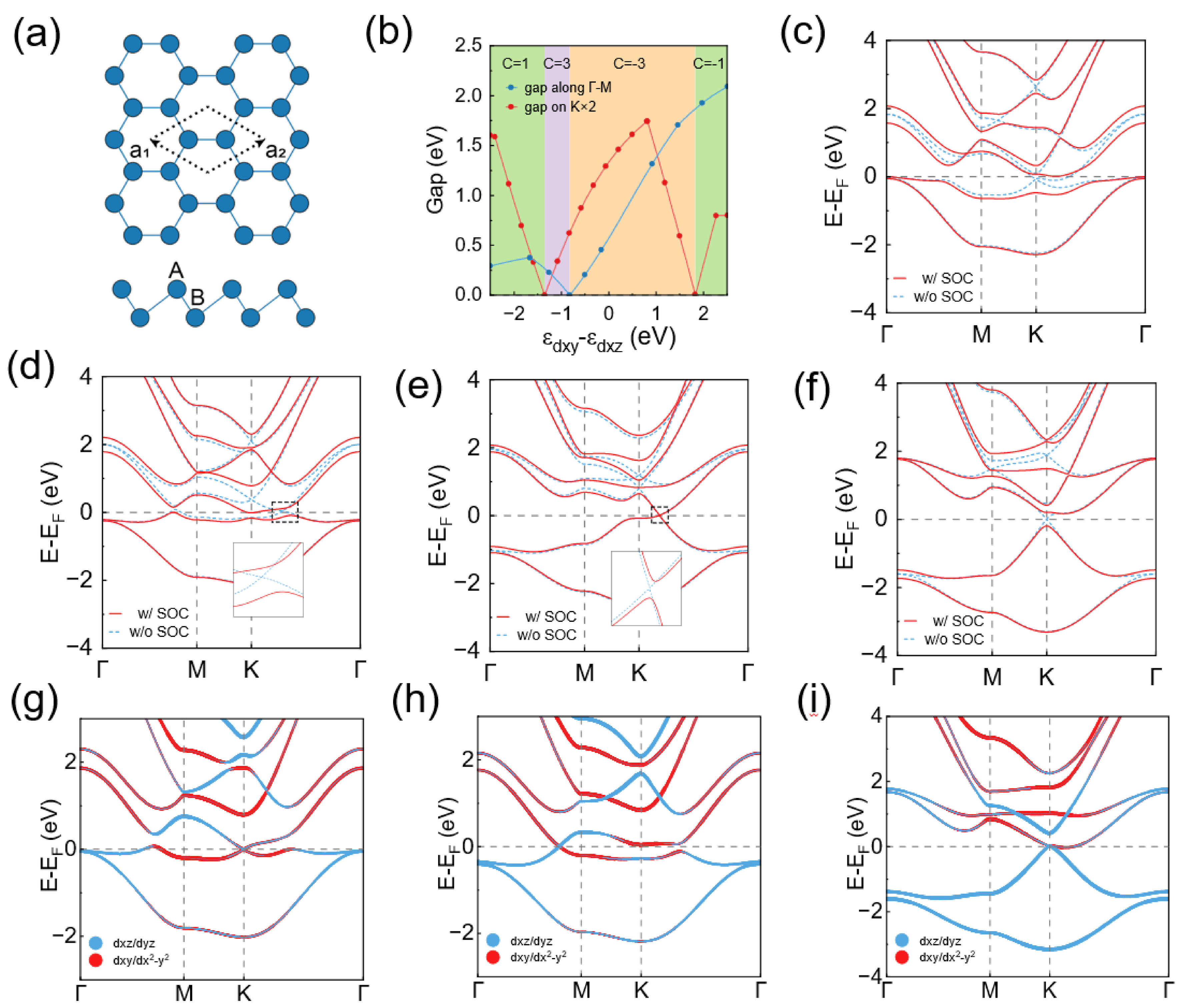
Introduction

The quantum anomalous Hall (QAH) effect has attracted significant attention due to its potential for low-dissipation devices and its connection to various quantum phenomena. However, experimentally realizing the QAH effect with high Chern numbers remains a significant challenge. In this study, based on a four-*d*-orbital tight-binding (TB) model in a buckled honeycomb lattice, we obtain rich QAH effects with the Chern numbers tuned between low values (±1) (LC) and high values (±3) (HC) by varying the difference of the on-site energies between *dxy* (*dx²-y²*) and *dxz* (*dyz*) or adjusting the magnetic orientation to retain specific symmetries.

