Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information for "Quantum Layer Spin Hall effect in sliding antiferromagnetic bilayers"

Yuping Tian, Chao-Bo Wang, Bing-Yuan Zhang, Xiangru Kong*, and Wei-Jiang Gong*
College of Sciences, Northeastern University, Shenyang 110819, China
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I. SUPPLEMENTARY FIGURES

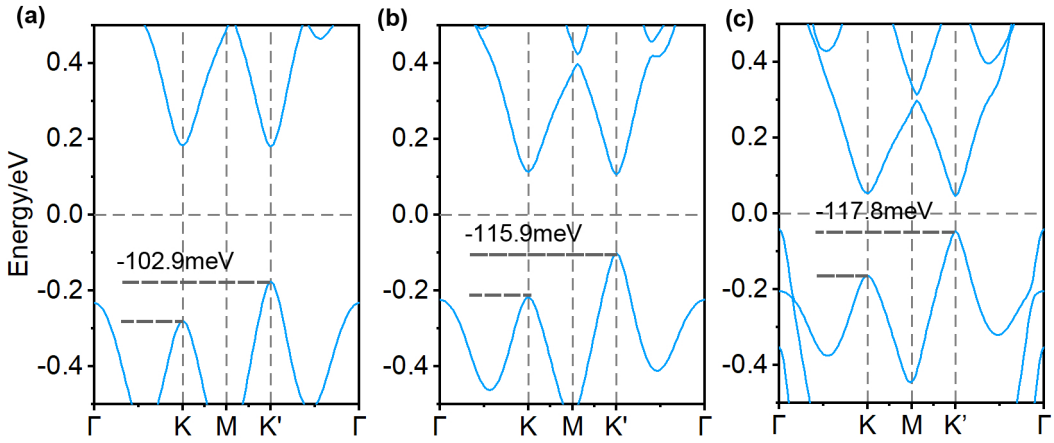

FIG. S1: The band structure of monolayer (a) $FeCl_2$, (b) $FeBr_2$ and (c) FeI_2.

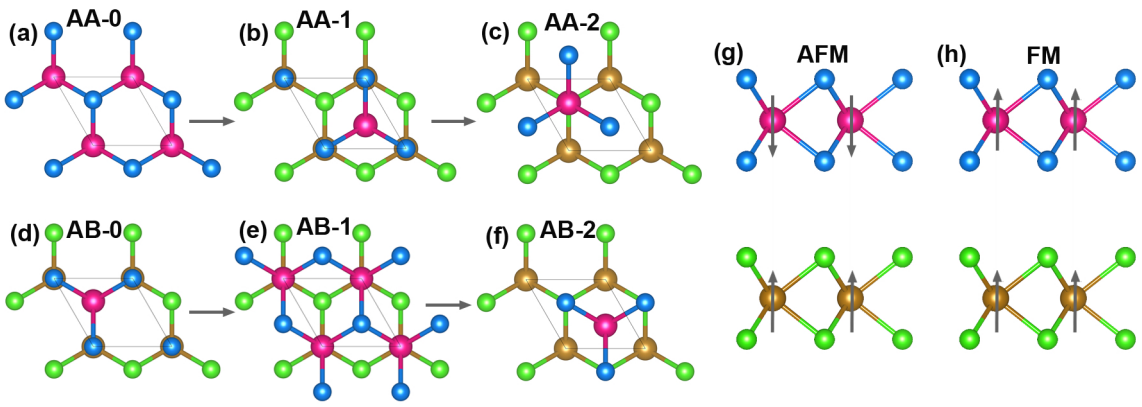

FIG. S2: The geometry structures of (a) AA-0, (b) AA-1, (c) AA-2, (d) AB-0, (e) AB-1 and (f) AB-2 stacking bilayer FeX_2. The (g) AFM and (h) FM magnetic ground states of bilayer FeX_2.

