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Janus Ga_2SeTe/In_2SSe heterostructures: Tunable electronic, optical, and photocatalytic properties

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Table S1 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 1 Ga_2SeTe/In_2SSe heterostructure (HS1) with five different stacking patterns using the vdW corrections of D2.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.89	3.89	3.99	-0.14
AB	3.89	3.89	3.15	-0.25
AC	3.89	3.89	3.67	-0.14
AD	3.90	3.90	3.10	-0.22
AE	3.90	3.90	3.08	-0.22

Table S2 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 2 Ga_2SeTe/In_2SSe heterostructure (HS2) with five different stacking patterns using the vdW corrections of D2.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.89	3.89	3.90	-0.16
AB	3.89	3.89	3.27	-0.28
AC	3.89	3.89	3.95	-0.16
AD	3.90	3.90	3.22	-0.25
AE	3.90	3.90	3.21	-0.26

Table S3 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 3 Ga_2SeTe/In_2SSe heterostructure (HS3) with five different stacking patterns using the vdW corrections of D2.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.89	3.89	3.78	-0.12
AB	3.90	3.90	3.05	-0.23
AC	3.89	3.89	3.76	-0.13
AD	3.89	3.89	3.03	-0.20
AE	3.89	3.89	3.02	-0.20

Table S4 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 4 Ga_2SeTe/In_2SSe heterostructure (HS4) with five different stacking patterns using the vdW corrections of D2.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.89	3.89	3.97	-0.14
AB	3.89	3.89	3.19	-0.26
AC	3.90	3.90	3.95	-0.15
AD	3.89	3.89	3.15	-0.23
AE	3.89	3.89	3.16	-0.24

Table S5 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 1 Ga_2SeTe/In_2SSe heterostructure (HS1) with five different stacking patterns using the vdW corrections of D3.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.97	3.97	3.83	-0.16
AB	3.98	3.98	3.18	-0.24
AC	3.97	3.97	3.83	-0.16
AD	3.98	3.98	3.10	-0.23
AE	3.98	3.98	3.20	-0.23

Table S6 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 2 Ga_2SeTe/In_2SSe heterostructure (HS2) with five different stacking patterns using the vdW corrections of D3.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.97	3.97	3.87	-0.17
AB	3.97	3.97	3.16	-0.25
AC	3.97	3.97	3.82	-0.16
AD	3.98	3.98	3.13	-0.24
AE	3.98	3.98	3.23	-0.24

Table S7 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 3 Ga_2SeTe/In_2SSe heterostructure (HS3) with five different stacking patterns using the vdW corrections of D3.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.98	3.98	3.86	-0.15
AB	3.98	3.98	3.18	-0.23
AC	3.97	3.97	3.83	-0.14
AD	3.98	3.98	3.10	-0.23
AE	3.98	3.98	3.22	-0.22

Table S8 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 4 Ga_2SeTe/In_2SSe heterostructure (HS4) with five different stacking patterns using the vdW corrections of D3.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.97	3.97	3.88	-0.16
AB	3.98	3.98	3.18	-0.24
AC	3.97	3.97	3.80	-0.15
AD	3.98	3.98	3.10	-0.23
AE	3.98	3.98	3.11	-0.24

Table S9 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 1 Ga_2SeTe/In_2SSe heterostructure (HS1) with five different stacking patterns using the vdW corrections of dDsC.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.95	3.95	3.81	-0.16
AB	3.95	3.95	3.22	-0.22
AC	3.94	3.94	4.00	-0.17
AD	3.95	3.95	3.08	-0.22
AE	3.94	3.94	3.30	-0.21

Table S10 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 2 Ga_2SeTe/In_2SSe heterostructure (HS2) with five different stacking patterns using the vdW corrections of dDsC.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.95	3.89	3.88	-0.16
AB	3.95	3.89	3.27	-0.22
AC	3.94	3.89	3.96	-0.16
AD	3.94	3.90	3.10	-0.21
AE	3.95	3.90	3.23	-0.21