Various QAH phases from TB model



TB model Hamiltonian:

$$H = H_0 + H_{SOC},$$

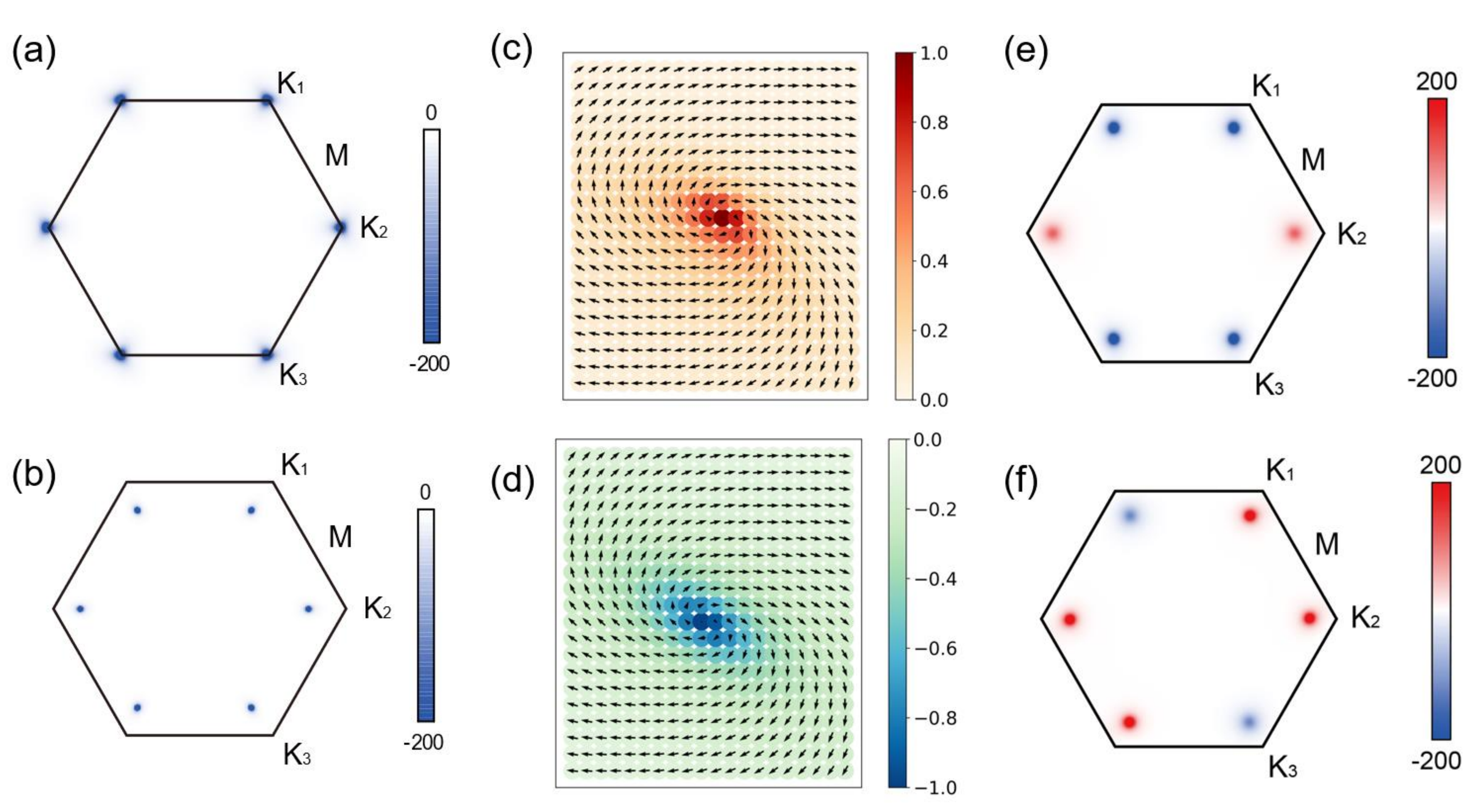
$$H_0 = \sum_i \epsilon_0 c_i^\dagger c_i + \sum_{\langle i,j\rangle} t_1 c_i^\dagger c_j + \sum_{\langle\langle i,j\rangle\rangle} t_2 c_i^\dagger c_j,$$

$$H_{SOC} = i\lambda \sum_i c_i^\dagger s c_i$$

The origin of the HC phase at small on-site energy differences between the two degenerate orbital sets can be understood from the band structure. When bands are formed predominantly by a single degenerate pair (e.g., *dxz/dyz*), band crossings are confined to high-symmetry points, which can only give rise to an LC phase. To realize an HC phase, band crossings must also occur at other locations such as high-symmetry lines, which requires hybridization with additional orbitals. In other words, the HC phase emerges from the interplay between multiple degenerate orbital channels.