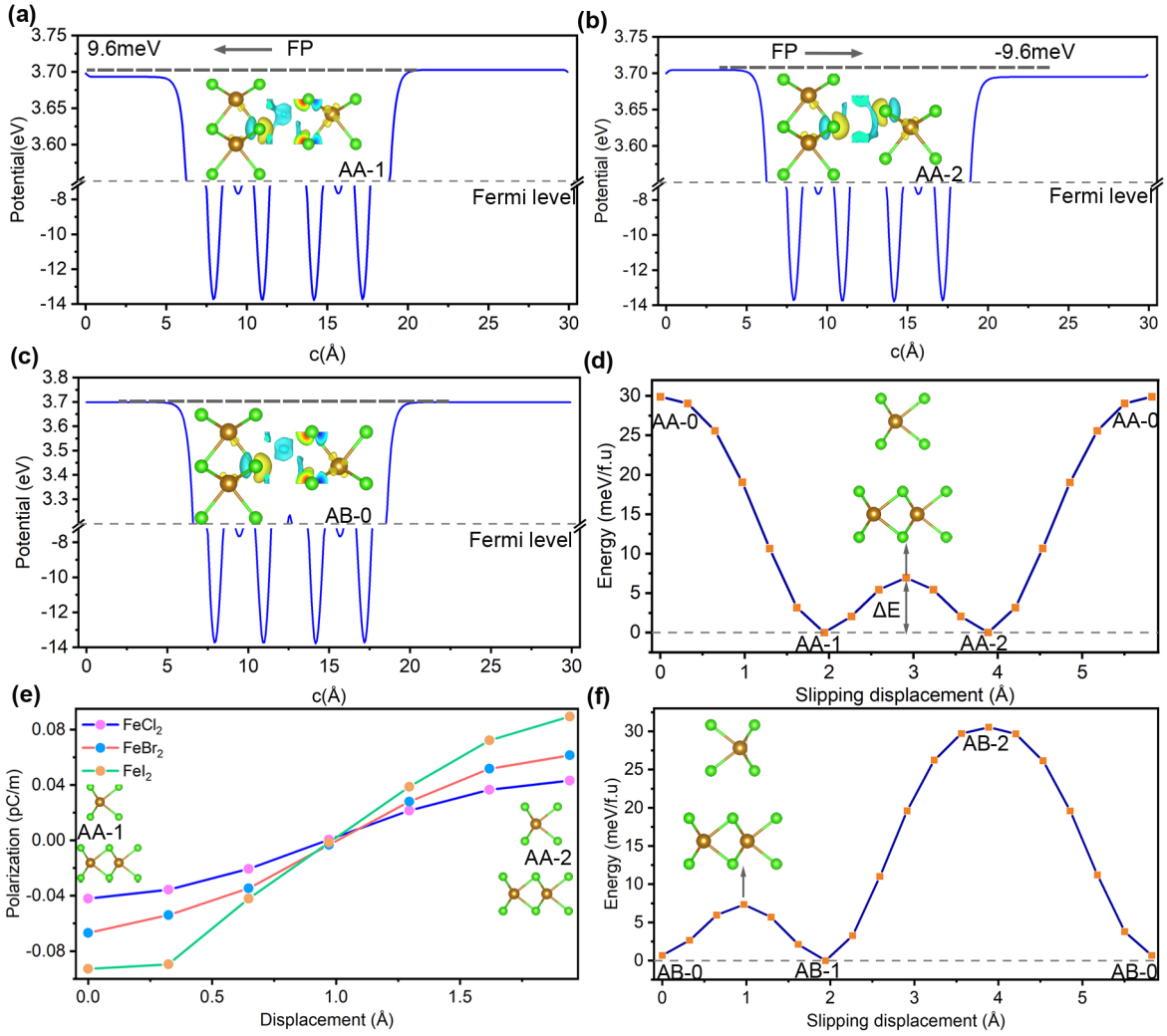

FIG. S3: Plane averaged electrostatic potential of (a) AA-1, (b) AA-2 and (c) AB-0 stacking bilayer $FeCl_2$ along the c direction. Insets describe the corresponding stacking structure and differential charge density diagram. The yellow and cyan area represents the accumulation and depletion of electrons, respectively. (e) The dependence of FP from AA-1 to AA-2 on the slipping displacement. Slipping energy barrier between upper and lower layers of (d) AA and (f) AB stacking bilayer $FeCl_2$.

