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

Supplementary information "Coexistence of intrinsic room-temperature ferromagnetism and piezoelectricity in monolayer $BiCrX_3$ (X = S, Se, and Te)"

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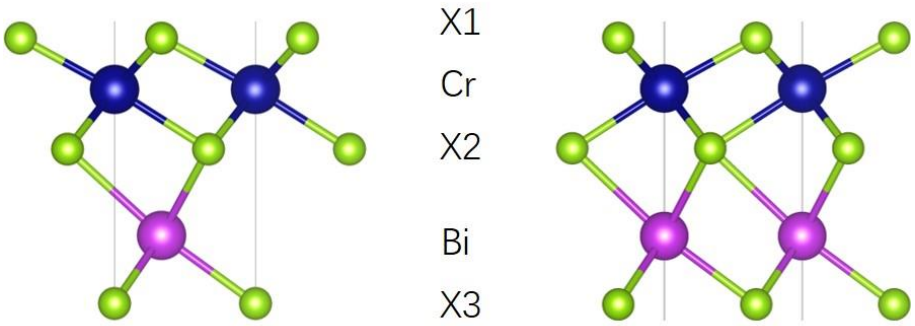

Figure S1. The number labels for X atoms in the ABCAB (left) and ABCBA (right) configurations. Magenta, blue, green represent Bi, Cr, and X (X = S, Se, and Te) atoms, respectively.

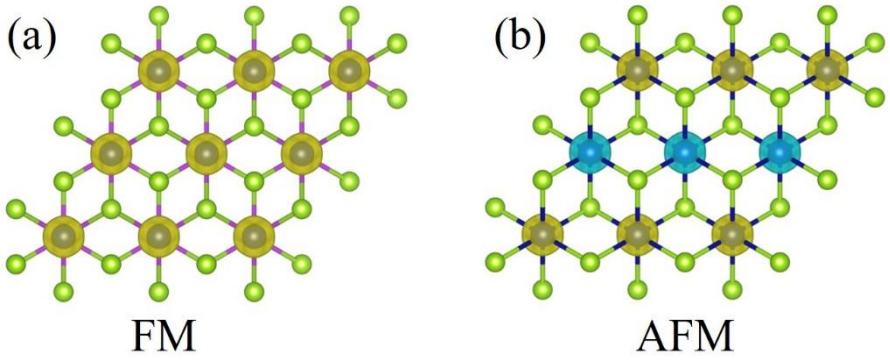

Figure S2. (a) FM, (b) AFM configurations. Magenta, blue, green represent Bi, Cr, and X (X = S, Se, and Te) atoms, respectively.

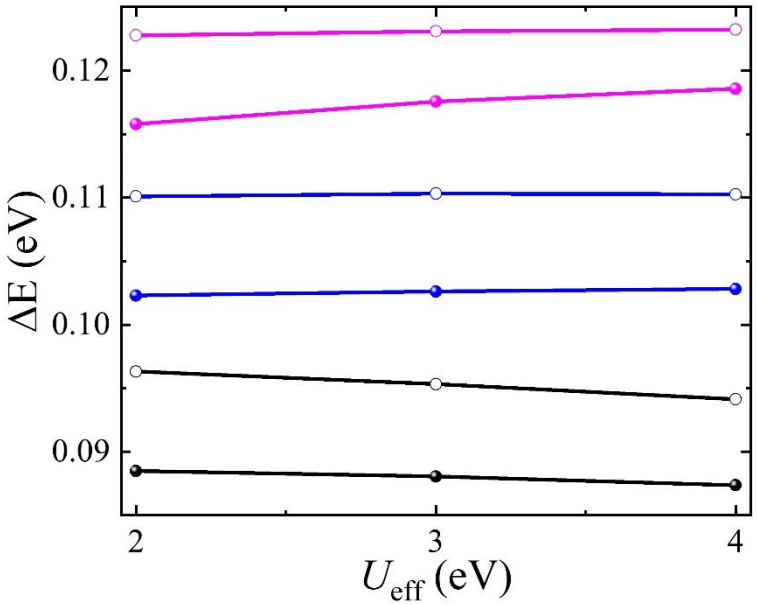

Figure S3. The calculated energy difference of $BiCrX_3$ monolayers as a function of U_{eff}. The black, blue, and magenta lines represent the $BiCrS_3$, $BiCrSe_3$, and $BiCrTe_3$, respectively. The solid and hollow points represent the ABCAB and ABCBA configurations, respectively.

