

Supplemental Materials for “Electronic-correlation induced sign-reversible Berry phase and Quantum anomalous valley Hall effect in Janus monolayer OsClBr”

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The purpose of this Supplemental Material is to provide additional information by means of some figures.

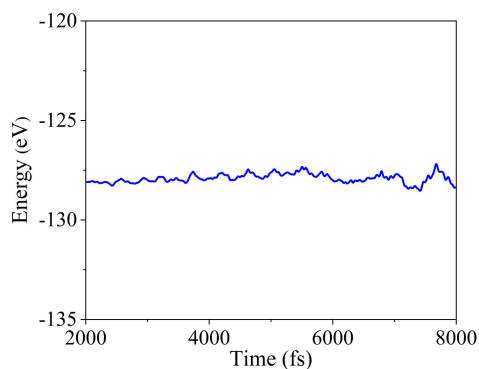


Fig. S1 The AIMD simulation of OsClBr at 300 K.

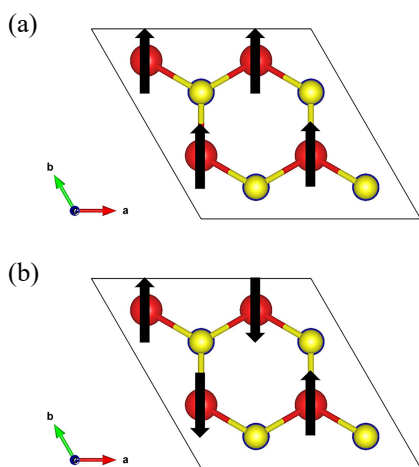


Fig. S2 The considered magnetic configurations of OsClBr: panel (a) is for FM configuration, and panel (b) is for AFM configuration. The black arrows represent the direction of the magnetic moments.

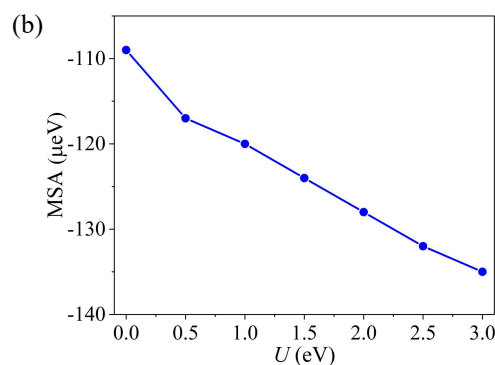
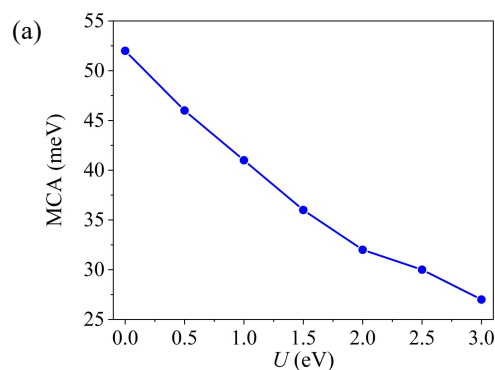


Fig. S3 The calculated (a) E_{MCA} and (b) E_{MSA} as a function of U values.

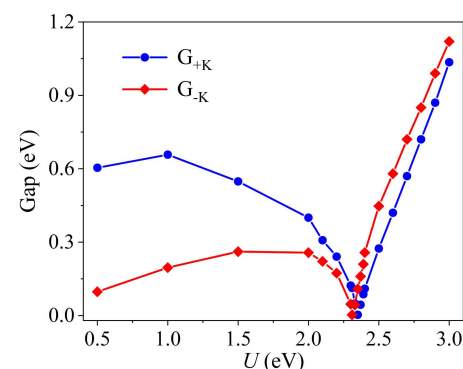


Fig. S4 The band gaps at +K/-K points as a function of U values (0.5-3 eV).

