Supporting information

Activating Hexagonal Boron Nitride Monolayer for Efficient Hydrogen Evolution Reaction by Strong Interfacial Interactions with 2D M_2X Electrides

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Table S1. The computed free energy change for H^* adsorption (ΔG_{H^*}) on the pristine BN and different M_2X electrides.

	ΔG_{H^*} (eV)
BN	2.44 on B site
BN	2.49 on N site
Ba_2N	2.73
Ca_2N	–0.61
Hf_2S	–1.26
Sc_2C	–0.42
Sr_2N	–0.56
Y_2C	–0.42

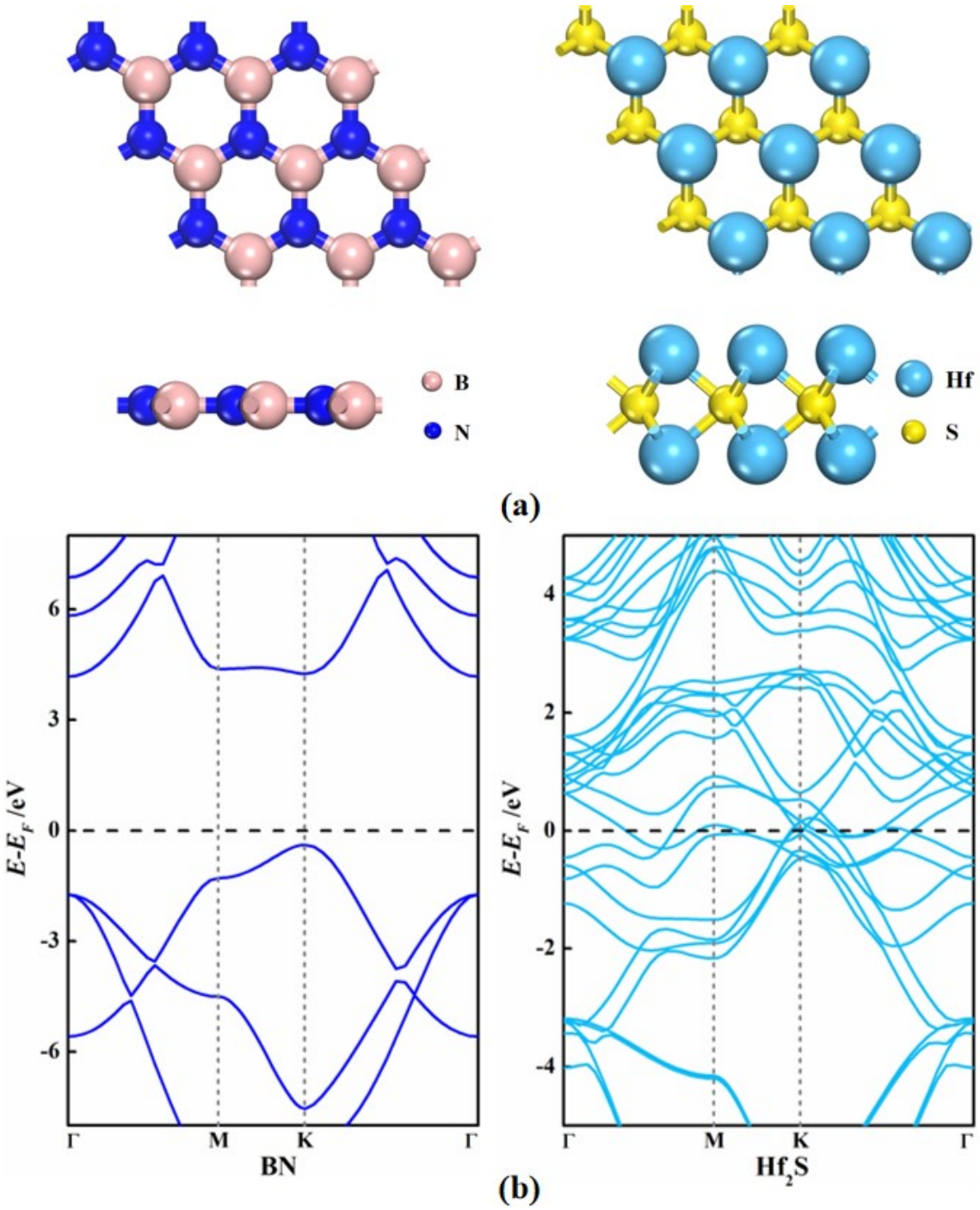
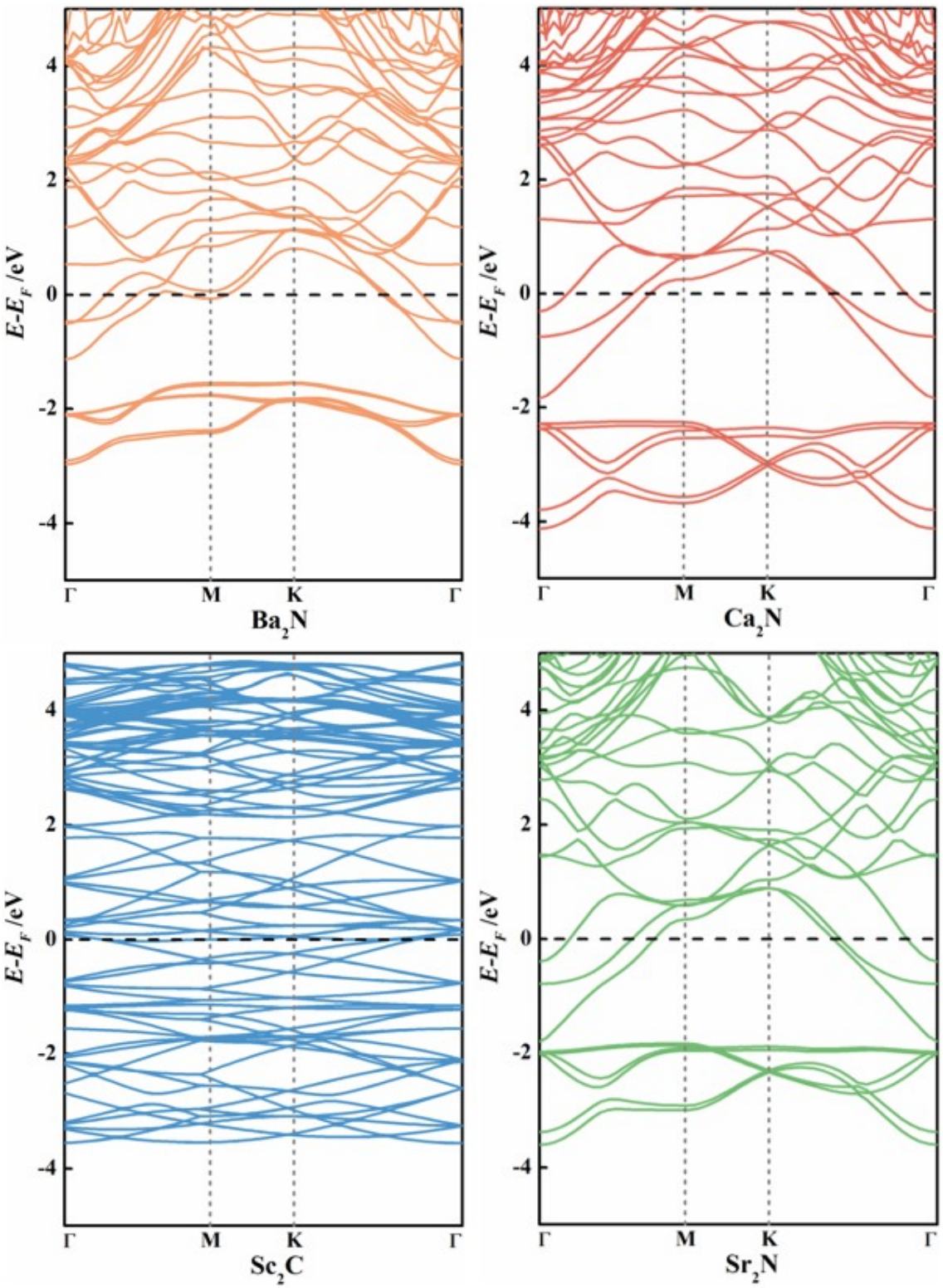