Table S11 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 3 Ga_2SeTe/In_2SSe heterostructure (HS3) with five different stacking patterns using the vdW corrections of dDsC.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.95	3.95	3.88	-0.14
AB	3.95	3.95	3.12	-0.22
AC	3.94	3.94	3.97	-0.15
AD	3.95	3.95	3.11	-0.23
AE	3.95	3.95	3.25	-0.22

Table S12 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 4 Ga_2SeTe/In_2SSe heterostructure (HS4) with five different stacking patterns using the vdW corrections of dDsC

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.94	3.94	3.85	-0.16
AB	3.95	3.95	3.20	-0.23
AC	3.94	3.94	3.96	-0.15
AD	3.95	3.95	3.18	-0.22
AE	3.95	3.95	3.20	-0.22

Table S13 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 1 Ga_2SeTe/In_2SSe heterostructure (HS1) with five different stacking patterns using the vdW corrections of TS.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.98	3.98	3.87	-0.16
AB	3.99	3.99	3.33	-0.25
AC	3.99	3.99	3.88	-0.16
AD	3.99	3.99	3.10	-0.23
AE	3.99	3.99	3.20	-0.24

Table S14 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 2 Ga_2SeTe/In_2SSe heterostructure (HS2) with five different stacking patterns using the vdW corrections of TS.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.98	3.98	3.90	-0.16
AB	3.99	3.99	3.24	-0.25
AC	3.99	3.99	3.87	-0.16
AD	3.98	3.98	3.13	-0.24
AE	3.99	3.99	3.28	-0.25

Table S15 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 3 Ga_2SeTe/In_2SSe heterostructure (HS3) with five different stacking patterns using the vdW corrections of TS

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.98	3.98	3.92	-0.16
AB	3.99	3.99	3.31	-0.25
AC	3.99	3.99	3.78	-0.15
AD	4.00	4.00	3.13	-0.23
AE	3.99	3.99	3.12	-0.24

Table S16 Calculated lattice parameters (*a* and *b*), and interlayer distance (*d*) and binding energy for model 4 Ga_2SeTe/In_2SSe heterostructure (HS4) with five different stacking patterns using the vdW corrections of TS.

Stacking patterns	*a*(Å)	*b*(Å)	*d*(Å)	E_b(eV)
AA	3.98	3.98	3.85	-0.16
AB	3.99	3.99	3.35	-0.26
AC	3.98	3.98	3.89	-0.15
AD	3.99	3.99	3.16	-0.25
AE	3.99	3.99	3.27	-0.25

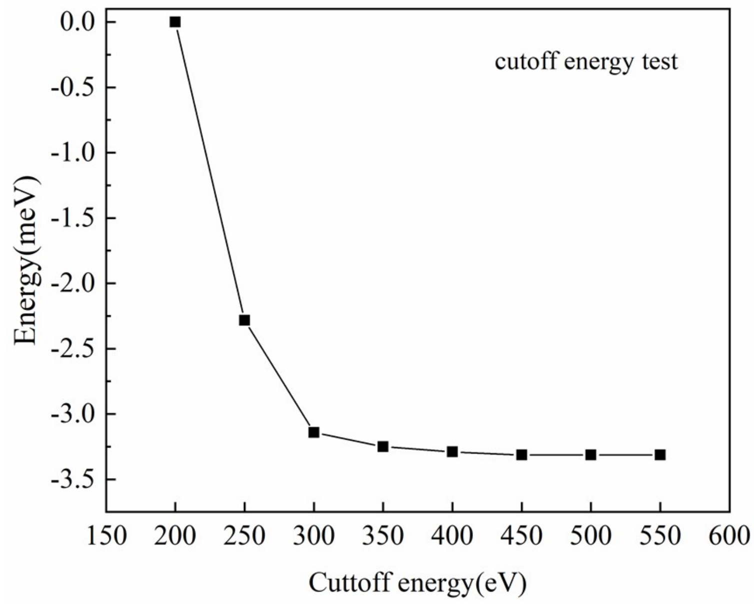

Figure S1. Cut off energy (E_{cut}) test for the Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructures system, where the energy at E_{cut} =200 eV has been set to 0.

