Supporting Information for

Charge transfer and strain tuned antiferromagnetism in two-dimensional $CrCl_3/[Mo_2C(-O)]_2$ heterojunction

Mingyu Zhao[1*], Xianqi Dai[2], Yanan Tang[3*]

1.School of Physics, Southeast University, Nanjing 211189, China

2.School of Physics, Henan Normal University, Henan 453000, China

3.School of Physics, Zhengzhou Normal University, Henan 450000, China

* Email: rmzhaomy@seu.edu.cn

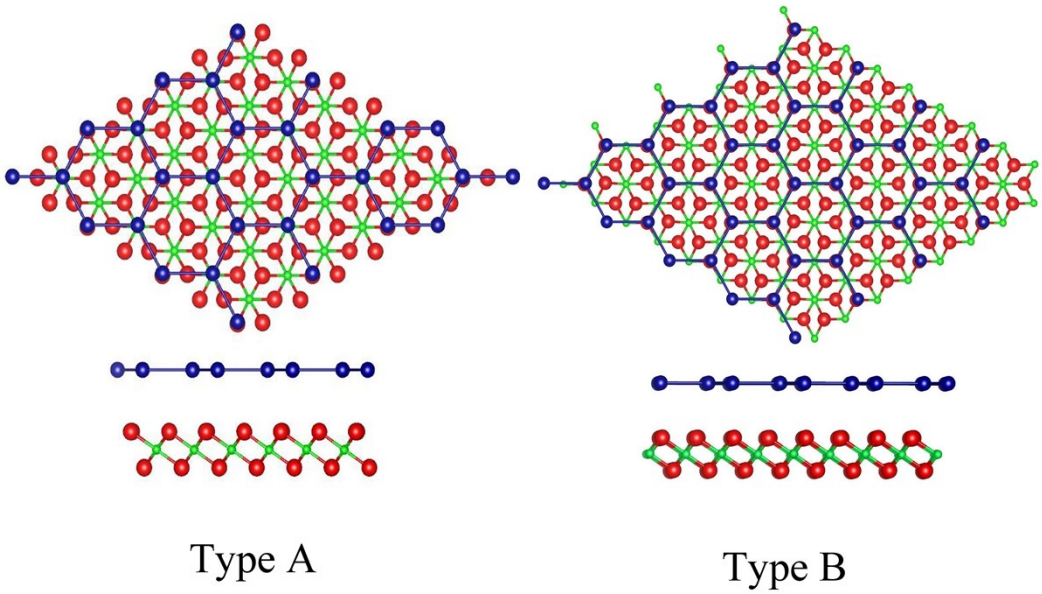

FIG. S1 Two different stacking modes for $CrCl_3/(Mo_2C)_2$ system (The skeleton of Cr is preserved in $CrCl_3$)

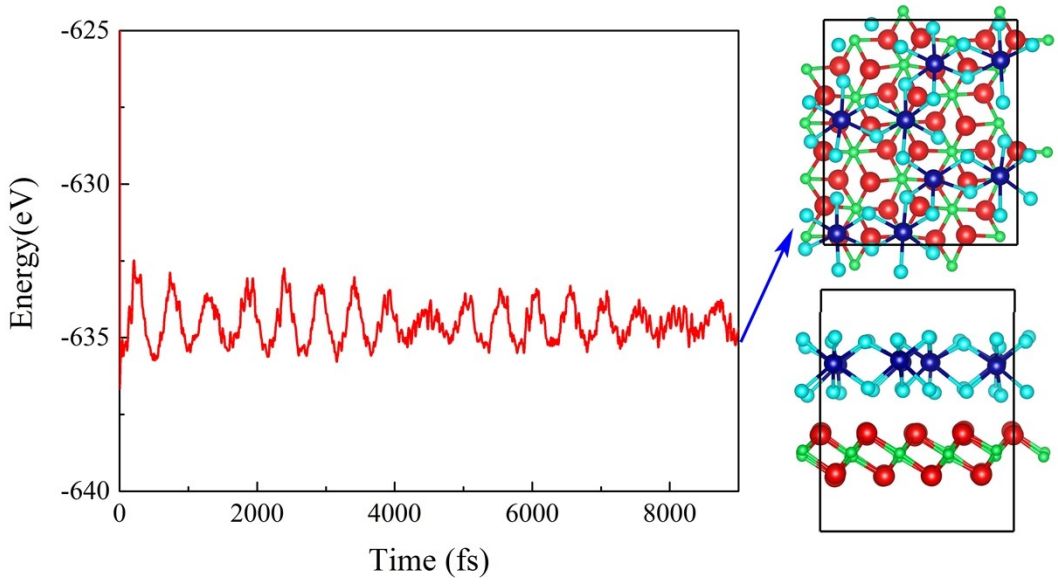

Fig. S2 The total energy fluctuations with time obtained by MD simulations at 300 K for 9 ps. The final configuration of the $CrCl_3/Mo_2C$ after the 9 ps MD simulation.s

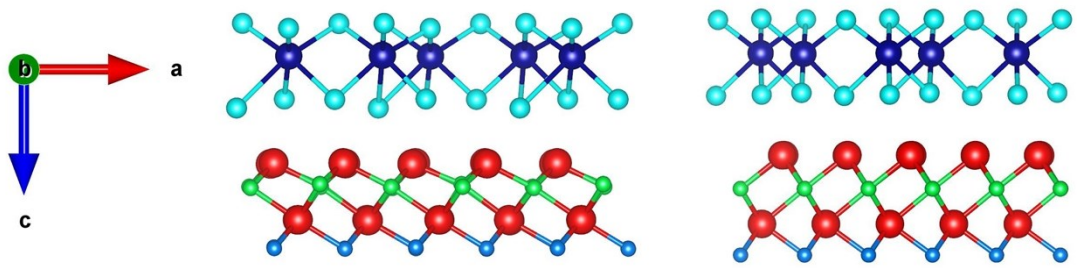

FIG. S3 Two different adsorption modes for O in $CrCl_3/Mo_2C$-O system

TABLE S1. The six-fold rotational symmetric magnetocrystalline anisotropy K^z and K^{xy} of $CrCl_3/Mo_2C$-O system and Néel temperature (T_N) under different strain.

strain	J (meV)	K^z (meV)	K^{xy} (meV)	T_N (K)
0%	6.83	-0.125	0.075	36
-1%	8.33	1.1125	1.1875	46
-2%	11.5	0.45	0.7	60
-3%	28.16	1.0125	0.8125	146