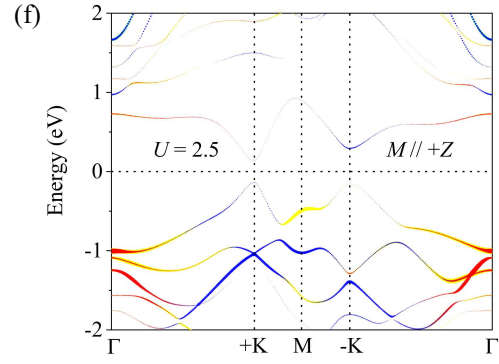
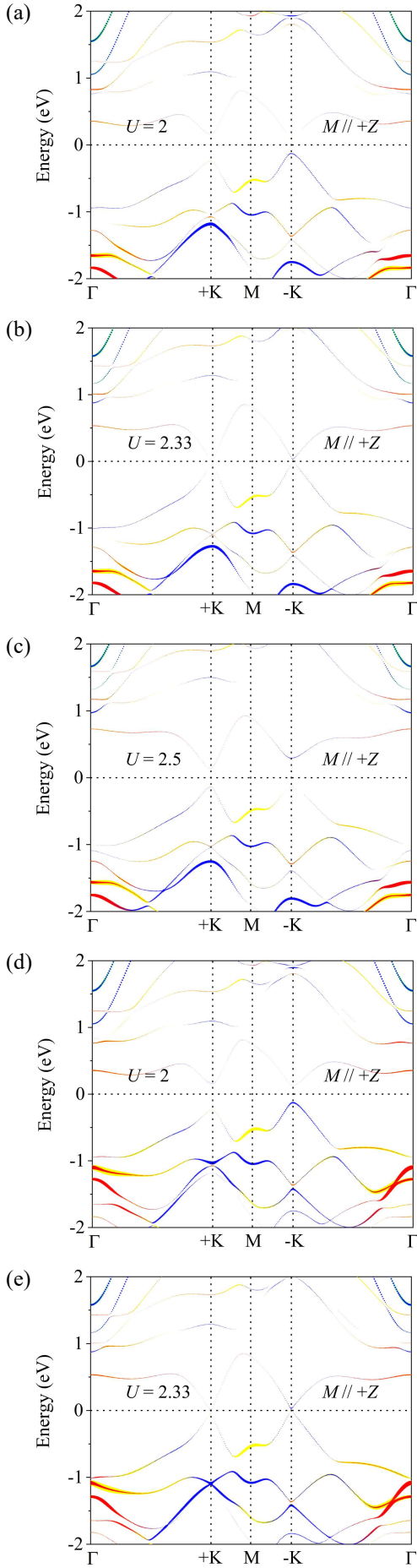
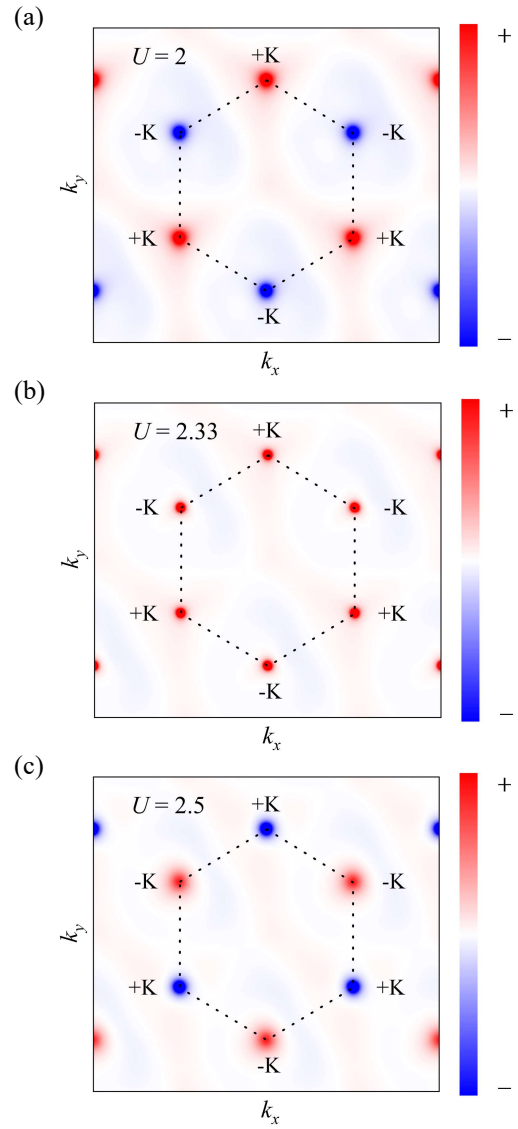


Fig. S5 (a)-(c):The orbital-projected band structures of Cl atoms for OsClBr. (d)-(f):The orbital-projected band structures of Br atoms for OsClBr. The green, yellow, red, and blue symbols represent the orbital components of s , p_x , p_y , and p_z of Cl (Br), respectively.