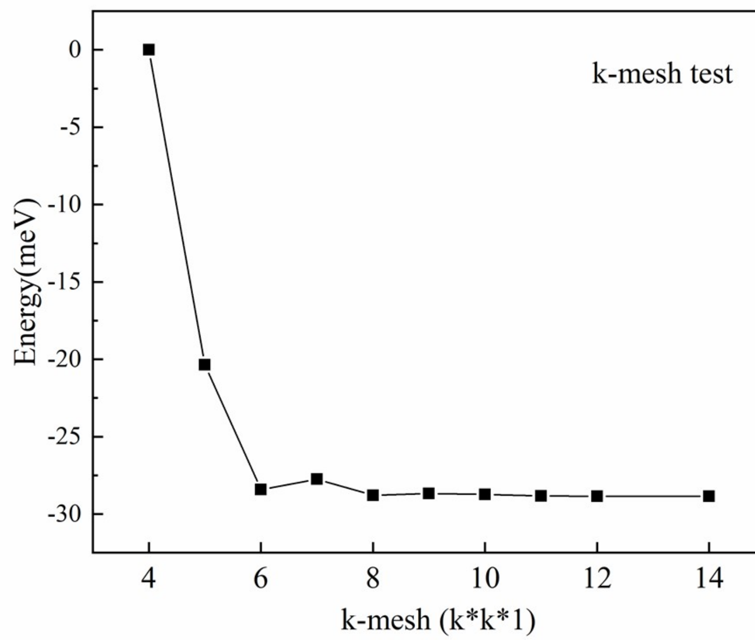

Figure S2. Total energy of Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructures as a function of k-mesh. Here, the energy of k-mesh=4*4*1 is set to 0.

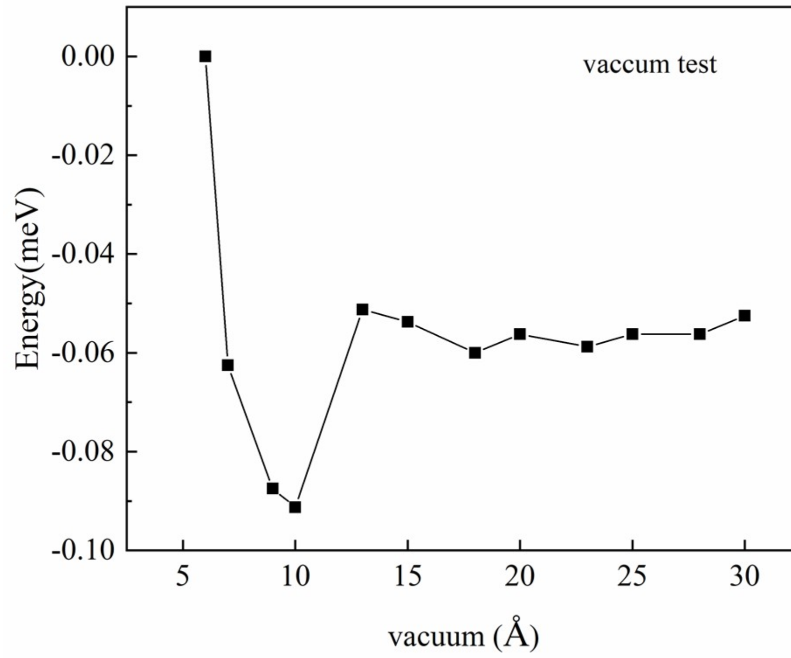

Figure S3. Total energy of Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructures as a function of vacuum region. Here, the energy with a vacuum region of 6 Å is set to 0.