Fig. S1. (a) The optimized structures of the pristine BN and H_2S nanosheets and (b) their corresponding band structures. The Fermi level was set as zero.


E-E_F /eV
4
2
0
-2
-4
Γ
M
K
Γ
Ba2N
Ca2N
Sc2C
Sr2N

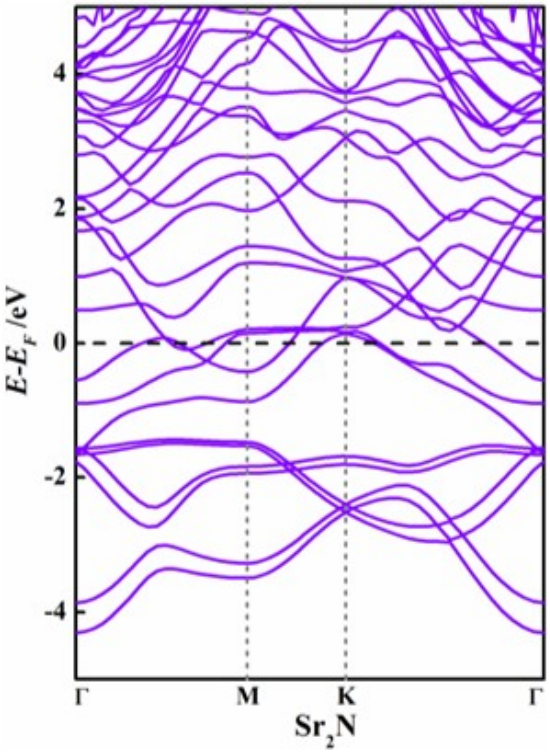


Fig. S2. The computed band structure of various M_2X materials.

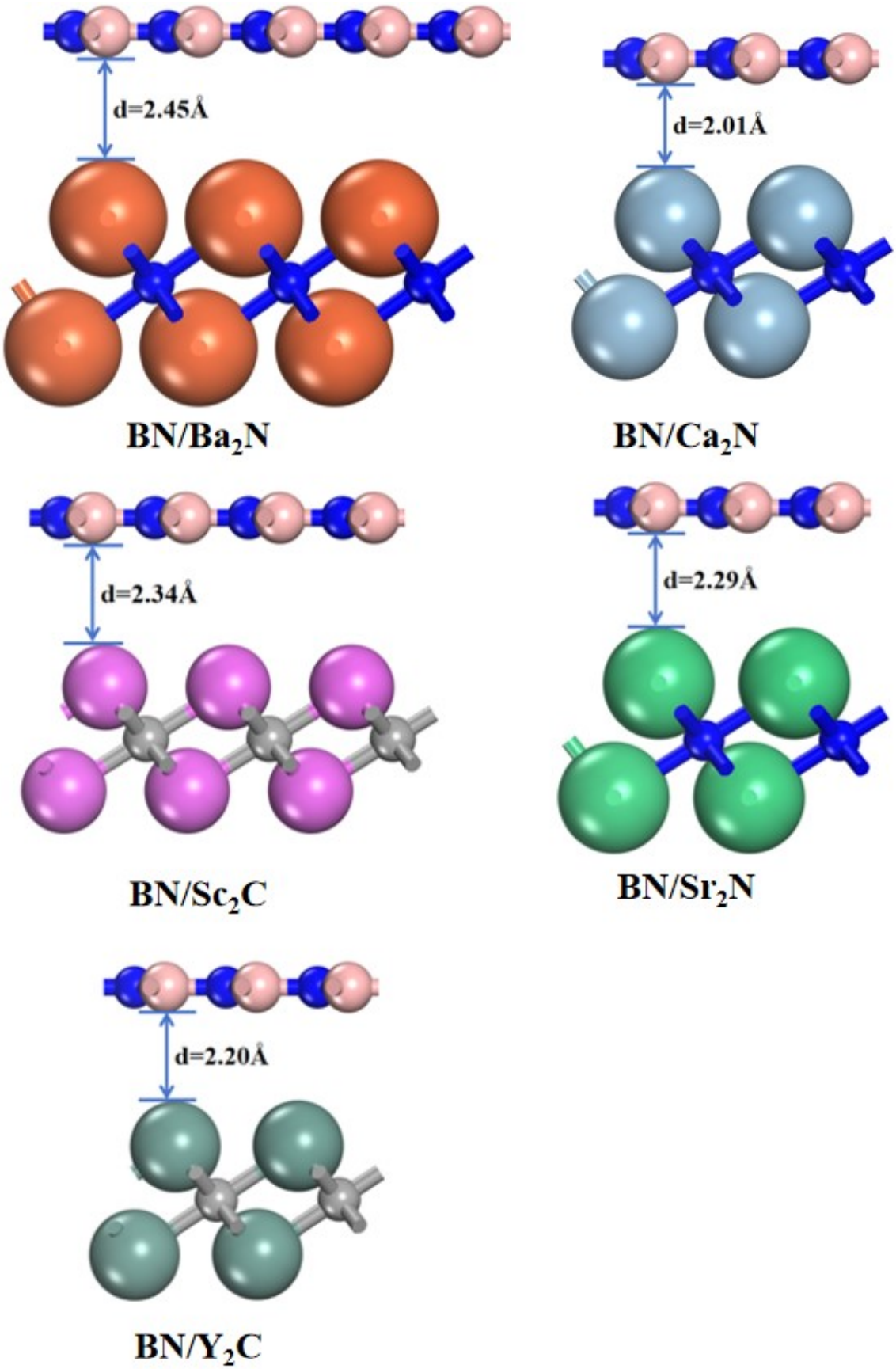


Fig. S3. The optimized configurations of various BN/M_2X heterostructures with the corresponding interlayer distance.

