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Supporting Information "Two-dimensional Janus MXenes: High-temperature Spin-polarized Semiconductor with Zero Magnetization"

Junjie He,[†] Pengbo Lyu,[†] L. Z. Sun,*[,§] Ángel Morales García[†] and Petr Nachtigall*[,†],

[†]*Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, 128 43 Prague 2, Czech Republic*

[§]*Hunan Provincial Key laboratory of Thin Film Materials and Devices, School of Material Sciences and Engineering, Xiangtan University, Xiangtan 411105, China*

E-mail: lz.sun@xtu.edu.cn, petr.nachtigall@natur.cuni.cz

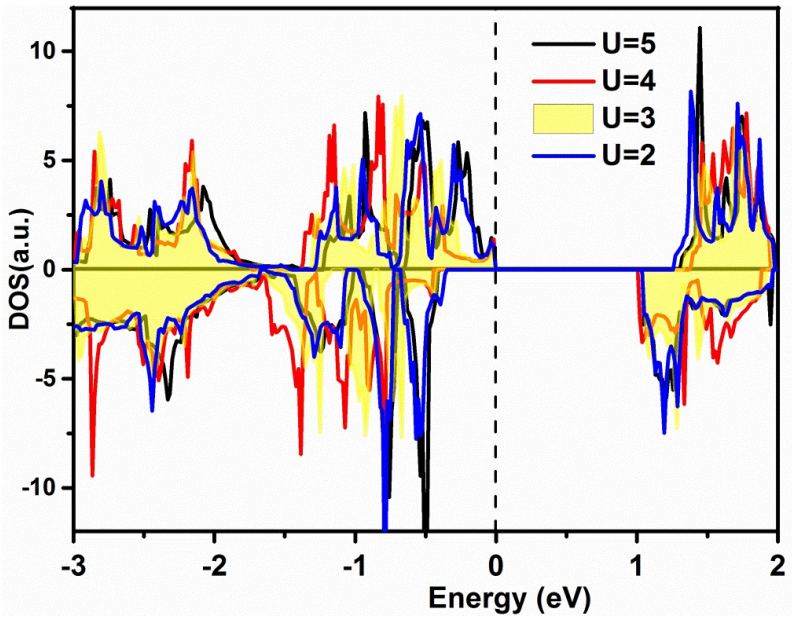

Fig. S1. The total DOS for Cr_2CFCl with various U value

Table S1: Calculated characteristics of Cr_2CX_2 materials. L is the lattice constant, E_{ex1} and E_{ex2} define the difference between $E_{Néel}$ and E_{FM}, $E_{Néel}$ and E_{zigzag}, respectively. The J_1 and J_2 represent the nearest neighbor and next nearest neighbor couplings constants, respectively.

	L (Å)	FM (eV)	AFM2 (eV)	J_1 (meV)	J_2 (meV)
H	2.992	0.758	0.931	-28.075	11.829
F	3.10	0.666	0.467	-24.654	0.643
Cl	3.269	0.588	1.160	-21.786	21.316
Br	3.368	0.525	1.161	-19.425	22.547
OH	3.121	0.663	0.441	-24.542	-0.019

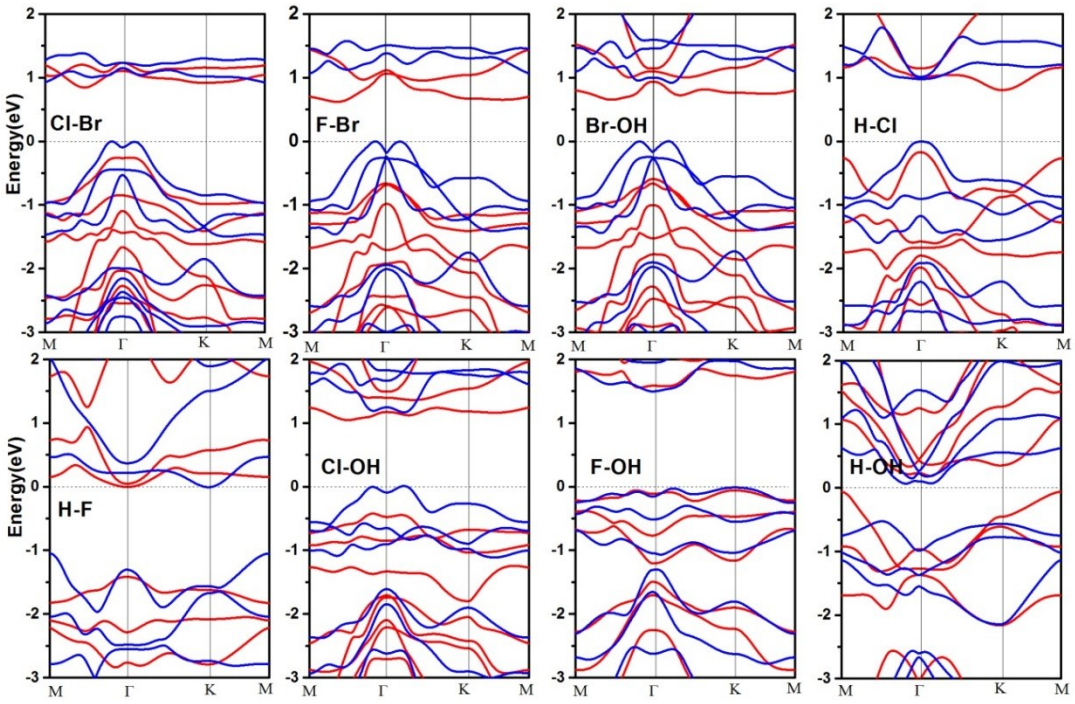

Fig. S2. The band structure for Janus Cr2CXX'**.** Red and blue lines represent the spin-up and spin-down directions, respectively.