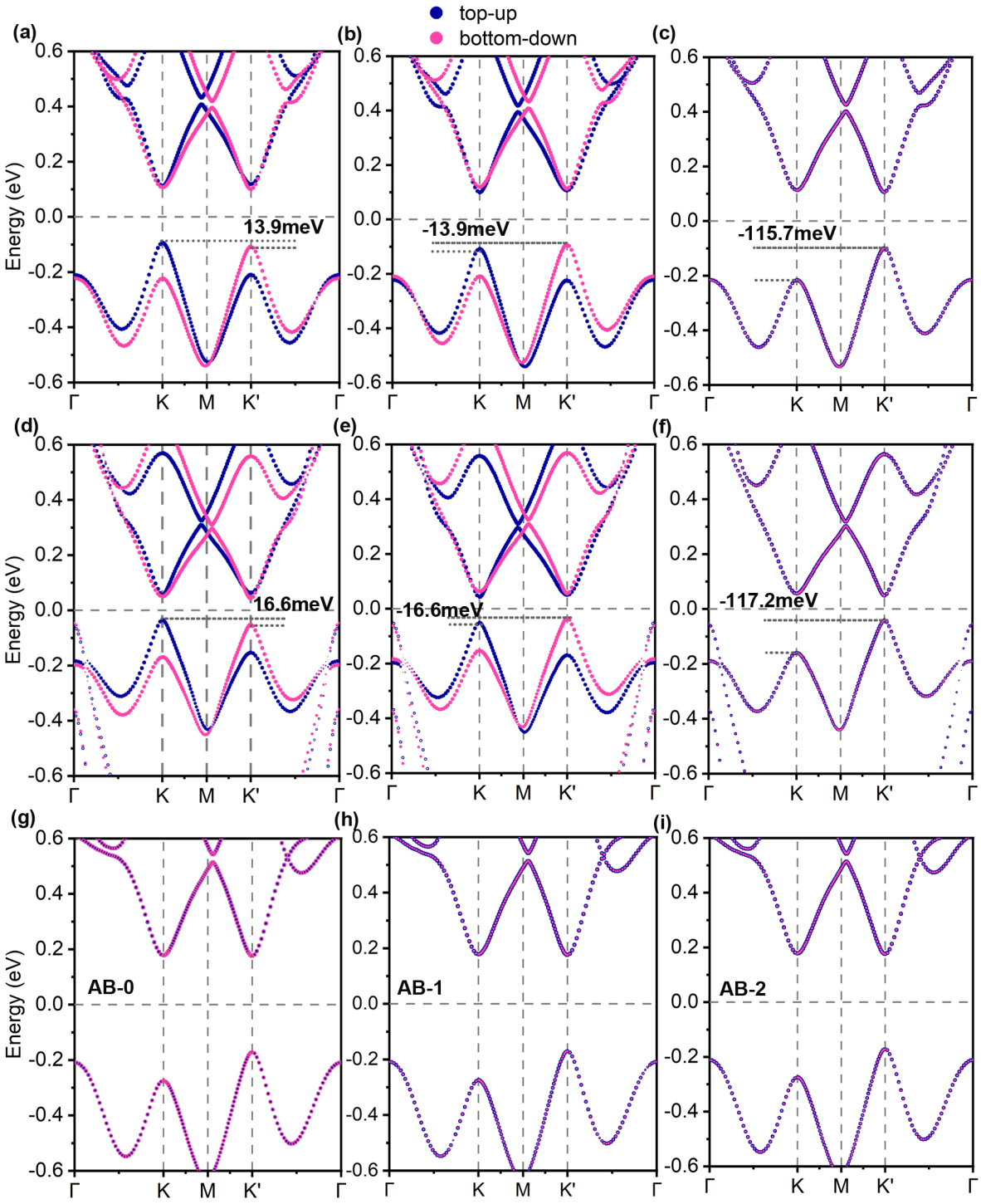

FIG. S4: The band structures under SOC effect of (a) AA-1 (b) AA-2 (c) AB-1 stacking bilayer $FeBr_2$, (d) AA-1 (e) AA-2 (f) AB-1 stacking bilayer FeI_2, and (g) AB-0 (h) AB-1 (i) AB-2 stacking bilayer $FeCl_2$, respectively.