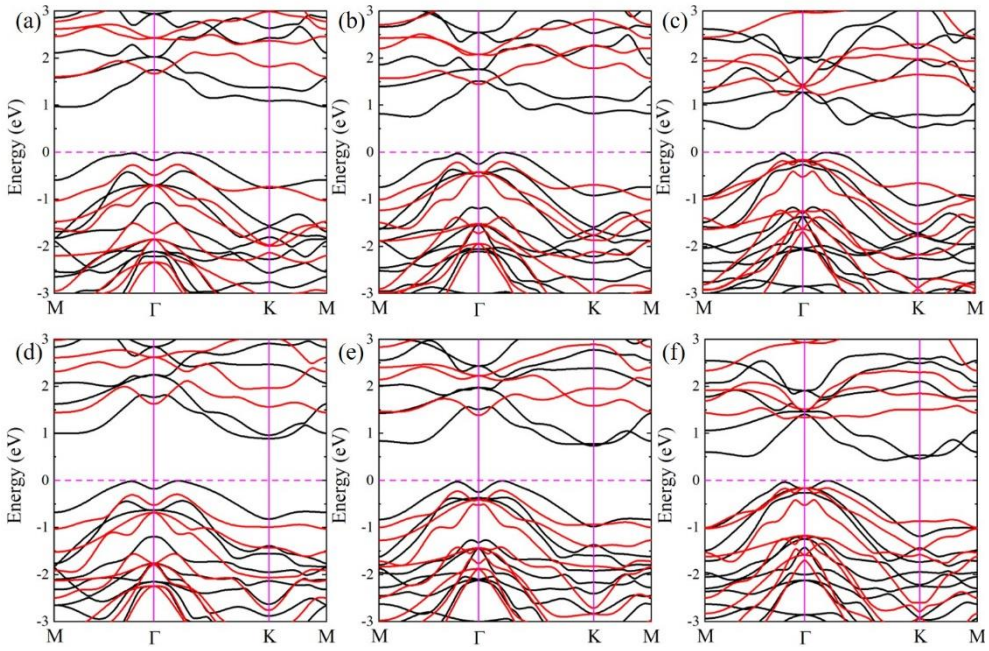

Figure S4. The calculated band-structure of $BiCrX_3$ monolayers with FM magnetic configuration. (a), (b), and (c) are the $BiCrS_3$, $BiCrSe_3$, and $BiCrTe_3$ with ABCAB configuration. (d), (e), and (f) are the $BiCrS_3$, $BiCrSe_3$, and $BiCrTe_3$ with ABCAB configuration. The carmine dashed lines represent the Fermi level set at 0 eV.

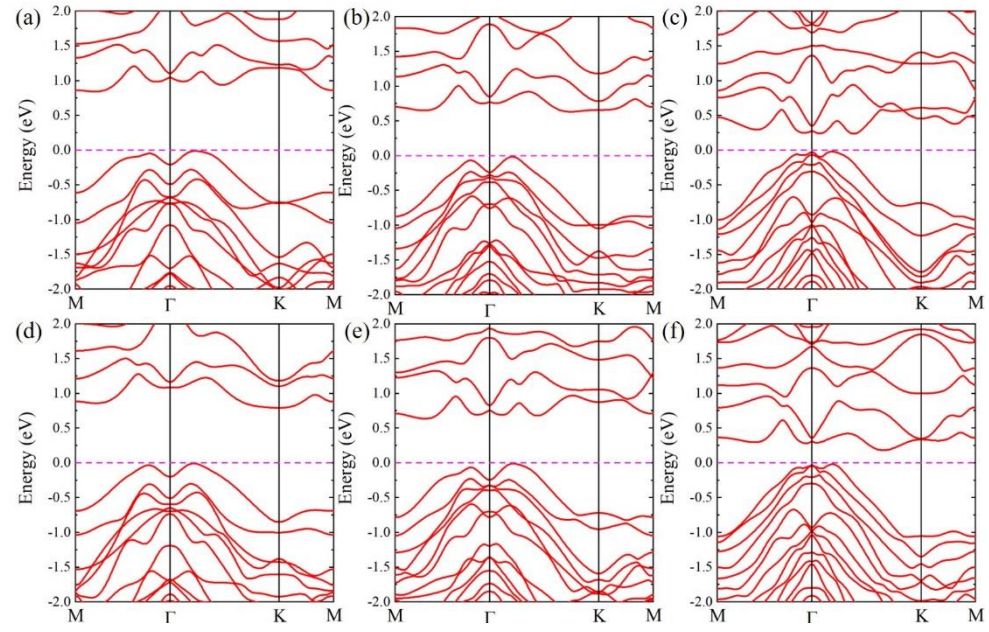

Figure S5. The calculated band-structure of $BiCrX_3$ monolayers with FM magnetic configuration including spin-orbital coupling effect. (a), (b), and (c) are the $BiCrS_3$, $BiCrSe_3$, and $BiCrTe_3$ with ABCAB configuration. (d), (e), and (f) are the $BiCrS_3$, $BiCrSe_3$, and $BiCrTe_3$ with ABCAB configuration. The carmine dashed lines represent the Fermi level set at 0 eV.

Table S1. The detailed structural information of $BiCrX_3$ monolayers. Cr-X1 and Cr-X2 are the bond lengths, which are in the unit of Å. Cr-X1-Cr and Cr-X2-Cr are the bond angles, which are in the unit of °. The X1 and X2 represent S, Se, and Te atoms, labeled in the Figure S2.

Materials	Configuration	Cr-X1	Cr-X2	Cr-X1-Cr	Cr-X2-Cr
$BiCrS_3$	ABCAB	2.464	2.592	100.48	93.86
	ABCBA	2.452	2.595	100.17	92.91
$BiCrSe_3$	ABCAB	2.603	2.708	98.97	93.91
	ABCBA	2.592	2.709	98.75	93.13
$BiCrTe_3$	ABCAB	2.818	2.894	97.62	94.22
	ABCBA	2.808	2.891	97.40	93.80

Table S2. The calculated total energies of $BiCrX_3$ monolayers with the magnetization along different directions, the MAE, and the single site magnetic anisotropy parameter. The energies of 001, 100, and 100 are in the unit of eV. The energies of MAE and the single site magnetic anisotropy parameter D are in the unit of meV.

Materials	Configuration	001	100	100	MAE	D
$BiCrS_3$	ABCAB	-26.399026	-26.398874	-26.398874	0.152	0.068
	ABCBA	-26.352365	-26.352186	-26.352186	0.179	0.080
$BiCrSe_3$	ABCAB	-24.524023	-24.523873	-24.523873	0.15	0.066
	ABCBA	-24.507651	-24.507487	-24.507487	0.164	0.073
$BiCrTe_3$	ABCAB	-22.644541	-22.644012	-22.644012	0.529	0.235
	ABCBA	-22.653195	-22.652573	-22.652573	0.622	0.276