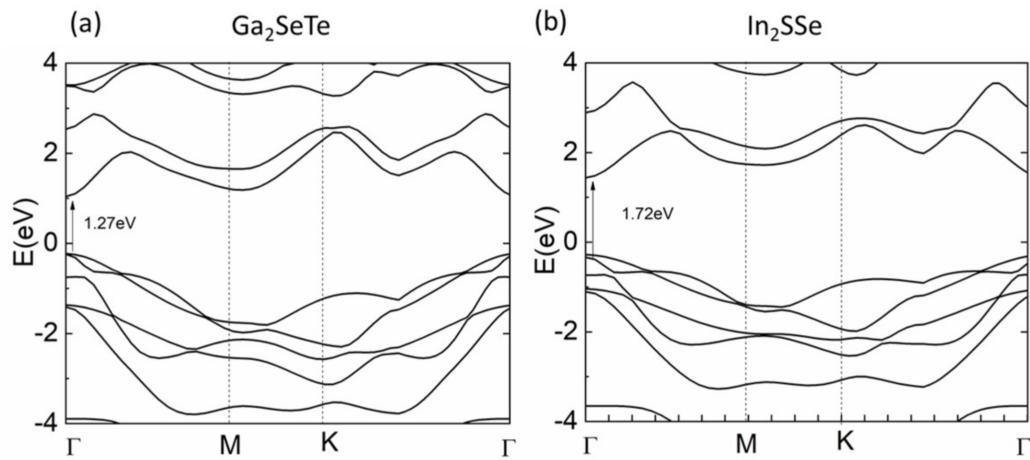

Figure S4. The PBE band structure of single layer janus Ga_2SeTe and In_2SSe.

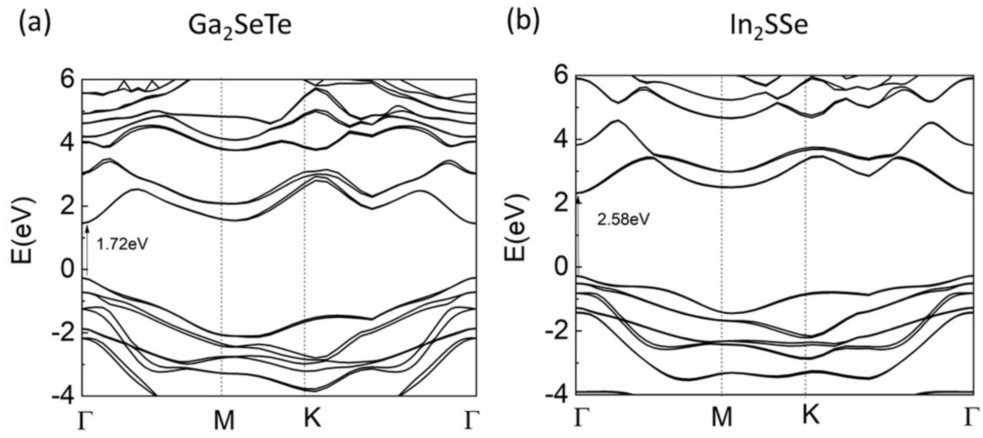

Figure S5. The HSE06+SOC band structure of single layer janus Ga_2SeTe and In_2SSe.

