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Prediction of Coexistence of Anomalous Valley Hall and Quantum Anomalous Hall Effects in Kagome-Honeycomb-Like Lattices

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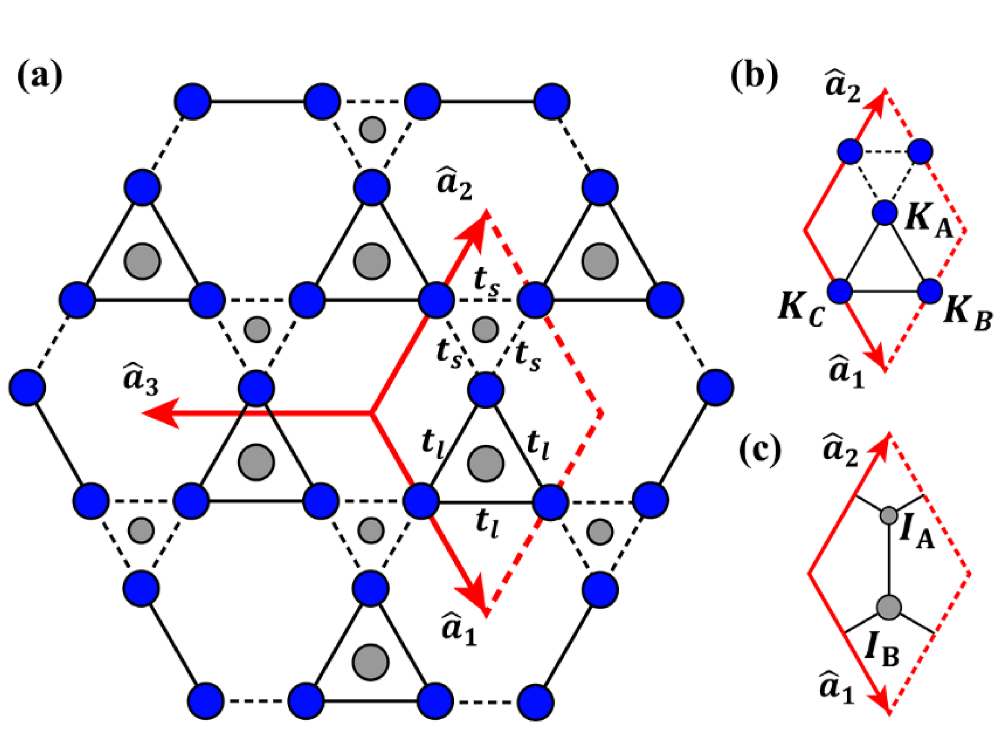
Abstract

