Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


Supplemental Material for

# Engineering topological states in two-dimensional honeycomb lattice

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**Tight-binding (TB) model analysis based on $d_{xz,yz}$ orbitals**

The 2 × 2 matrix elements without considering spin-orbit coupling (SOC) based on $d_{xz,yz}$ orbitals are expressed as

$$
\begin{aligned}
&H_0 = \begin{vmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{vmatrix}, \\
&h_{11} = \varepsilon + 2t_{dd\delta}\cos\sqrt{3}k_y + (\frac{3}{2}t_{dd\pi} + \frac{1}{2}t_{dd\delta})\left[\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right)\right], \\
&h_{22} = \varepsilon + 2V_{dd\pi}\cos\sqrt{3}k_y + (\frac{1}{2}t_{dd\pi} + \frac{3}{2}t_{dd\delta})\left[\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right)\right], \\
&h_{12} = \frac{\sqrt{3}}{2}(t_{dd\pi} - t_{dd\delta})\left[\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) - \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right)\right], \\
&h_{21} = h_{12}.
\end{aligned}
\tag{1}
$$

Here, $\varepsilon$ denotes on-site energy, and $t_{dd\sigma}$, $t_{dd\delta}$, and $t_{dd\pi}$ represent hopping parameters. The on-site SOC term is written as

$$
H_{SOC} = \lambda_{SOC}\begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}, \tag{2}
$$

The electronic band structure of the TB model without including SOC is given in Fig. S3, showing that linear Dirac and non-Dirac bands locate around the K/K' and Γ points point, respectively. Here, the parameters are set to $\varepsilon$ = 0.0 eV, $t_{dd\pi}$ = 0.06 eV, and $t_{dd\delta}$ = -0.06 eV. After considering SOC ($\lambda_{SOC}$ = 0. 02 eV), a global band gap is opened, as seen in Fig. 3(b). Detailed Berry curvature and Chern number calculations confirm that the band gap is topologically trivial, which is the same as that of the two-band TB model based on $d_{x^2-y^2,xy}$ orbitals.

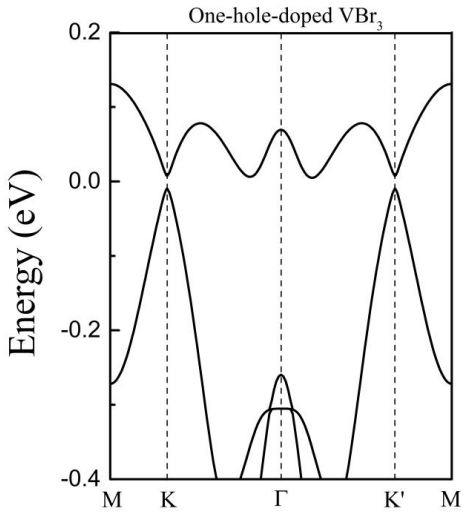


Fig. S1 The electronic band structure of one-hole-doped $VBr_3$ monolayer with including spin-orbit coupling (SOC), where the Fermi level is tuned into the band gap.

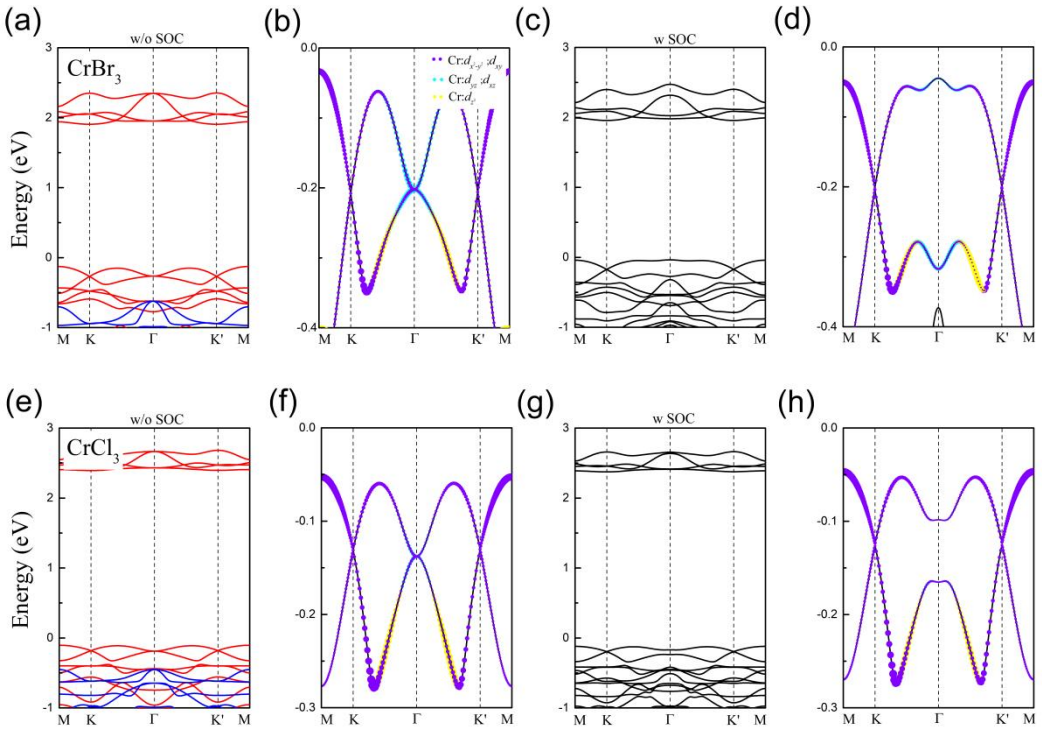


Fig. S2 (a) The electronic band structure of ferromagnetic $CrBr_3$ monolayer without SOC, where red and blue lines represent spin-up and spin-down channels, respectively. (b) Magnified valence bands near Fermi level. Here, the projected bands of Cr are also given. (d,e) The same as (b,c) with considering SOC. Here, the projected bands of Cr are also given. (e-h) The same as (a-d) for $CrCl_3$ monolayer. The Fermi levels are set to zero.

