

## Supplemental materials for “First-Principles Prediction of Intrinsic Ferrovalley Properties in Janus Rare-Earth PrXY (X≠Y=Cl, Br, I) Monolayers”

Huai-Jin Zhang<sup>1</sup>, Yu-Ping Tian<sup>1</sup>, Cui Jiang<sup>2</sup>, Xiangru Kong<sup>1,\*</sup> and Wei-Jiang Gong<sup>1†</sup>

1. College of Sciences, Northeastern University, Shenyang 110819, China

2. Basic Department, Shenyang Institute of Engineering, Shenyang 110136, China

(Dated: December 23, 2024)

system	PrBrCl	PrBrI	PrClI
a=b(Å)	4.000	4.164	4.108
d <sub>Pr-X</sub> (Å)	3.021	3.046	2.912
d <sub>Pr-Y</sub> (Å)	2.893	3.216	3.209
Valley Polarization(meV)	38	84	68

FIG. S1: The lattice constants (a=b), bond lengths between Pr and X/Y atoms and valley polarization for Janus PrXY (X≠Y = Cl,Br,I) monolayers.

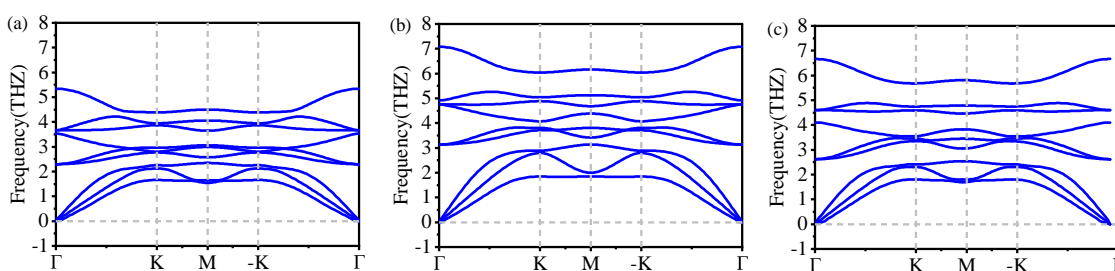


FIG. S2: Phonon dispersion of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI .

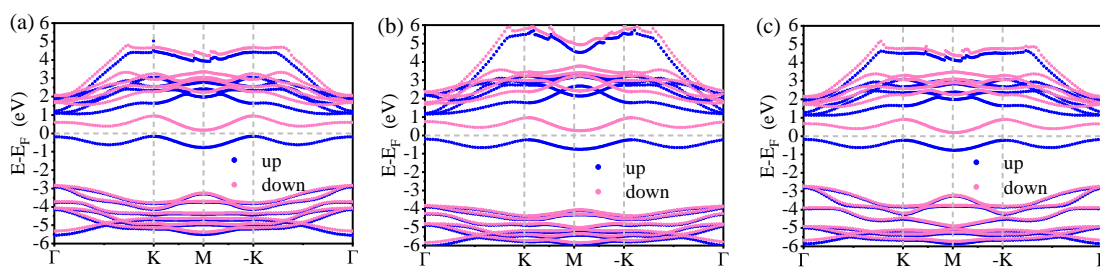


FIG. S3: Spin-polarized band structures of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI without considering the SOC.

\*Electronic address: kongxiangru@mail.neu.edu.cn

†Electronic address: gwj@mail.neu.edu.cn

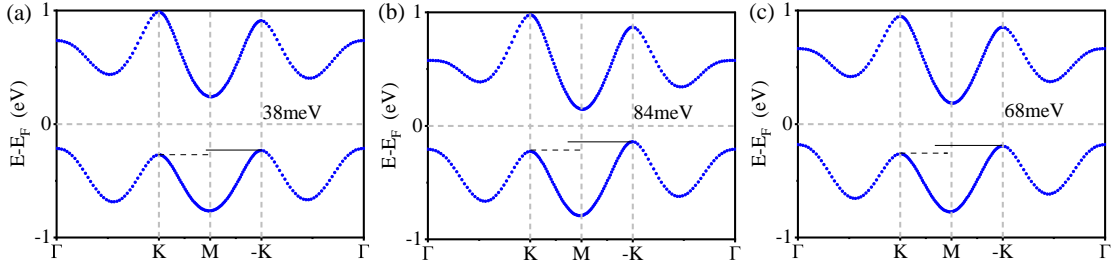


FIG. S4: Band structures of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI when the SOC is taken into account.