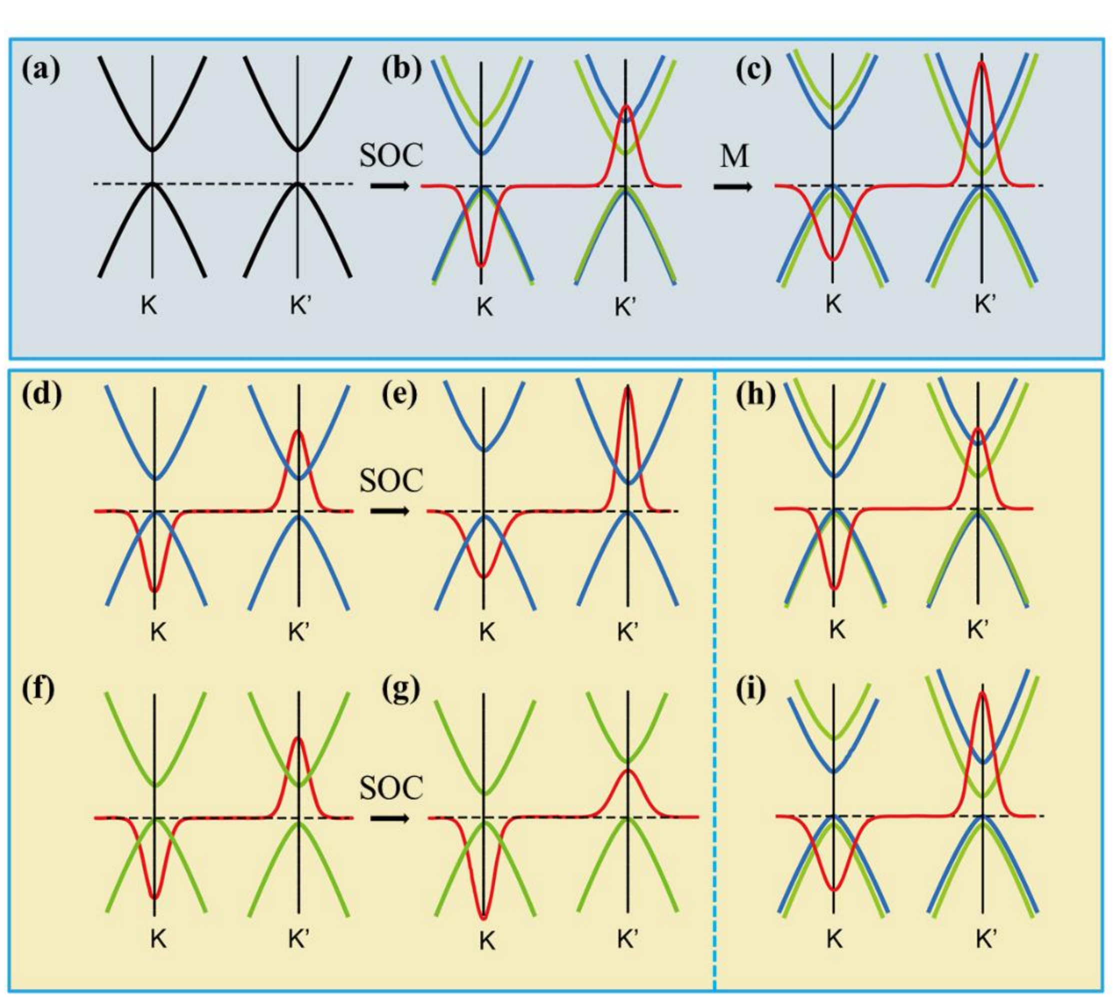
To explore the mechanism of valley degrees of freedom, we employ the kagome-honeycomb-like (KHL) lattice to reveal the evolution of Dirac bands under time-reversal symmetry (TRS), space-inversion symmetry (SIS), and spin-orbital coupling (SOC) effect. Utilizing the composed structure of different lattice features, and based on tight-Binding (TB) model, we illustrate clearly the valley effects in spin subspace in the kagome-featured band structures. The characteristic non-Dirac bands of the honeycomb-featured lattice contribute to the quantum anomalous Hall (QAH). At the different points in Brillouin zone (BZ), the QAH and anomalous valley Hall (AVH) effects are found coexisting in the system with appropriate parameters adopted in the KHL lattice.

Geometry structure of the kagome-honeycomb-like (KHL) lattice



(a) Geometry structure of the kagome-honeycomb-like (KHL) lattice. The corner-sharing triangles describe a kagome-featured lattice. The dashed and solid lines represent different hopping parameters t_s (for the small triangles) and t_l (for the large triangles), respectively. Lattice vectors are labeled by a_1 , a_2, a_3. There are five atoms in each unit cell, and can be separated into a kagome-featured lattice and a honeycomb-featured lattice, as shown in (b) and (c), respectively.

Valleytronics of kagome bands



(a-c) The mechanism of valley effects in previous studies. As with SIS breaking, SOC and exchange interacitons are successively considered for the calculations of the band structures and Berry curvatures (d-i) The mechanism of valley effects in the kagome-featured lattice. The valley degree of freedom independently exist in the each spin subspace. When spin bands overlap, the superposition of Berry curvatures at valleys are determined by unbreaking or breaking of TRS.

Tight-binding model of the KHL lattice

$$H = H_K \oplus H_H$$

$$H_K = H_t + H_{K-soc} + H_M$$

$$H_t = -(t_l c^\dagger_{\mathbf{R}B} c_{\mathbf{R}A} + t_s c^\dagger_{(\mathbf{R}-\mathbf{a}_1)B} c_{\mathbf{R}A} + t_l c^\dagger_{\mathbf{R}c} c_{\mathbf{R}B} + t_s c^\dagger_{(\mathbf{R}-\mathbf{a}_2)C} c_{\mathbf{R}B} + t_l c^\dagger_{\mathbf{R}A} c_{\mathbf{R}C} + t_s c^\dagger_{(\mathbf{R}-\mathbf{a}_3)A} c_{\mathbf{R}C}) + H.c.,$$

