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Supplementary information

Janus transition metal dichalcogenides in combination with MoS2 for high-efficiency photovoltaic applications

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Table. S1 Optimal lattice parameters as well as other information (MoSSe_MoS_2 Heterostructure)
AAI

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.1541	-3.86	-1328.984	90	560	0.003281	0.000386
relax	1514.8826	6.0849	3.1015	0.27	-1328.989	90	560	0.003225	0.000023

AAI-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.1541	-3.86	-1328.984	90	560	0.003281	0.000386
relax	1514.8826	6.0849	3.1015	0.27	-1328.989	90	560	0.003225	0.000023

AAII:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.7438	15.85	-1328.923	90	560	0.006867	0.000215
relax	1514.8826	6.0849	3.5387	0.32	-1328.992	90	560	0.004120	0.000020

AAII-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.882	6.0849	3.3540	2.58	-1328.97	90	560	0.006333	0.000332

	6				3				
Relax	1514.8826	6.0849	3.1369	0.24	-1328.994	90	560	0.004170	0.000035

ABI:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.24	1533.7595	6.1227	3.8745	0.76	-1328.949	90	560	0.009543	0.000227
Relax	1533.7595	6.1227	3.4421	-4.05	-1328.991	90	560	0.004060	0.000006

ABI-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.23	1524.3065	6.1038	3.3136	-2.63	-1328.978	90	560	0.005814	0.000439
Relax	1524.3065	6.1038	3.0787	-1.82	-1328.993	90	560	0.004253	0.000027

ABII:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.23	1524.3065	6.1038	3.8269	6.17	-1328.946	90	560	0.007854	0.000138
Relax	1524.3065	6.1038	3.5171	-1.81	-1328.992	90	560	0.004067	0.000011

ABII-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction

3.22	1514.8826	6.0849	3.0750	-4.78	-1328.984	90	560	0.004091	0.000299
Relax	1514.8826	6.0849	3.1545	0.84	-1328.994	90	560	0.004120	0.000024

Table. S2 Optimal lattice parameters as well as other information (WSSe_MoS_2 Heterostructure)

AAI:

Lattice constant (Ao) a=	unit-cell volume (a.u.)^3	attice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.6647	-4.61	-1725.333	90	560	0.005128	0.000481
relax	1514.8826	6.0849	3.5931	0.58	-1725.337	90	560	0.005062	0.000065

AAI-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.3524	-3.90	-1725.331	90	560	0.005265	0.000064
relax	1514.8826	6.0849	3.2965	-0.34	-1725.338	90	560	0.004932	0.000054

AAII:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.8826	6.0849	3.9495	15.45	-1725.276	90	560	0.008698	0.000311
Relax	1514.8826	6.0849	3.7488	0.96	-1725.343	90	560	0.006267	0.000034

AAII-Se:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.22	1514.882	6.0849	3.3740	-5.06	-1725.34	90	560	0.006242	0.000427

	6				0				
relax	1514.8826	6.0849	3.3381	0.17	-1725.344			0.006149	0.000044

ABI:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.24	1533.7595	6.1227	3.9650	4.75	-1725.285	90	560	0.014114	0.000318
Relax	1533.7595	6.1227	3.9847	24.94	-1725.318	90	560	0.011711	0.000146

ABI-Se

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.24	1533.7595	6.1227	3.6072	-1.76	-1725.313	90	560	0.010838	0.000189
relax	1533.7595	6.1227	3.2248	-3.99	-1725.342	90	560	0.005931	0.000021

ABII:

Lattice constant (A°) a=	unit-cell volume (a.u.)^3	lattice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	Ecutrho	Total Dispersion Force	Total SCF correction
3.23	1524.3065	6.1038	4.0552	7.13	-1725.293	90	560	0.009531	0.000118
Relax	1524.3065	6.1038	3.6658	-2.89	-1725.343	90	560	0.005988	0.000008

ABII-Se:

Lattice constant (Ao) a=	unit-cell volume (a.u.)^3	attice parameter (alat) a.u	the Fermi energy (ev)	hydrostatic pressure (kbar)	total energy (Ry)	Ecutwfc	ECutrho	Total Dispersion Force	Total SCF correction
3.23	1524.3065	6.1038	3.4190	-5.94	-1725.336	90	560	0.008042	0.000122
relax	1524.3065	6.1038	3.3490	0.44	-1725.344	90	560	0.006184	0.000031

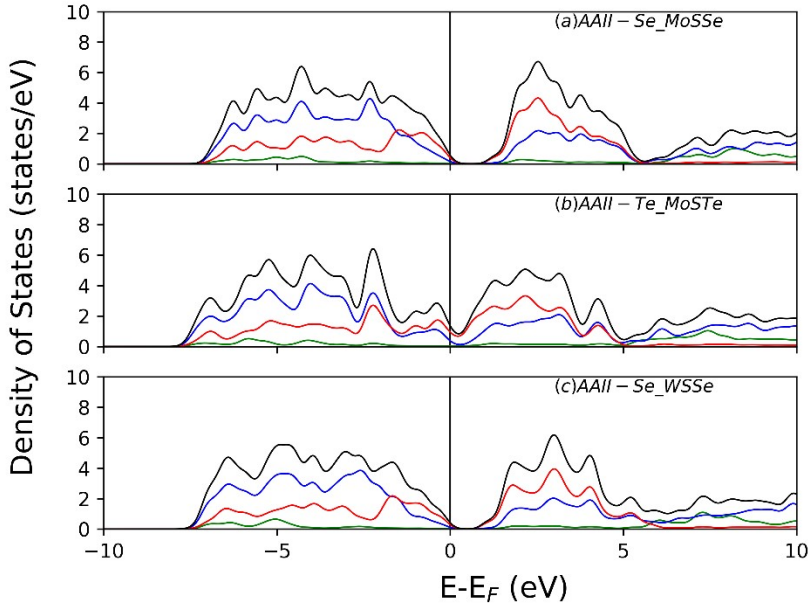

Figure S1: Density of state of the three heterostructures are presented. The green, blue, red and black line represents the s-orbital, p- orbital, d- orbital and sum of the orbitals.