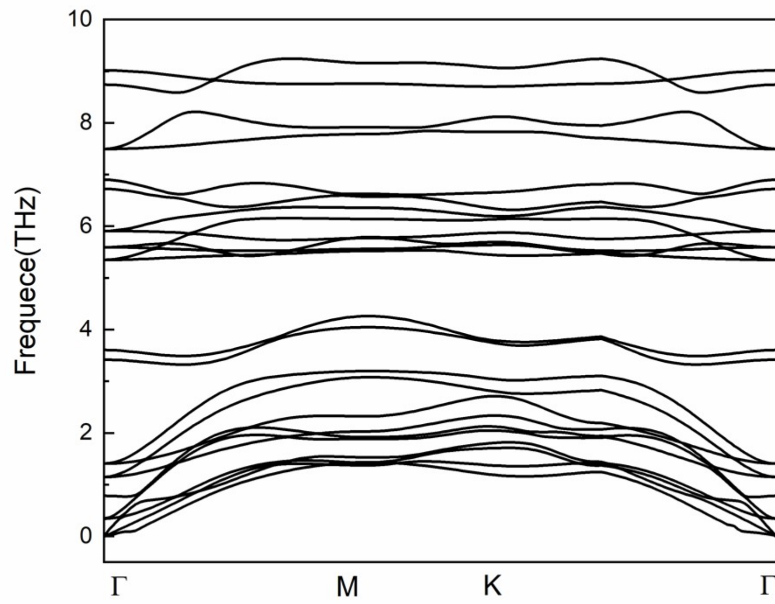

Figure S6. Phonon spectrum of Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructures.

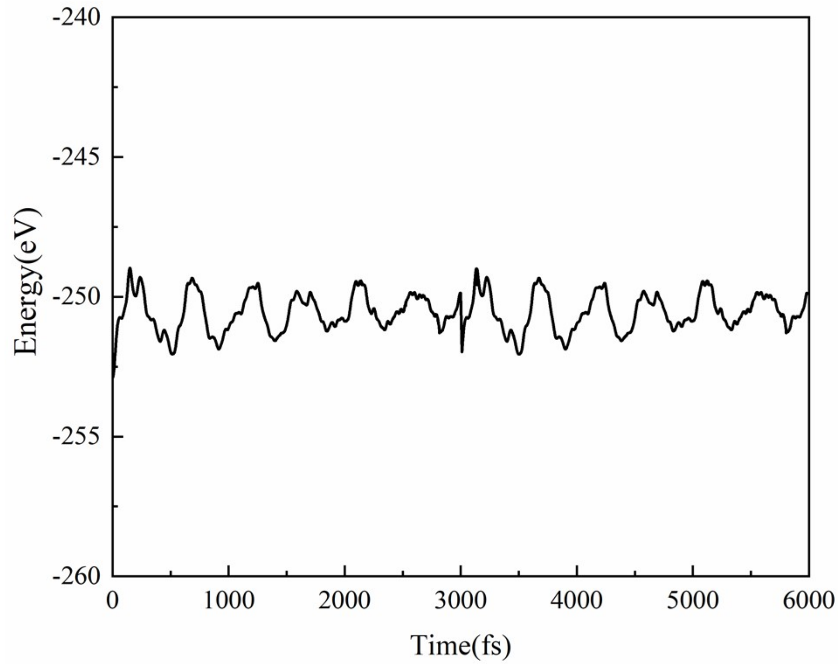

Figure S7. The variation of total energy of Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructures as a function of time at temperature 300 K.