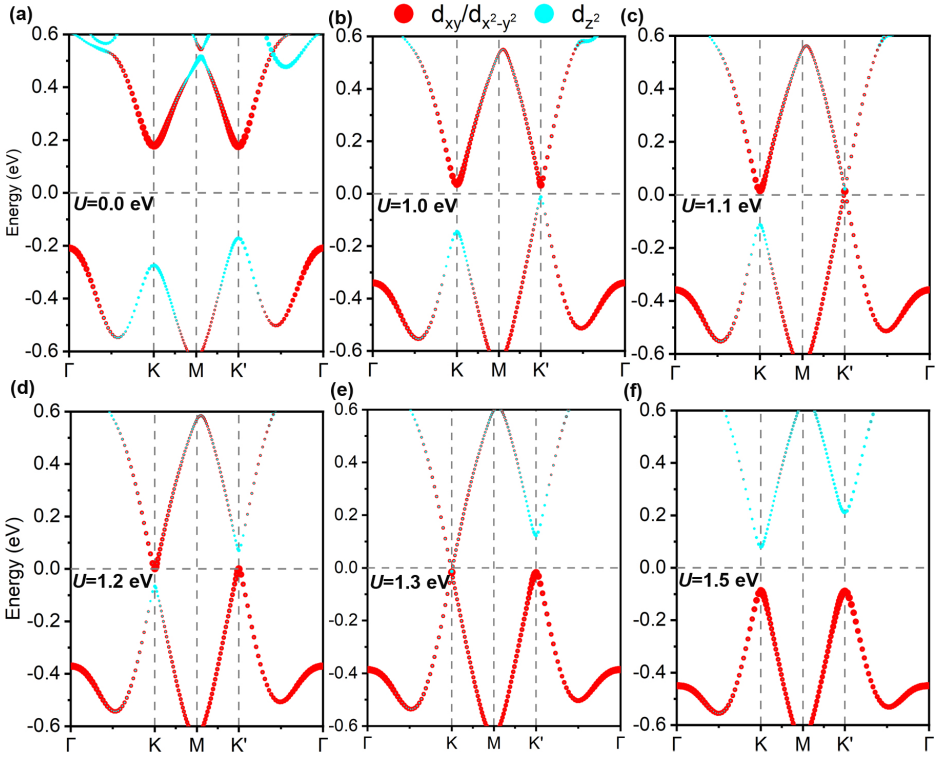

FIG. S5: The band structure of AB-1 stacking bilayer $FeCl_2$ calculated at (a) $U = 0$ eV, (b) $U = 1.0$ eV, (c) $U = 1.1$ eV, (d) $U = 1.2$ eV, (e) $U = 1.3$ eV, and (f) $U = 1.5$ eV, respectively. The cyan and red dots represents Fe-$d_{x^2-y^2}$ /d_{xy} and Fe-d_{z^2} orbitals, respectively.