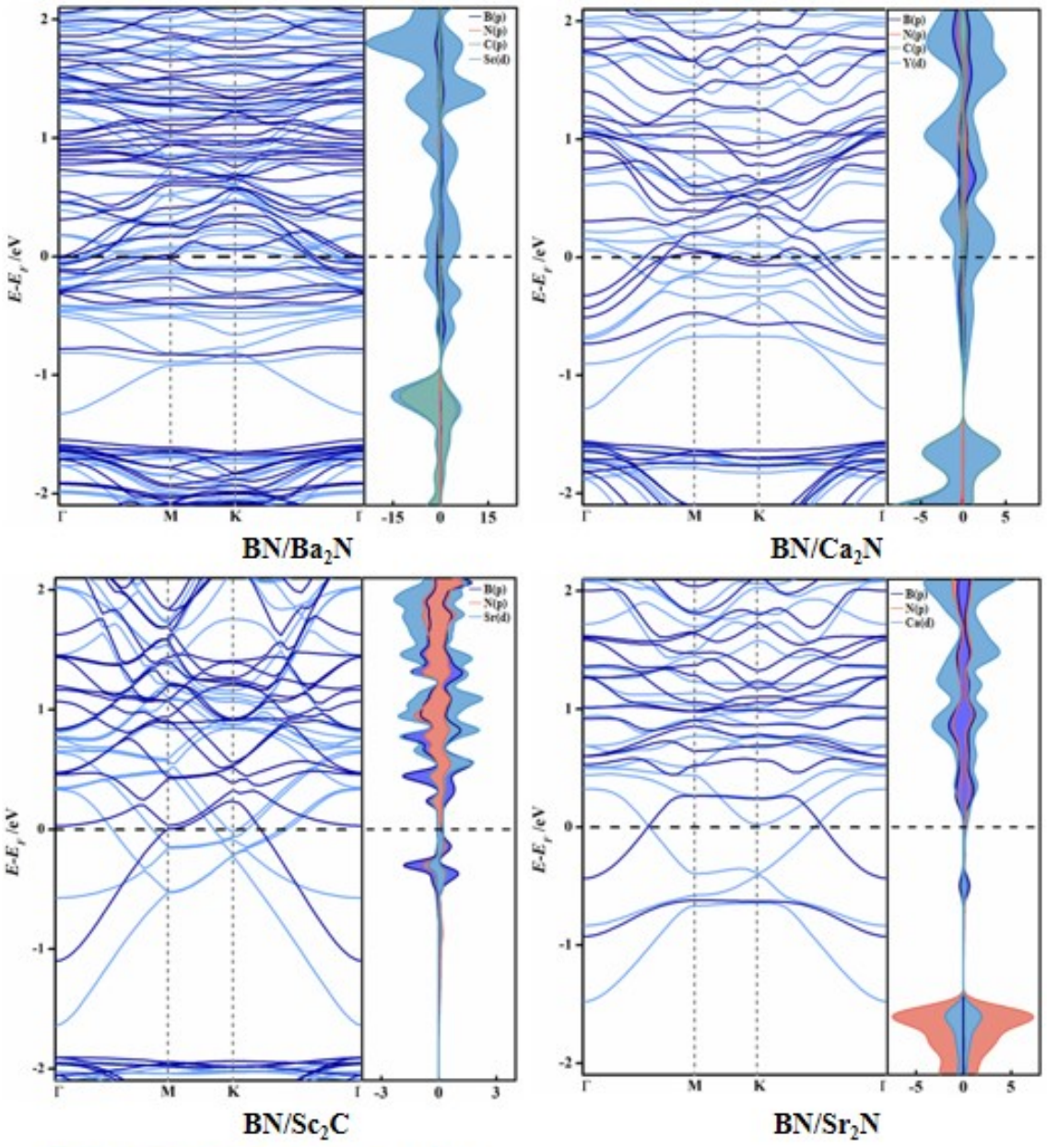

E-E_F /eV
Γ
M
K
Γ
B(p)
N(p)
C(p)
Sc(d)
BN/Ba2N
B(p)
N(p)
C(p)
Y(d)
BN/Ca2N
B(p)
N(p)
Sr(d)
BN/Sc2C
B(p)
N(p)
Ca(d)
BN/Sr2N

Fig. S4. The computed band structures and partial density of states (PDOS) of various BN/M_2X heterostructures.