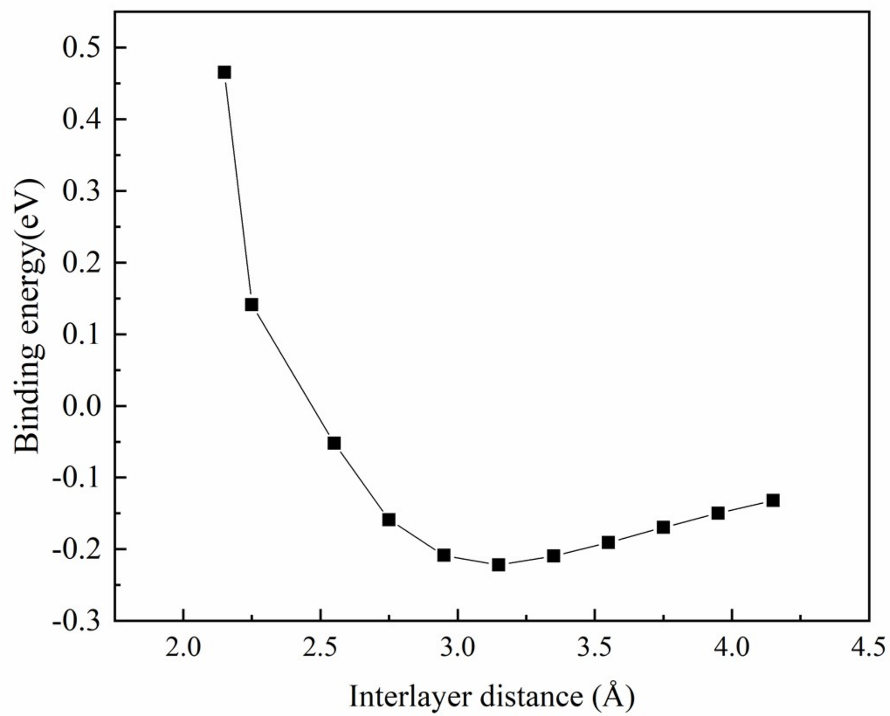

Figure S8. The variation of the binding energy of Ga_2SeTe/In_2SSe (HS1-AB) vdw heterostructure as a function of interlayer distance.

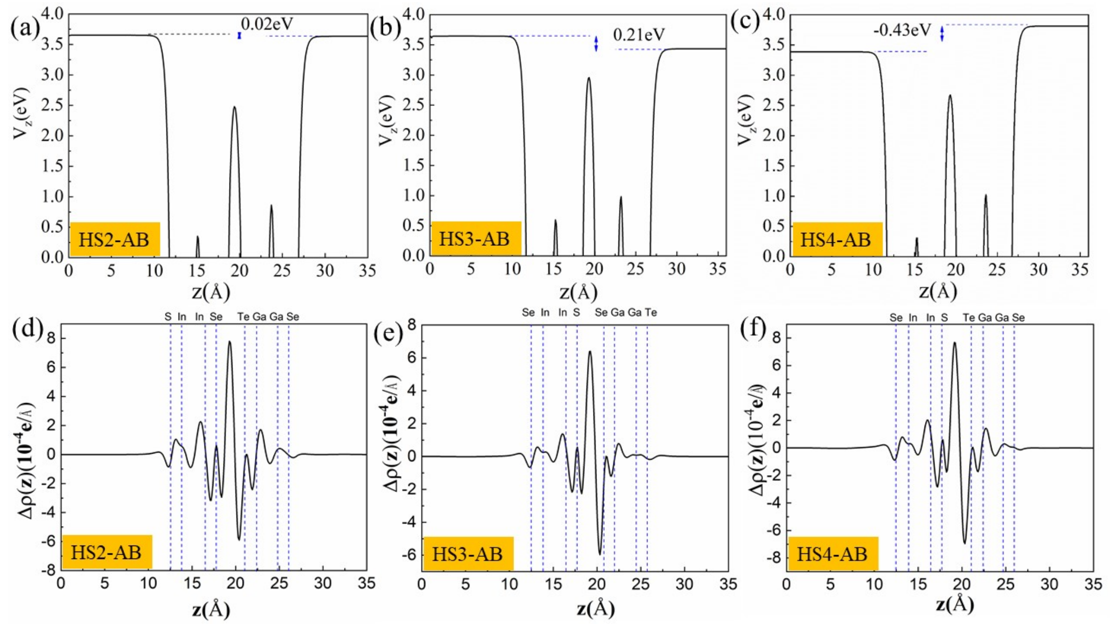

Figure S8. The average potential energy of janus Ga_2SeTe /In_2SSe heterostructures: (a) HS2-AB, (b) HS3-AB, and (c) HS4-AB. Planar averaged charge density difference of janus Ga_2SeTe /In_2SSe heterostructures: (d) HS2-AB, (e) HS3-AB, and (f) HS4-AB.