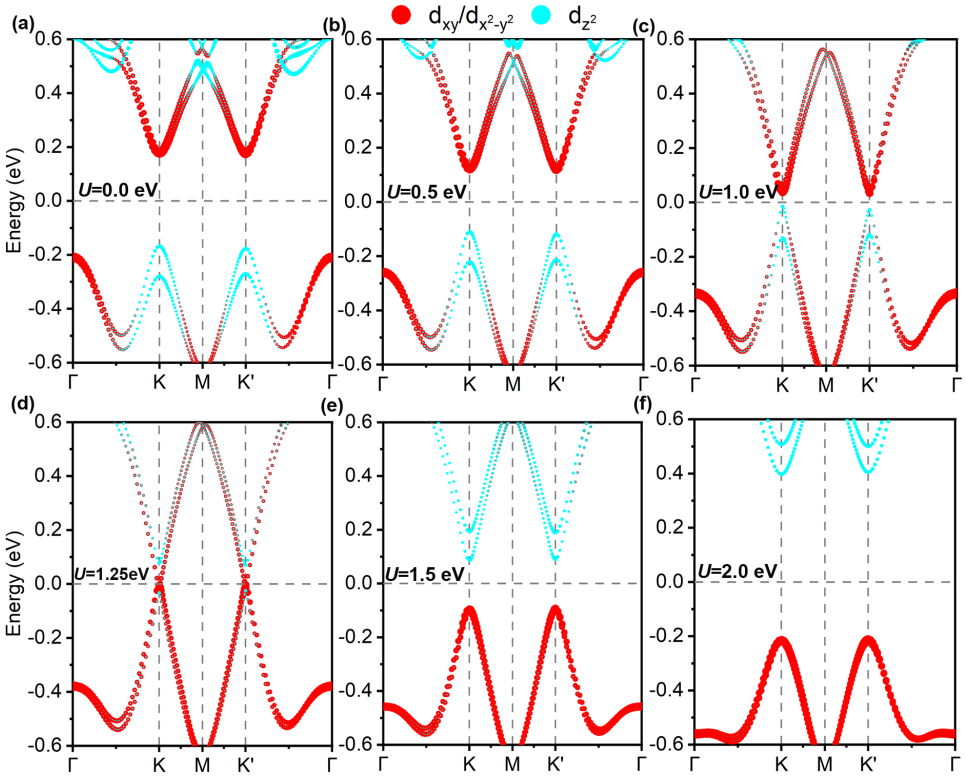

FIG. S6: The band structure of AA-1 stacking bilayer $FeCl_2$ calculated at (a) $U = 0$ eV, (b) $U = 0.5$ eV, (c) $U = 1$ eV, (d) $U = 1.25$ eV, (e) $U = 1.5$ eV, and (f) $U = 2$ eV, respectively. The cyan and red dots represents Fe-$d_{x^2-y^2}$ /d_{xy} and Fe-d_{z^2} orbitals, respectively.

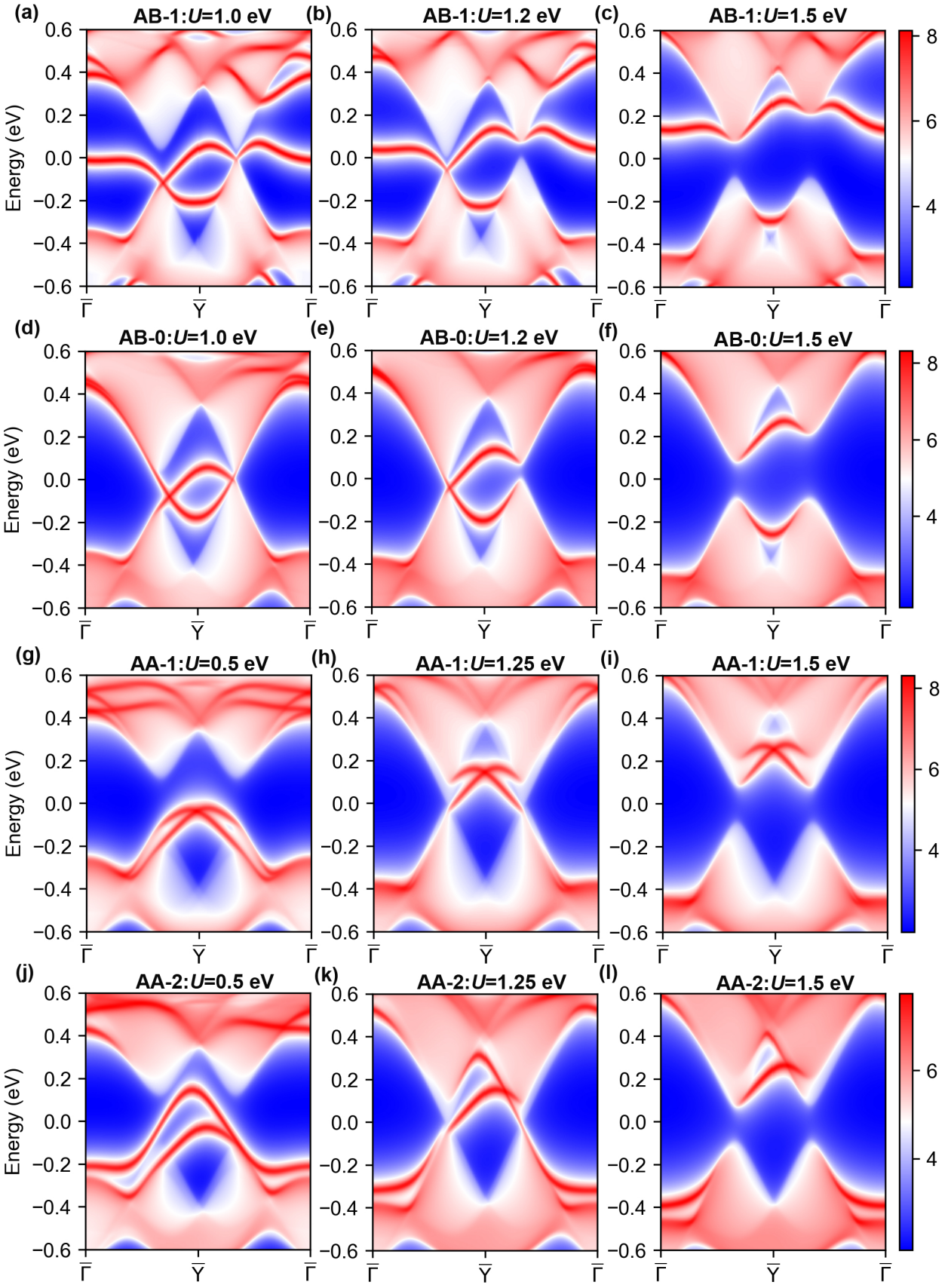

FIG. S7: Topological left edge states of AB-1, AB-0, AA-1 and AA-2 stacking bilayer $FeCl_2$ along the (100) direction calculated at different correlation strengths.