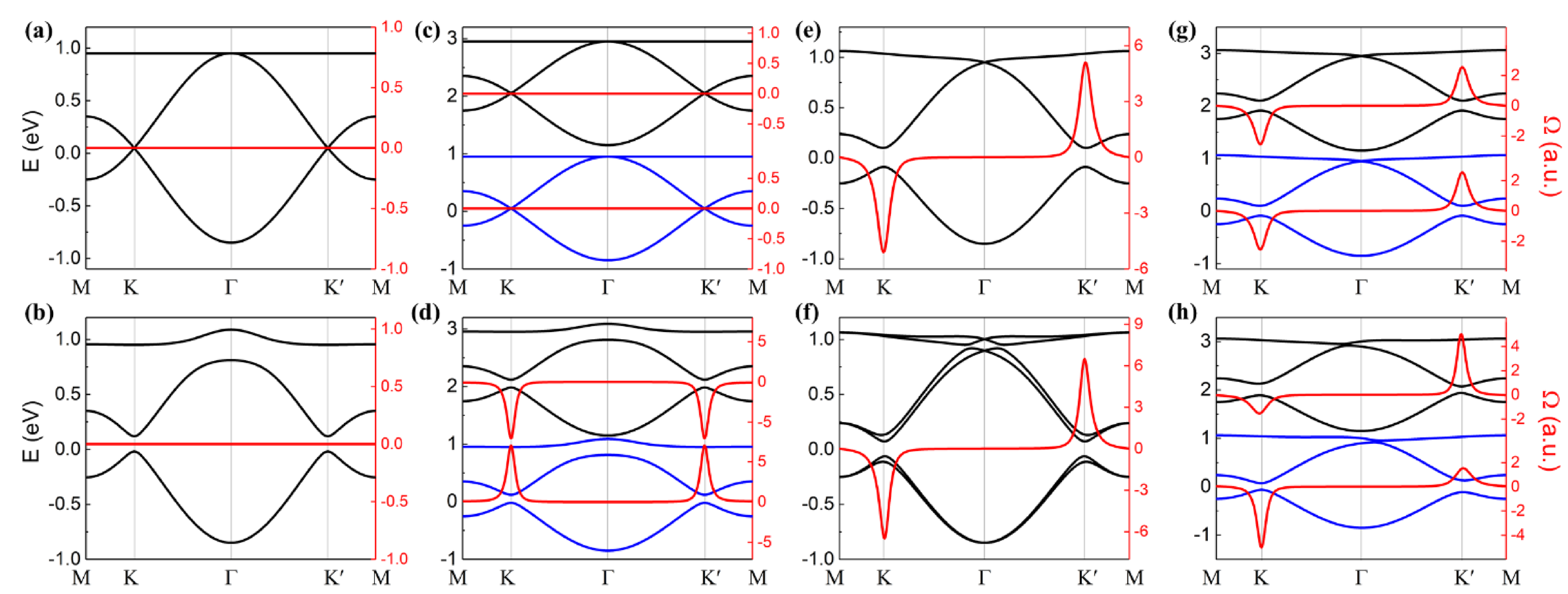
$$H_{K-soc} = \pm 2i(\lambda_l c^\dagger_{\mathbf{RB}} c_{\mathbf{RA}} + \lambda_s c^\dagger_{(\mathbf{R}\text{-}\mathbf{a}_1)B} c_{\mathbf{RA}} + \lambda_l c^\dagger_{\mathbf{RC}} c_{\mathbf{RB}} + \lambda_s c^\dagger_{(\mathbf{R}\text{-}\mathbf{a}_2)C} c_{\mathbf{RB}} + \lambda_l c^\dagger_{\mathbf{RA}} c_{\mathbf{RC}} + \lambda_s c^\dagger_{(\mathbf{R}\text{-}\mathbf{a}_3)A} c_{\mathbf{RC}}) + H.c.,$$

$$H_M = M_K \sum_{\alpha\sigma} c^\dagger_{\alpha\sigma} \mathbf{s}_z c_{\alpha\sigma}$$

$$H_H = -t_{nn} \sum_{<ij>,\sigma} d^\dagger_{i\sigma} d_{j\sigma} - t_{nnn} \sum_{<<ii>>,\sigma} d^\dagger_{i\sigma} d_{i\sigma} + (\lambda_p \oplus \lambda_d) \vec{L} \cdot \vec{S} + M_H \sum_{i\sigma} d^\dagger_{i\sigma} \mathbf{s}_z d_{i\sigma}$$