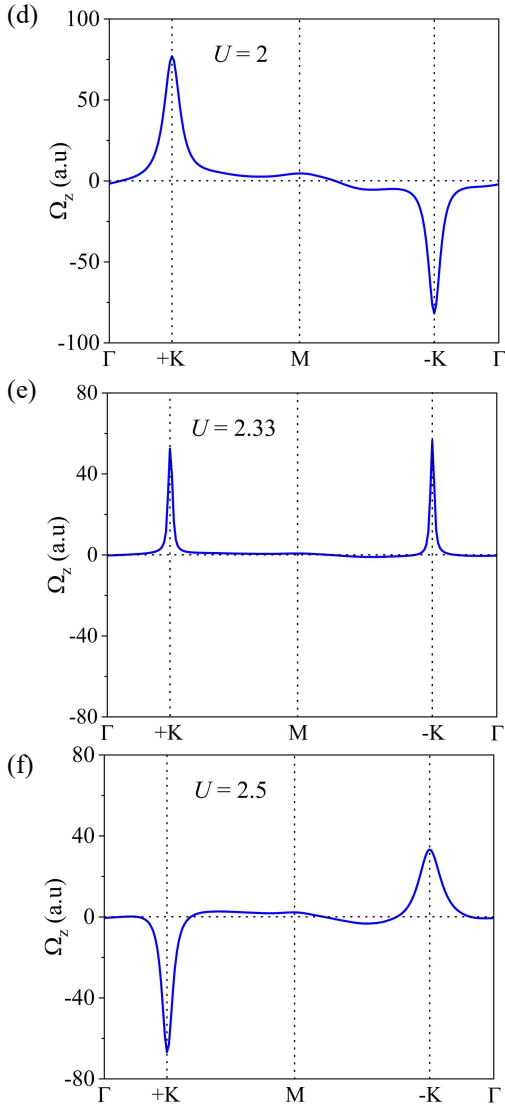


Fig. S6 The Berry curvature of OsClBr in the 2D BZ with (a) $U = 2$ eV, (b) $U = 2.33$ eV, and (c) $U = 2.5$ eV. The Berry curvature along the high symmetry points with (d) $U = 2$ eV, (e) $U = 2.33$ eV, and (f) $U = 2.5$ eV.

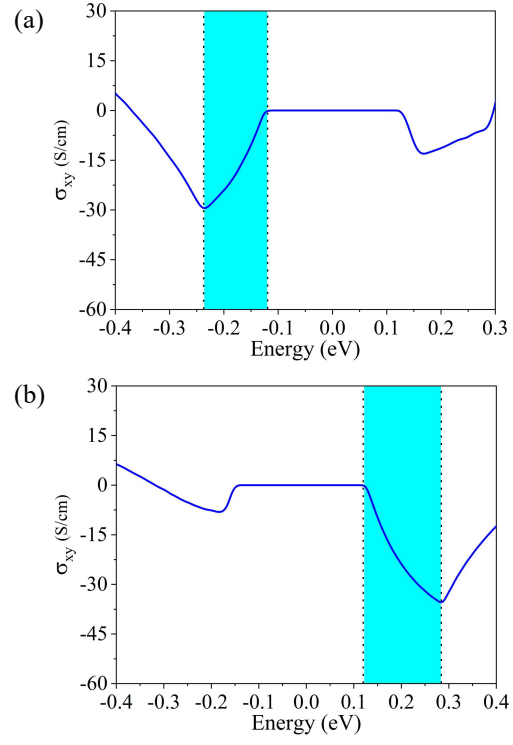


Fig. S7 The AHC of (a) $U = 2$ eV and (b) $U = 2.5$ eV as a function of Fermi energy.

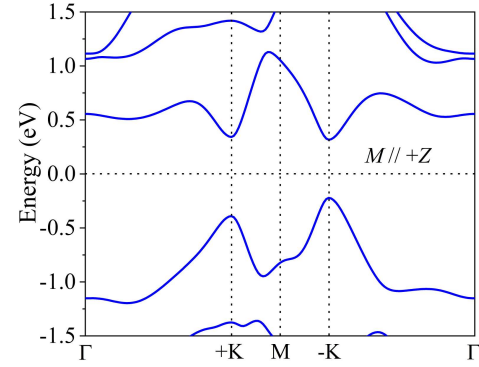


Fig. S8 The band structure of OsClBr by HSE06+SOC with the magnetization direction of Os along +Z.

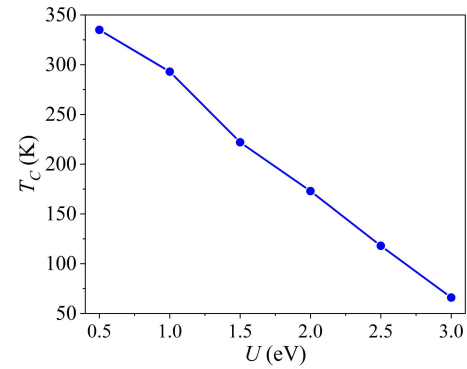


Fig. S9 The T_C as a function of U values (0.5-3 eV).