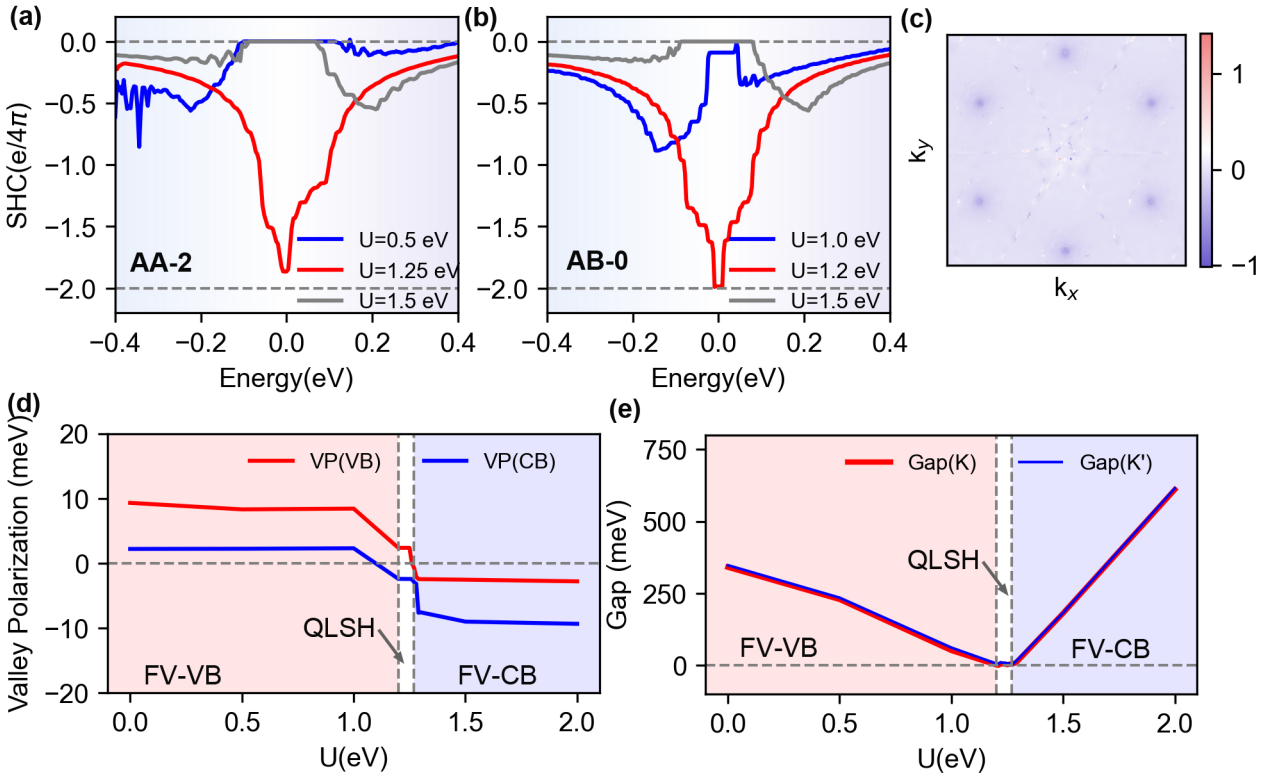

FIG. S8: The SHC of (a) AA-2 and (b) AB-0 structure under different values of U. (c) SHC of AA-1 stacking systems in a slice of the BZ calculated at $U = 1.25$ eV. (d) and (e) show the variation of valley polarization and band gap at K and K' points of AA-1 structures with U-values.

