Supplementary Information

Two-dimensional $Cs_3Sb_2I_9/C_2N$ van der Waals type-II heterostructure: A Promising Photocatalyst for high efficiency water-splitting

Hui Wang,[a] Baozeng Zhou,*[a]

[a] *Tianjin Key Laboratory of Film Electronic & Communicate Devices, School of Integrated Circuit Science and Engineering, Tianjin University of Technology, Tianjin 300384, China*

*Corresponding Authors

baozeng@tju.edu.cn (B. Zhou)

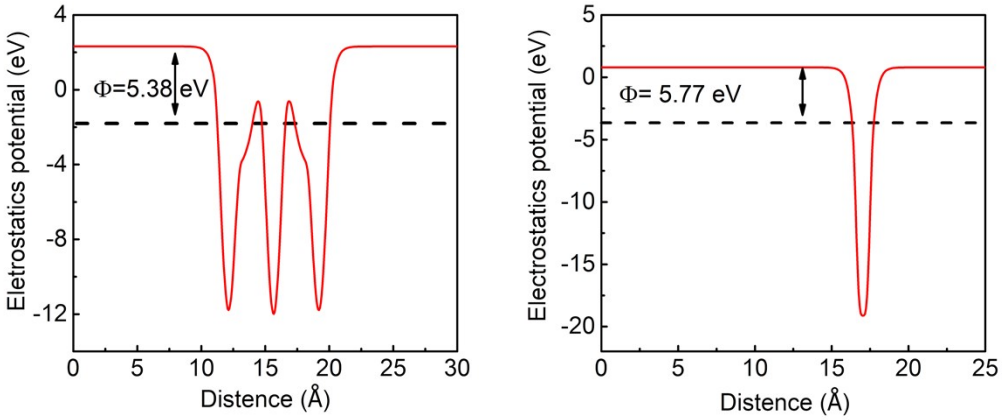

Fig. S1. (a) The plane-average electrostatic potential of (a) the $Cs_3Sb_2I_9$ monolayer and (b) C_2N monolayer.

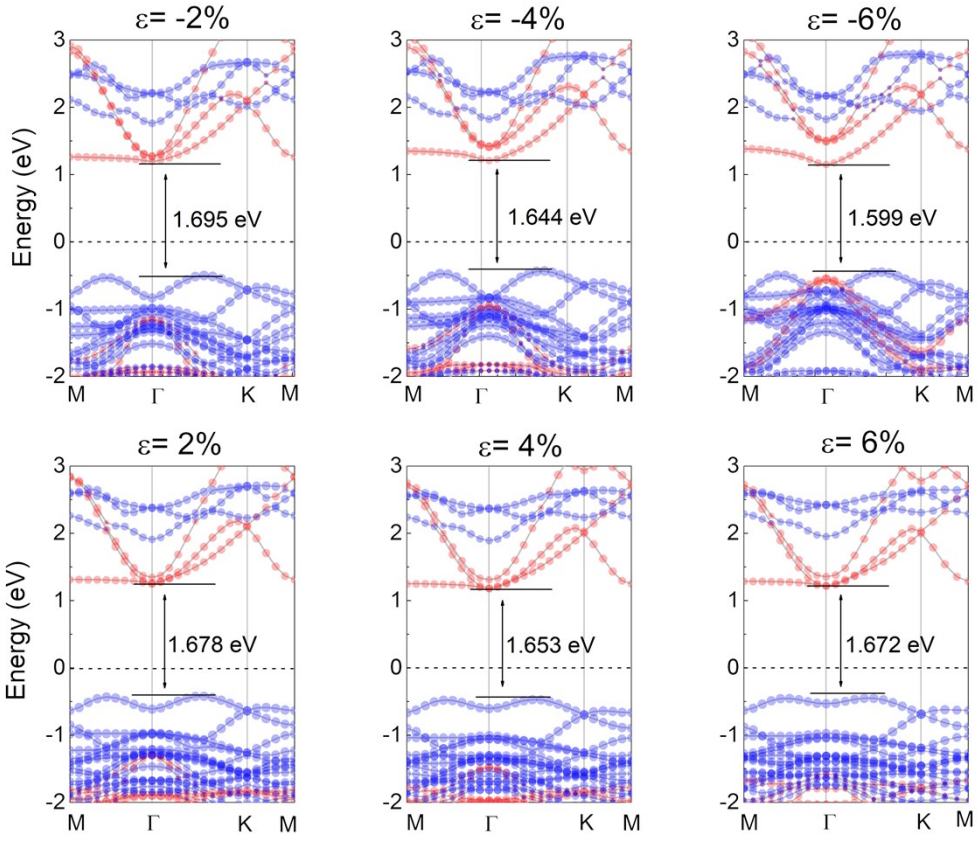

Fig. S2. The band structures of the $Cs_3Sb_2I_9/C_2N$ heterostructure under different in-plane biaxial strains based on HSE06 method. The Fermi level is set to zero.

