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

Supporting Information

Prediction of 2D ferromagnetism and monovalent europium ions in the EuBr/graphene heterojunctions

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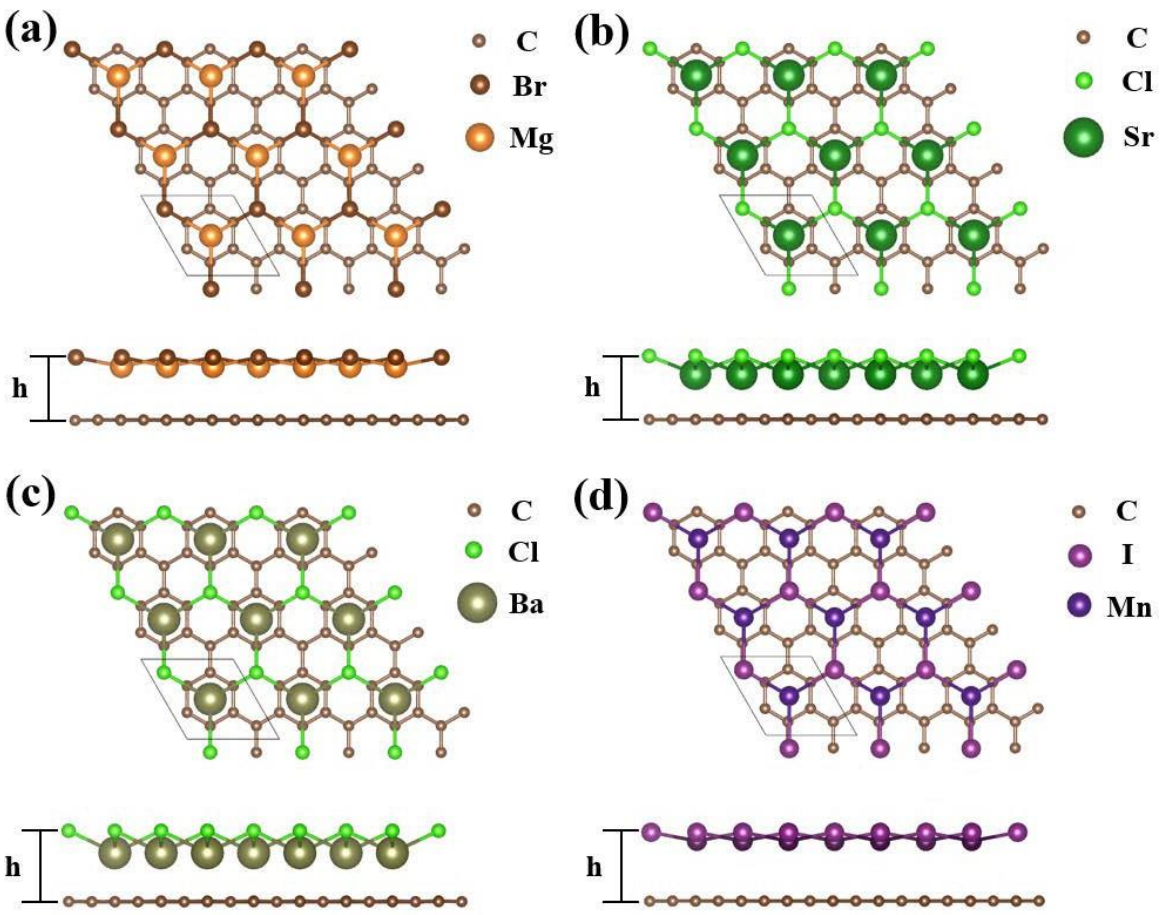

Figure S1. Geometric structures of 3×3 supercells of (a) MgBr/graphene heterojunctions, (b) SrCl/graphene heterojunctions, (c) BaCl/graphene heterojunctions and (d) MnI/graphene heterojunctions.

Table S1. Lattice constants, bond length, h, cohesive energy and heterojunction formation energy of different heterojunctions and isolated crystals.

Materials	Lattice Constants a=b (nm)	Bond Length of Metal Halide (nm)	h (nm)	Cohesive Energy (eV/atom)	Heterojunction Formation Energy (eV/atom)
MgBr/graphene heterojunctions	0.493	0.288	0.340	6.76	0.019
Isolated MgBr crystals	0.369	0.268	\	2.09	\
SrCl/graphene heterojunctions	0.496	0.303	0.344	7.05	0.081
Isolated SrCl crystals	0.429	0.293	\	3.08	\
BaCl/graphene heterojunctions	0.497	0.311	0.381	7.10	0.104
Isolated BaCl crystals	0.472	0.308	\	3.21	\
MnI/graphene heterojunctions	0.491	0.287	0.372	6.78	0.408
Isolated MnI crystals	0.409	0.273	\	1.97	\

Table S2. Energy and magnetic moment of 2×2 supercells of MnI/graphene heterojunctions with different magnetic configurations.

Magnetic Configurations	Energy (eV)	Magnetic Moment (μ_B)
FM	-331.85749	17.8
AFM1	-332.30736	0.0
AFM2	-332.30792	0.0
AFM3	-332.31102	0.0
FIM	-332.13208	8.4

Table S3. Energy of 2×2 supercells of EuBr/graphene heterojunction with different Hubbard on-site Coulomb potential set for Eu.

U-J	FM (eV)	AFM1 (eV)	AFM2 (eV)	AFM3 (eV)	FIM (eV)
4.0	-358.59578	-358.59003	-358.59003	-358.59003	-358.59122
8.0	-357.92893	-357.90797	-357.90797	-357.90797	-357.91293

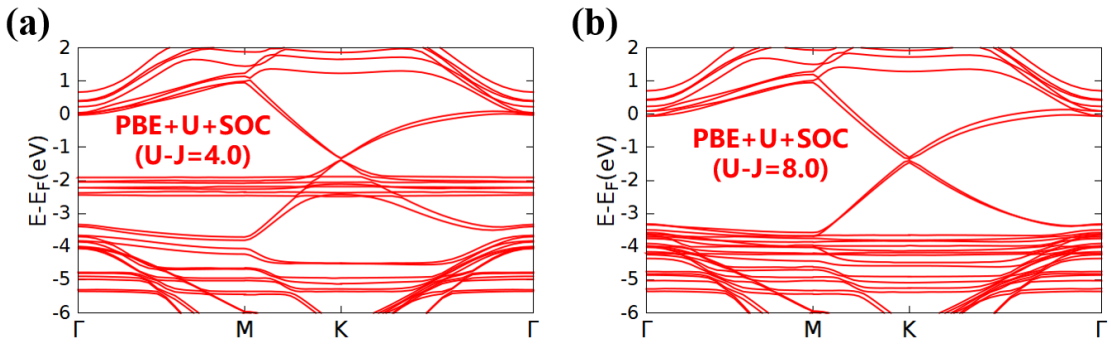

Figure S2. Band structure of EuBr/graphene heterojunctions with different Hubbard on-site Coulomb potential set for Eu ions of (a) U-J = 4.0 and (b) U-J = 8.0.