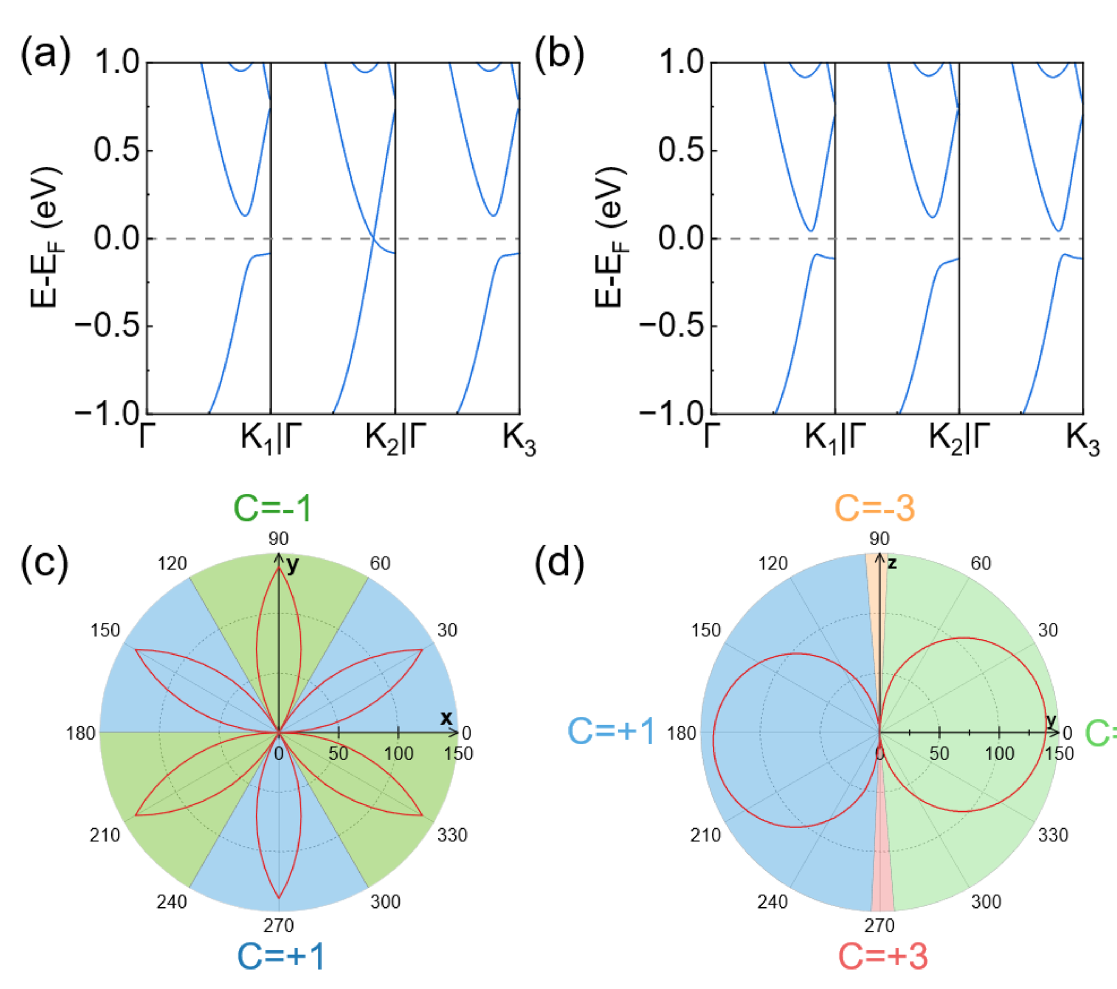
(a) The lattice geometry of buckled honeycomb. (b) Topological phase diagram with on-site energy difference ε_{dxy} - ε_{dxz}, including low Chern and high Chern phases. (c-f) The fitted bands based on the TB model with C=1, 3, -3 and -1 respectively. Blue dashed line and red solid line represents without or with SOC. (g-i) Projected band structures of topological transformation critical state in TB between C = +1 and +3 (g), C = +3 and -3 (h), and C = -3 and -1 (i).

Topological mechanisms



(a, b) The distribution of the Berry curvatures for TB model of C=-1 and C=-3. (c, d) Topological pseudospin texture of C=3 and C=-3 respectively. The color represents the z-direction strength of the arrow. (e, f) The distribution of the Berry curvatures for TB model in the same parameters with C=-3 but magnetization direction in xy plane with φ =90° and 30°.

Tunable Chern numbers



(a, b) Band structure of TB with SOC in the same parameters of C=-3 except for the magnetization along x and y direction, respectively. (c, d) Phase diagram of Chern number as a function of magnetization direction in x-y plane and y-z plane, respectively. The polar radius indicates the value of band gap (in meV).