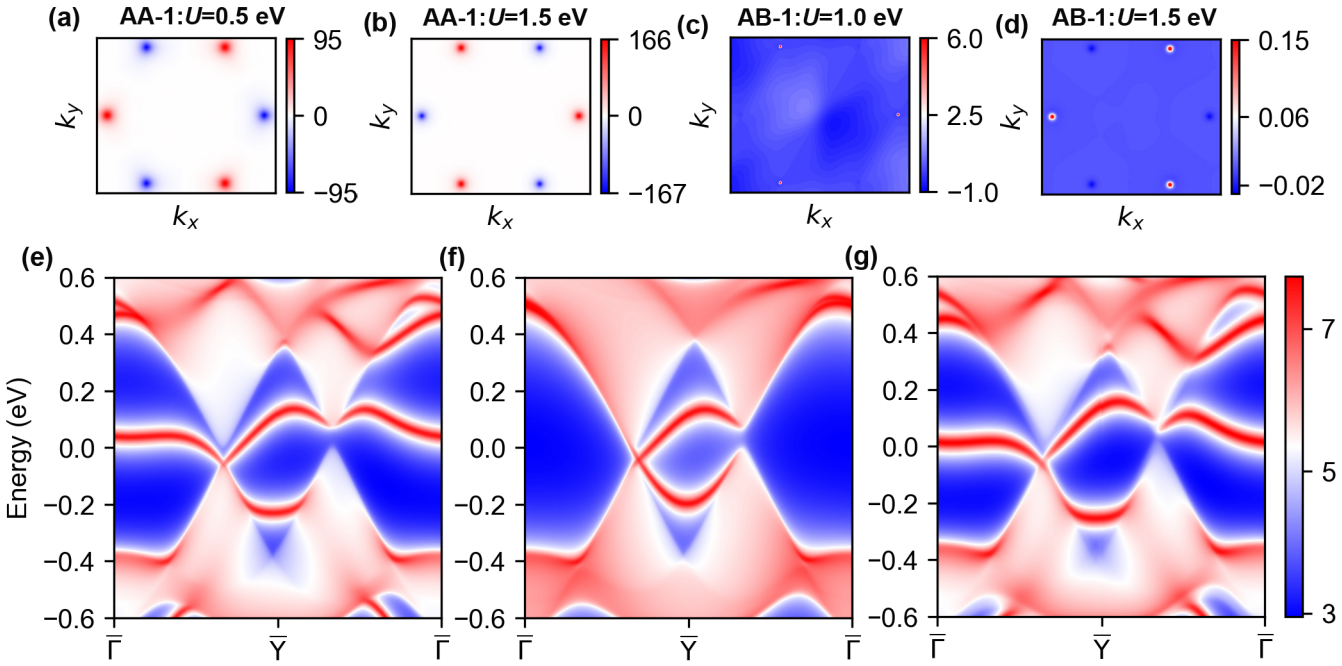

FIG. S9: The Berry curvature of AA-1 stacking bilayer $FeCl_2$ at (a) $U = 0.5$ eV and (b) $U = 1.5$ eV. The Berry curvature of AB-1 stacking bilayer $FeCl_2$ at (c) $U = 1.0$ eV and (d) $U = 1.5$ eV. (e) Topological right edge states of AB-1 stacking bilayer $FeCl_2$ along the (010) direction calculated at $U = 1.2$ eV. (f) Topological right edge states of AB-0 stacking bilayer $FeCl_2$ along the (100) direction calculated at $U = 1.2$ eV. (g) Topological left edge states of AB-1 stacking bilayer $FeCl_2$ along the (100) direction calculated at $U = 1.2$ eV under the external electrical field E = 0.05 V/Å.