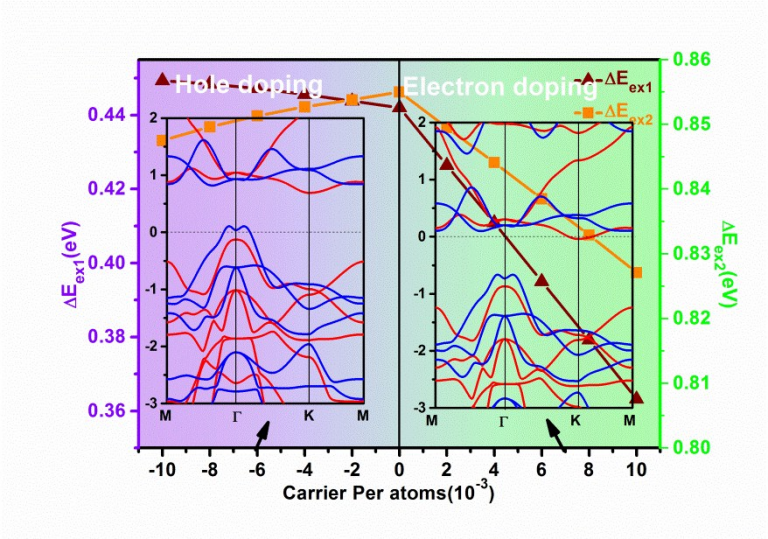

Fig. S3. Positive and negative values characterize the electron and hole doping in Cr_2CHBr, respectively. The calculated band structures for electron doping and hole doping for various carrier concentrations are presented as well; red and blue lines represent the spin-up and spin-down directions, respectively.

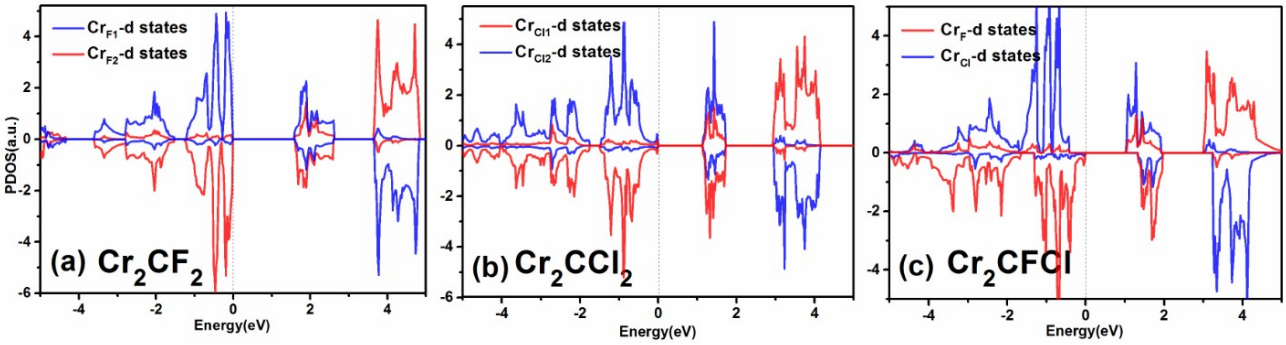

Fig. S4. *d* states of Cr atoms calculated for Cr_2CF_2 (a), Cr_2CCl_2 (b) and Cr_2CFCl

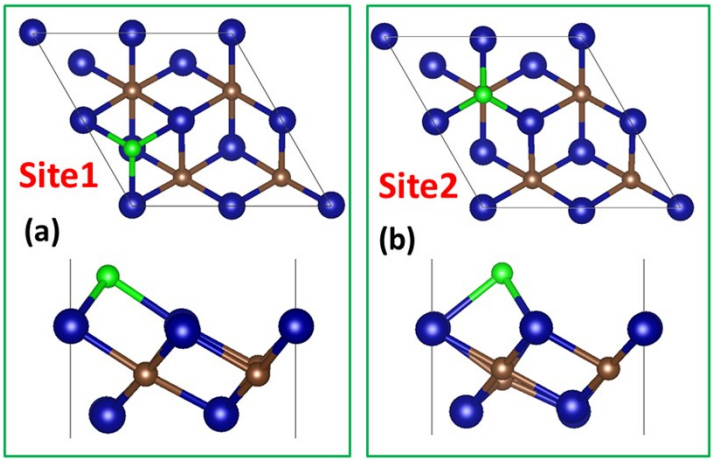

Fig. S5. Two possible sites for functional atoms/groups, site 1 and site 2 are shown in parts (a) and (b), respectively; top and side views are shown in upper and lower panels, respectively.

Table S2. Total energies of the Cr_8C_4X unit cells with functionalizing group in sites 1 or 2 calculated for X = H, OH, F, Cl, Br.

	Functional group				
Functional group position	H (eV)	OH (eV)	F (eV)	Cl (eV)	Br (eV)
Site1	-90.88	-99.07	-93.12	-91.69	-91.16
Site2	-90.16	-98.53	-92.58	-90.17	-90.85