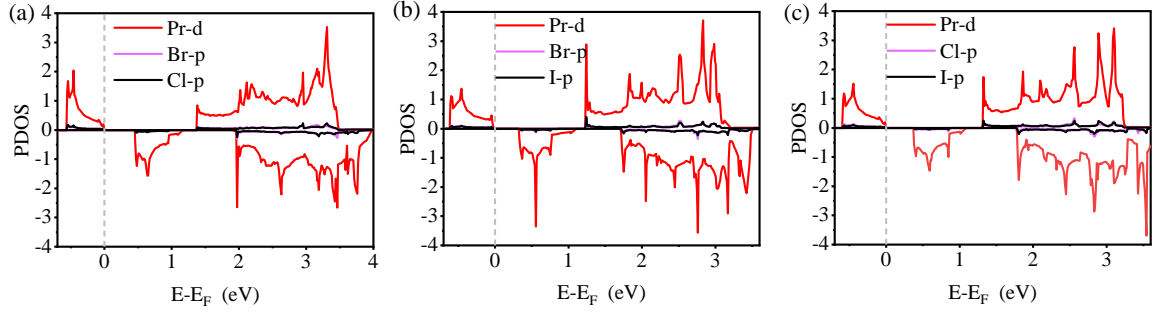


FIG. S5: The PDOS of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI, respectively.

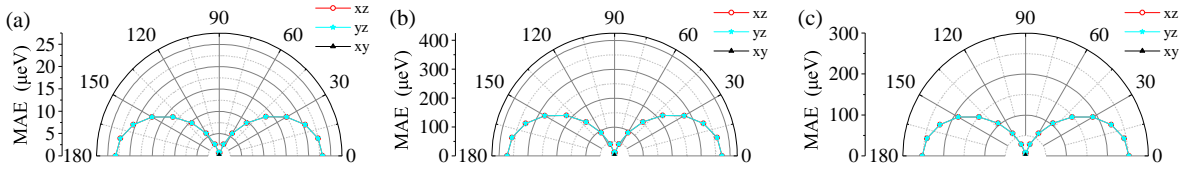


FIG. S6: The projections of MAE of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI on the  $xz$  plane,  $yz$  plane, and  $xy$  plane.

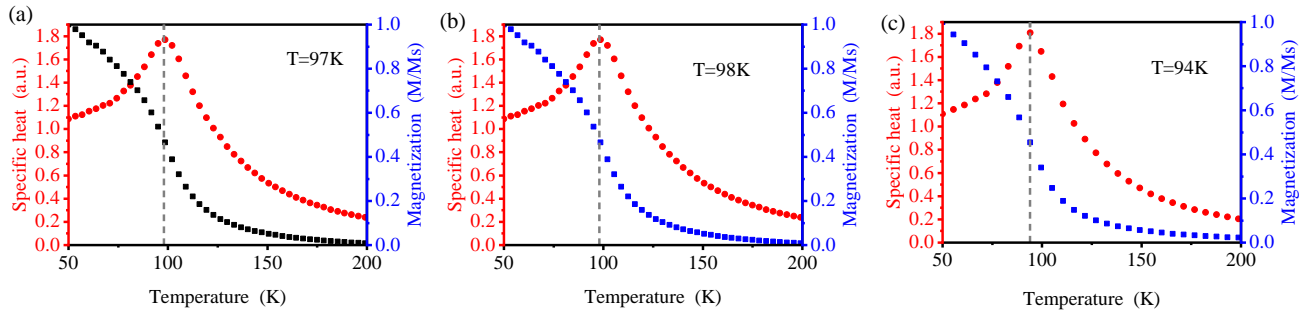


FIG. S7: The variation of average magnetic moment of monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI versus temperature.