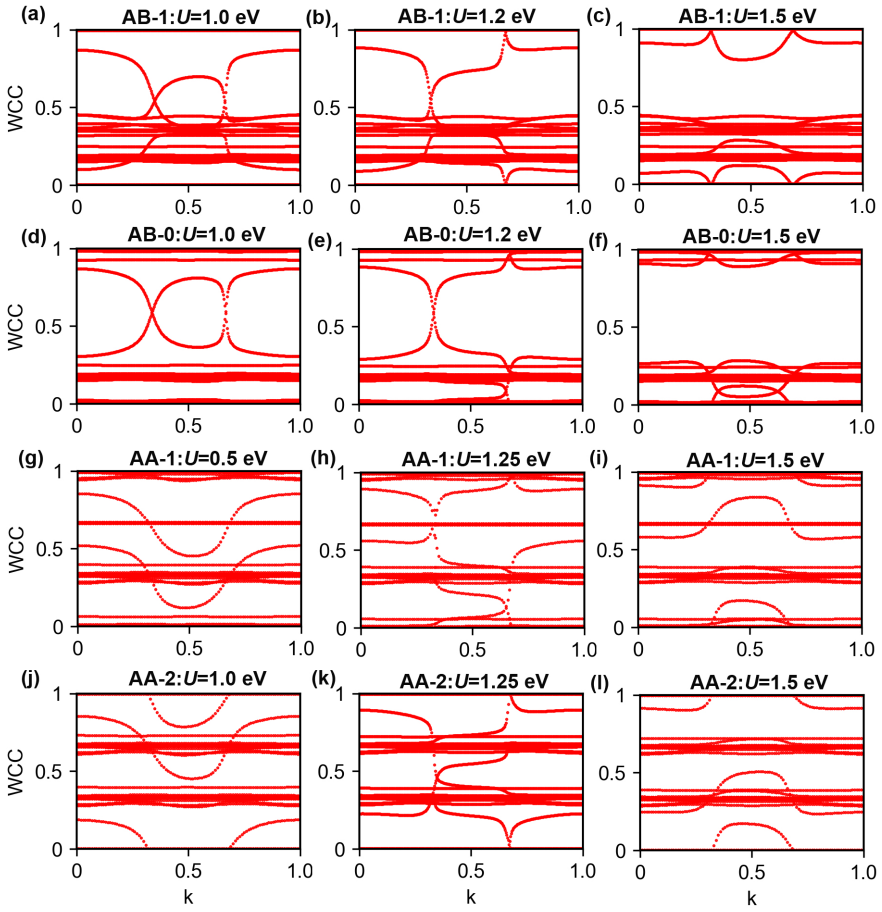

FIG. S10: The Wannier charge center (WCC) of AB-1, AB-0, AA-1 and AA-2 stacking bilayer $FeCl_2$ under different correlation strengths.

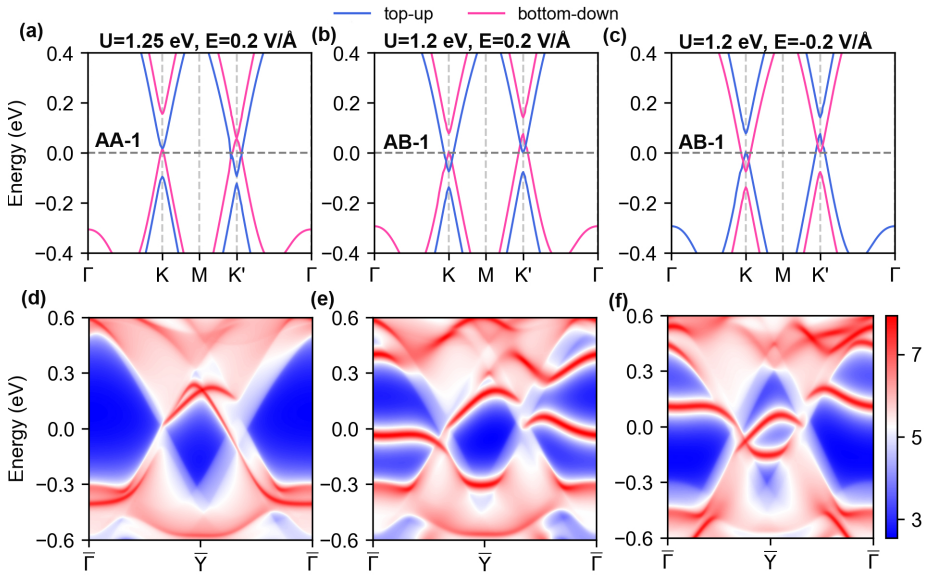

FIG. S11: (a) The spin-polarized band structure and (d) topological left edge states along the (100) direction of AA-1 stacking bilayer $FeCl_2$ at $U = 1.25$ eV under the external electrical field E = 0.2V/Å. (b) The spin-polarized band structure and (e) topological left edge states along the (100) direction of AB-1 stacking bilayer $FeCl_2$ at $U = 1.2$ eV under the external electrical field E = 0.2V/Å. (c) The spin-polarized band structure and (f) topological left edge states along the (100) direction of AA-1 stacking bilayer $FeCl_2$ at $U = 1.2$ eV under the external electrical field E = -0.2V/Å.