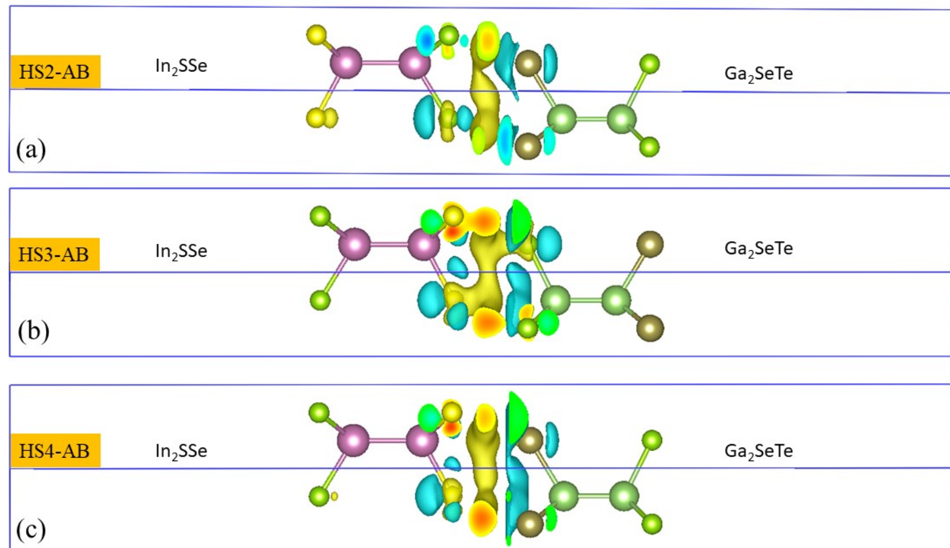

Figure S9. 3D isosurface of the differential electron density of janus Ga_2SeTe/In_2SSe heterostructures (with the isovalue 0.0001e/ Å^3): (a) HS2-AB, (b) HS3-AB, and (c) HS4-AB, where the yellow and cyan regions represent electron accumulation and depletion.

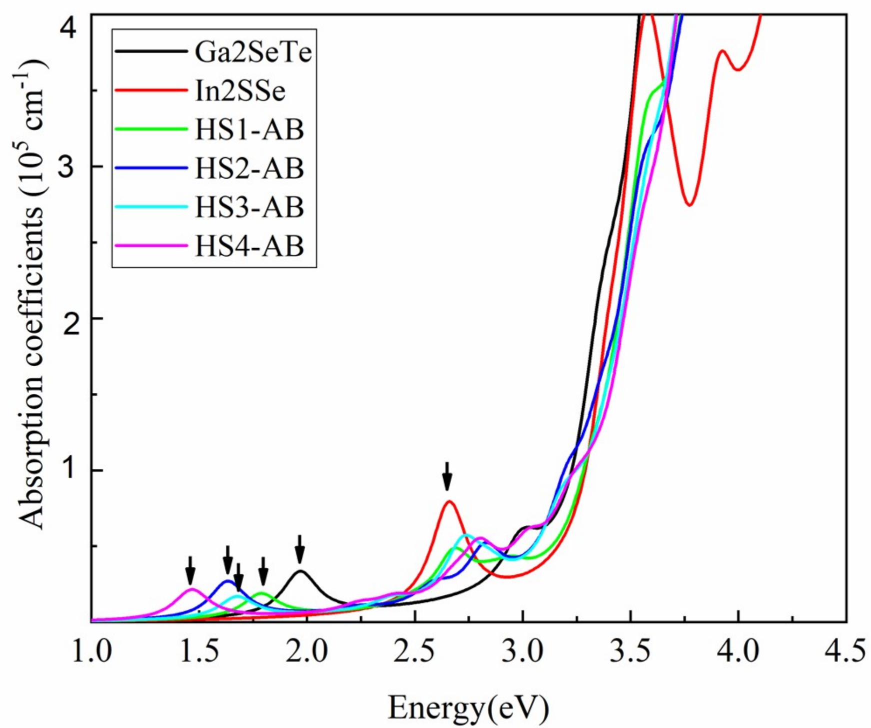

Figure S10. (a) Calculated absorption coefficients of the Janus Ga_2SeTe monolayer, Janus In_2SSe monolayer, and Janus Ga_2SeTe/In_2SSe heterostructures using GW-BSE approach. The first absorption peaks are marked by the arrows.