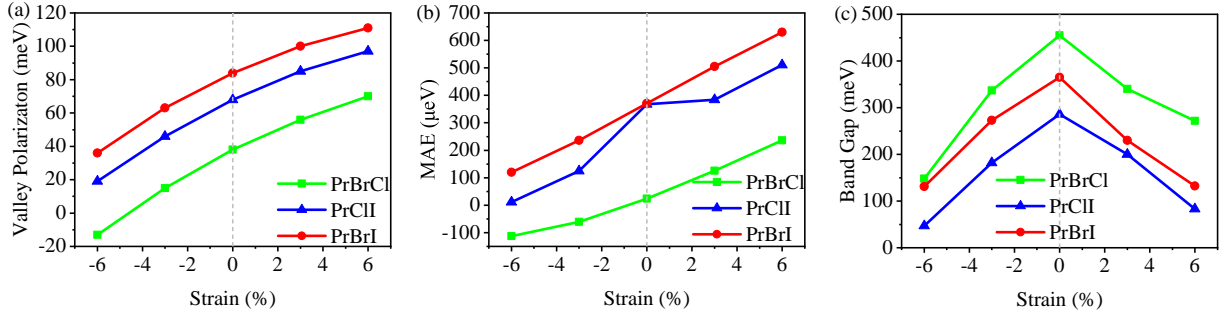


FIG. S8: The variation of valley polarization (a), MAE (b), and band gap (c) for PrXY monolayers versus biaxial strain.

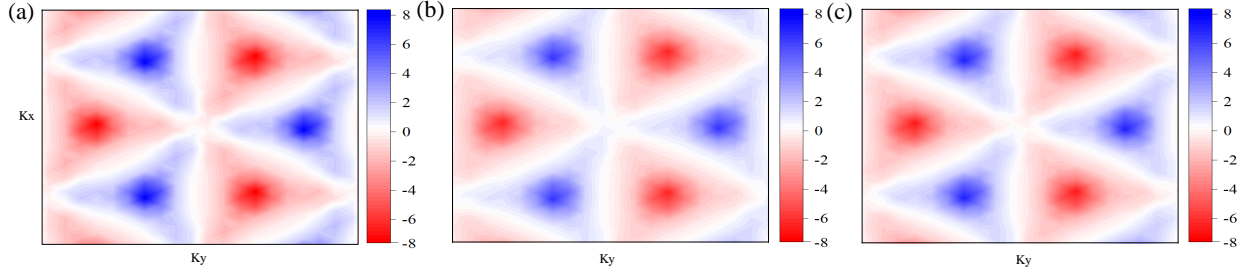


FIG. S9: Berry curvatures for monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI, respectively.

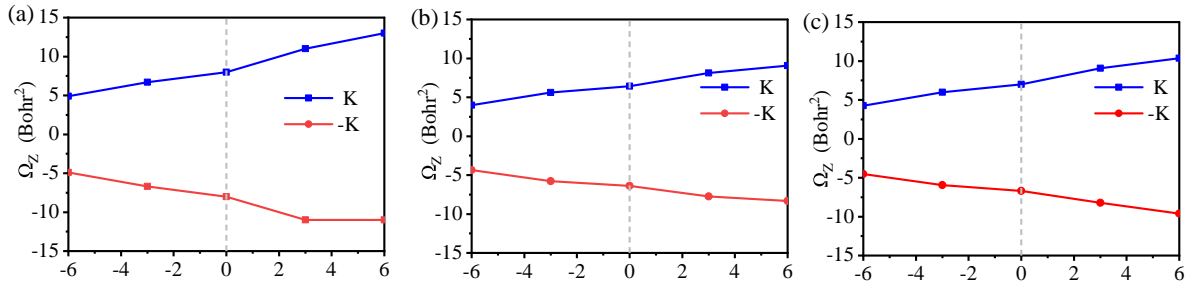


FIG. S10: The variation of Berry curvature versus strain for monolayer (a) PrBrCl, (b) PrBrI, and (c) PrClI.