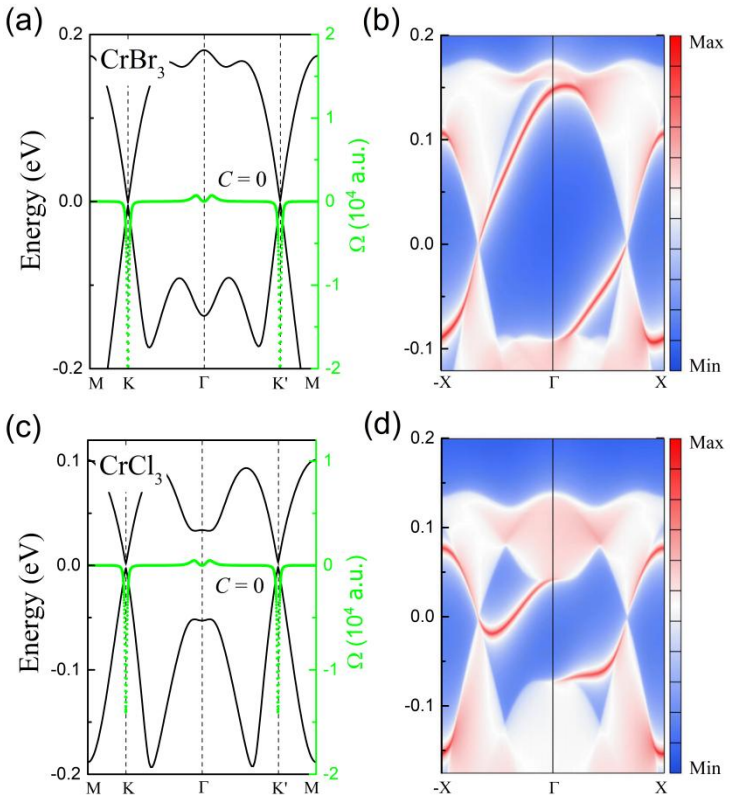


Fig. S3 (a) Green dashed lines represent the calculated 1D Berry curvature distribution along the high-symmetry path. (b) The corresponding edge state. (c,d) The same as (a,b) for $CrCl_3$ monolayer. Here, the Fermi levels are tuned into the global band gaps. The calculated Chern number ($C$) is 0 for each system.

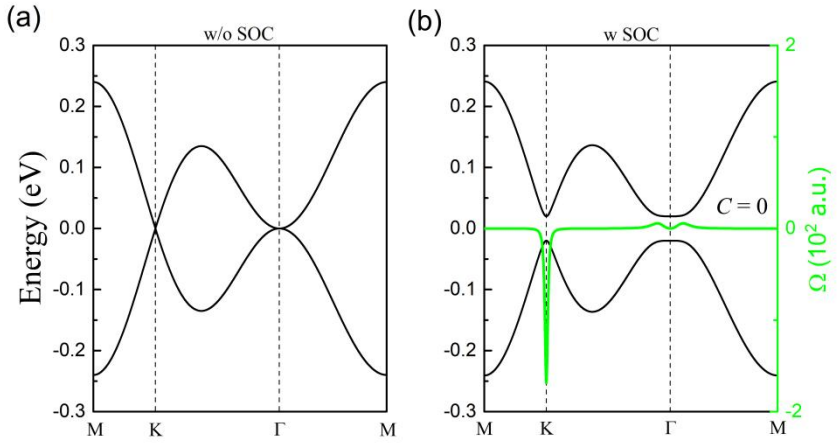


Fig. S4 Band structures obtained from two-band tight-binding (TB) model without (a) and with (b) considering SOC based on $d_{xz,yz}$ orbitals. The green dashed lines in (b) denote 1D Berry curvature distribution.

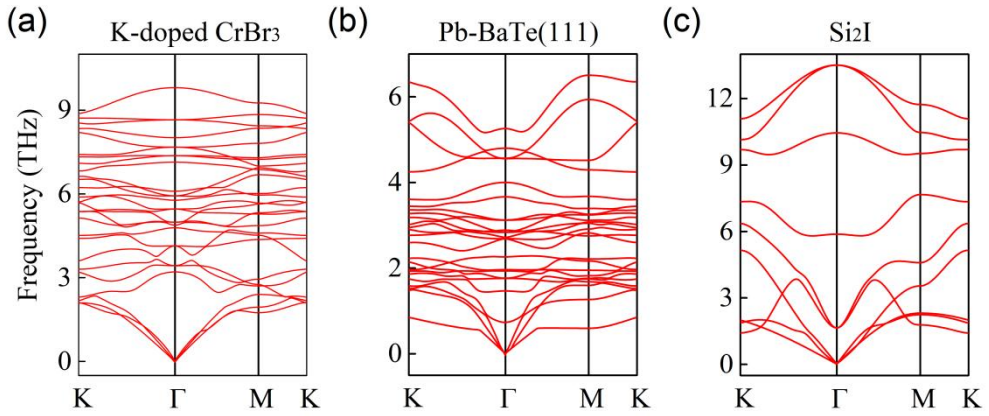


Fig. R5. Calculated phonon spectrum of K-doped $CrBr_3$ (a), Pb/BaTe(111) (b), and $Si_2I$ (c), respectively.