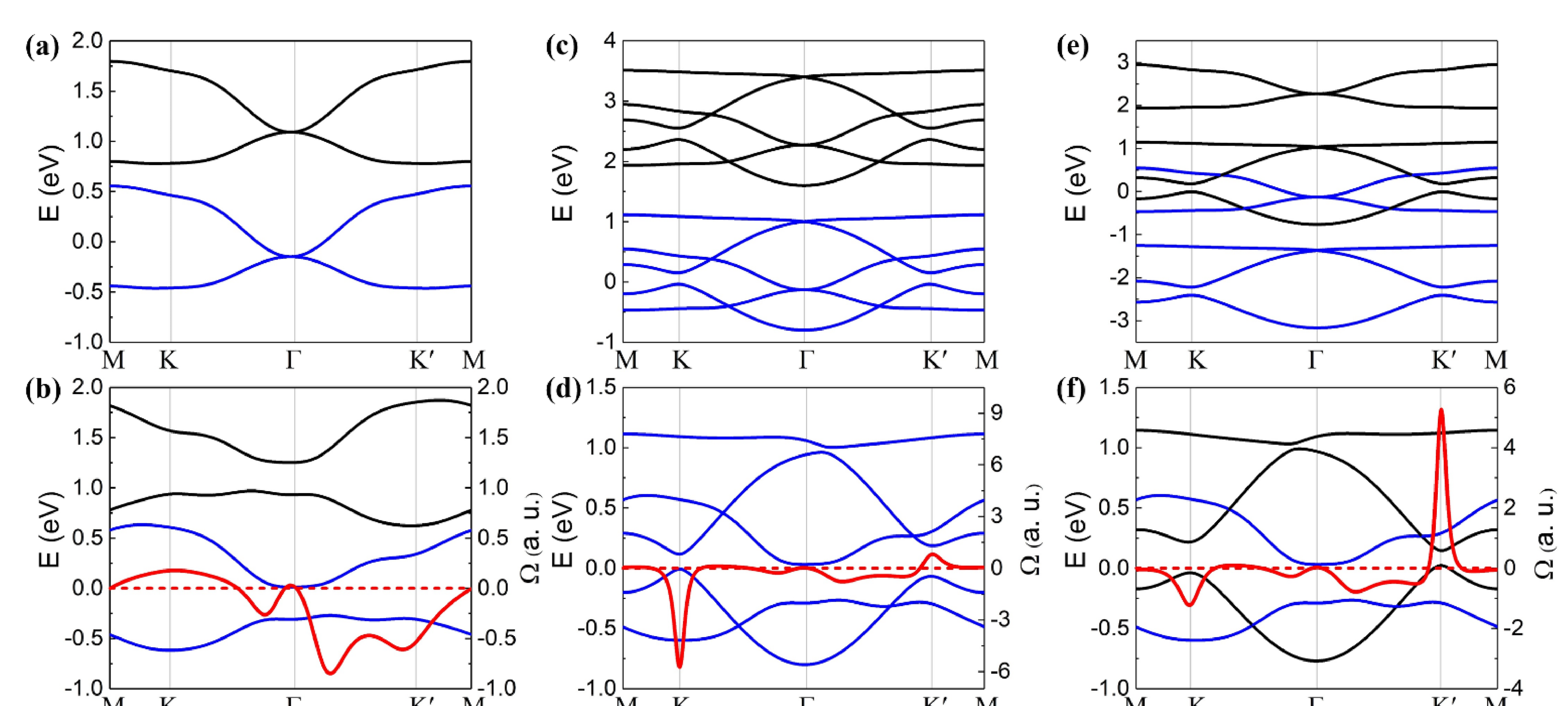
We consider only p_z orbitals on K_A, K_B, K_C, and d_{xy}/d_{x2-y2}, p_x/p_y orbitals on I_A, I_B. In this way, according to the orthogonality, there is no hopping term between the orbital in the z-direction and the orbitals in the x-y plane in a planar structure without buckling. Thus, the band structures of the kagome-feature and honeycomb-feature can be analyzed separately.

The results of kagome-feature model



The parameters of the system are tuned appropriately with (a-b) both TRS and SIS, (c-d) SIS and broken TRS, (e-f) TRS and broken SIS, (g-h) both broken TRS and SIS. The upon and bottom panels are distinguished by without and with SOC, respectively.

The results of honeycomb-feature model and composite states of QAH and AVH effects



(a-b) Results of the TB model of the hexagonal-featured lattice. The NN hopping parameters and NNN hopping parameters are tuned to make the degeneracy localized at Γ point. (c-f) The composite states of QAH and AVH effects in KHL lattice, with appropriate TB parameters. The blue and black bands represent different spins and the red curves are for the Berry curvatures.

Conclusions

- The valleytronics of the kagome-feature lattice are explored based on a TB model of the KHL lattice. The QAH effect is easily tuned in the honeycomb-feature bands.
- Novel coexistence states of QAH and AVH effects occur when the characteristic bands are tuned properly.

References: 1. A. Bolens and N. Nagaosa, Physical Review B 99 (2019). 2. X. Guo, Z. Liu, B. Liu, Q. Li, and Z. Wang, Nano Lett 20, 7606 (2020).

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