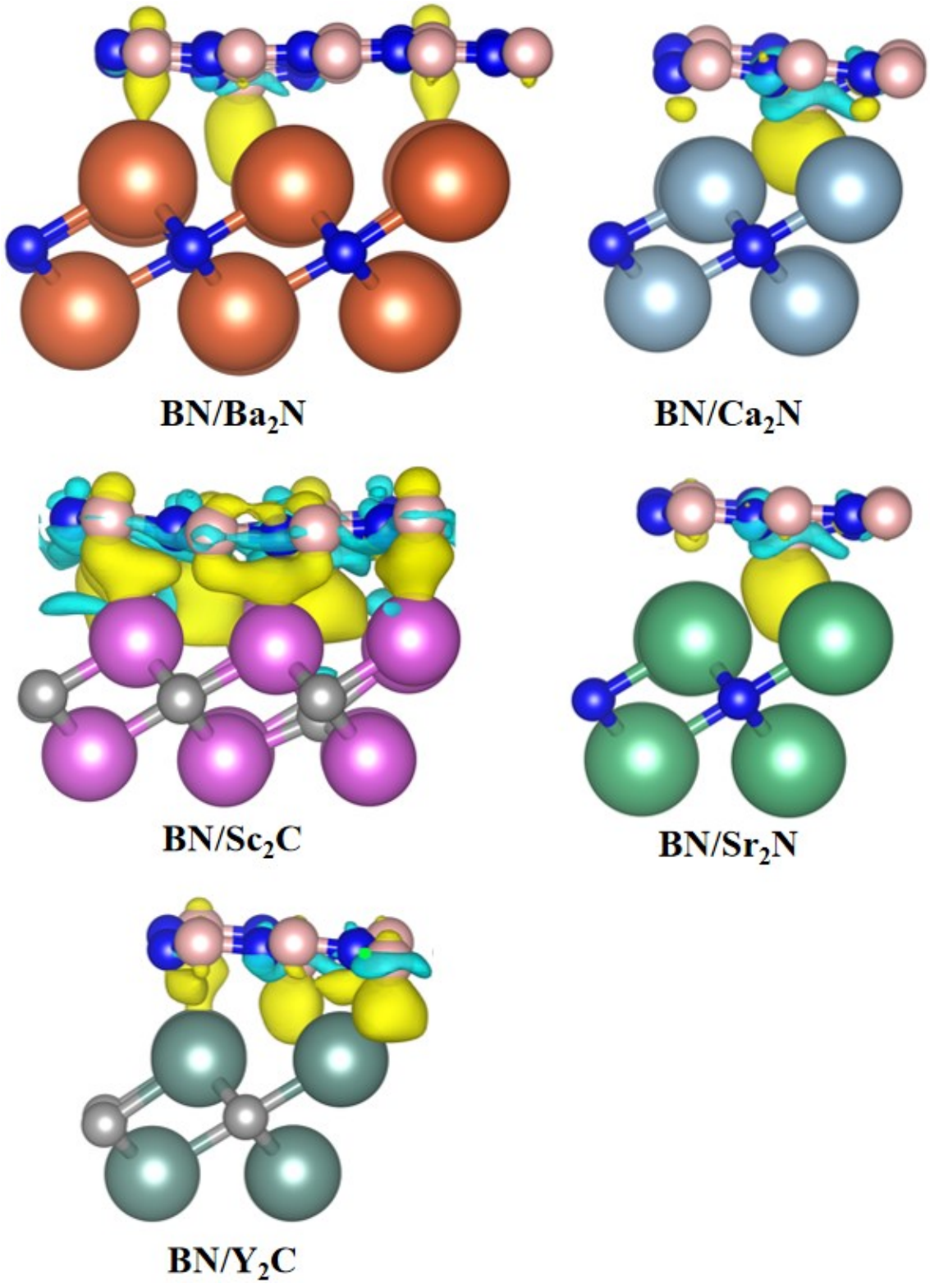


Fig. S5. Charge density differences of of BN/M_2X materials. The isosurface value was set to 0.004 e $Å^{-3}$.