Table S1. The lattice vectors and fractional coordinates of each atom in $Cs_3Sb_2I_9$ monolayer.

a[Å]	8.5765446220052617	-0.0002483203601371	0.0000000000000000
b[Å]	-4.2884873627427877	7.4273813591313695	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	32.1162986754999977
Cs	0.0000002237613942	-0.0000002237613942	0.4875089798720780
Cs	0.6666679102651420	0.3333321277348610	0.3905298179730471
Cs	0.3333319586159192	0.6666680163840821	0.5845802267985640
Sb	0.6666626182419404	0.3333374197580630	0.5521316682149298
Sb	0.3333370739032921	0.6666629010967093	0.4229951740651128
I	0.5000007257513797	0.4999992662486263	0.4875472781026999
I	0.5000010587203817	0.0000018559277786	0.4875474395715557
I	0.0000018589277753	0.4999989362796215	0.4875474395715557
I	0.1672293732362382	0.8327706017637556	0.3755004512061940
I	0.1672354562808724	0.3344718348744096	0.3755026605971554
I	0.6655281451255890	0.8327645207191219	0.3755026605971554
I	0.3345019687295104	0.1672500300588584	0.5995945960560164
I	0.8327499609411444	0.6654980282704923	0.5995945960560164
I	0.8327553923549754	0.1672445926450276	0.5995968793179001

Table S2. The lattice vectors and fractional coordinates of each atom in C_2N monolayer.

a[Å]	8.3287319581807910	-0.0000086375643439	0.0000000000000000
b[Å]	-4.1643734594268507	7.2128776652686950	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	28.6035003661999987
C	0.6649572866375831	0.1584761652715319	0.5955600433095020
C	0.3349885443879356	0.8415201333268880	0.5956595566038005
C	0.8414926157747485	0.5064955199102057	0.5955571754278379
C	0.1584452948996779	0.4934817062717273	0.5956610035639622
C	0.4934733252926527	0.3350109869042917	0.5955641888062967
C	0.5064836582225742	0.6649773415631767	0.5956531663188126
C	0.1584470410483025	0.6649779869047788	0.5956589147980300
C	0.8414891099342869	0.3350094274929322	0.5955609477713283
C	0.5064848012035074	0.8415210432113602	0.5956545249771583
C	0.4934729002164080	0.1584767113576188	0.5955655530966505
C	0.3349890260971121	0.4934829240720786	0.5956606190163212
C	0.6649577975526456	0.5064937770785224	0.5955574130945321
N	0.0000345343050144	0.6688782423430601	0.5955862260575377
N	0.0000303720937557	0.3311047793888947	0.5955904449498829
N	0.3310876579249200	0.3311005900158068	0.5955960398514453
N	0.6688635075330792	0.6688793235882384	0.5955784847071436
N	0.6688656689146286	0.0000004111987619	0.5955828544814462
N	0.3310887337587158	-0.0000013558998655	0.5955944541683168

Table S3. The lattice vectors and fractional coordinates of each atom in $Cs_3Sb_2I_9/C_2N$ heter -ostructure.

a[Å]	8.3456922733198695	-0.0000000000007894	0.0000000000000000
b[Å]	-4.1728461366112484	7.2275815208635814	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	35.1968994141000024
C	0.6649359999399138	0.1585395468799504	0.6402403861571315
C	0.8414605311200489	0.5063965070599608	0.6402403861571315
C	0.4936034989400397	0.3350640050600902	0.6402403861571315
C	0.8414605061200504	0.3350640050600902	0.6402403861571315
C	0.4936034909400391	0.1585395468799504	0.6402403861571315
C	0.6649360049399107	0.5063965070599608	0.6402403861571315
C	0.3350396862159499	0.8415186379211264	0.6400909004273174
C	0.1584813800788680	0.4935210612948140	0.6400909004273174
C	0.5064789727051888	0.6649603207840471	0.6400909004273174
C	0.1584813760788677	0.6649603207840471	0.6400909004273174
C	0.5064789517051835	0.8415186379211264	0.6400909004273174
C	0.3350397102159519	0.4935210612948140	0.6400909004273174
N	0.9998523075193120	0.6683765496921765	0.6401666884638502
N	0.3316234353078187	0.3314757498271277	0.6401666884638502
N	0.6685242401728715	0.0001476944806882	0.6401666884638502
N	0.3316234253078179	0.0001476944806882	0.6401666884638502
N	0.6685242421728717	0.6683765496921765	0.6401666884638502
N	0.9998523145193090	0.3314757498271277	0.6401666884638502
Cs	0.0000000000000000	0.0000000000000000	0.4349319845023842
Cs	0.6666666710000015	0.3333333420000031	0.3434549864300251
Cs	0.3333333420000031	0.6666666839999991	0.5258608464019332
Sb	0.6666666710000015	0.3333333420000031	0.4938071562099040
Sb	0.3333333420000031	0.6666666839999991	0.3756653220506507
I	0.4997778994005557	0.5002221205994388	0.4348345988707436
I	0.4997778924005587	0.9995557848011174	0.4348345988707436
I	0.0004442221988796	0.5002221205994388	0.4348345988707436
I	0.1638879755788878	0.8361120214211155	0.3318777061109088
I	0.1638879885788853	0.3277759771577777	0.3318777061109088
I	0.6722240748422266	0.8361120214211155	0.3318777061109088
I	0.3289453482912208	0.1644726761456070	0.5378518953901192
I	0.8355272998543910	0.1644726761456070	0.5378518953901192
I	0.8355272968543872	0.6710547067087802	0.5378518953901192