Electronic supplementary information (ESI)

Effects of stacking method and strain on the electronic properties of the few layered group-IVA monochalcogenides heterojunctions

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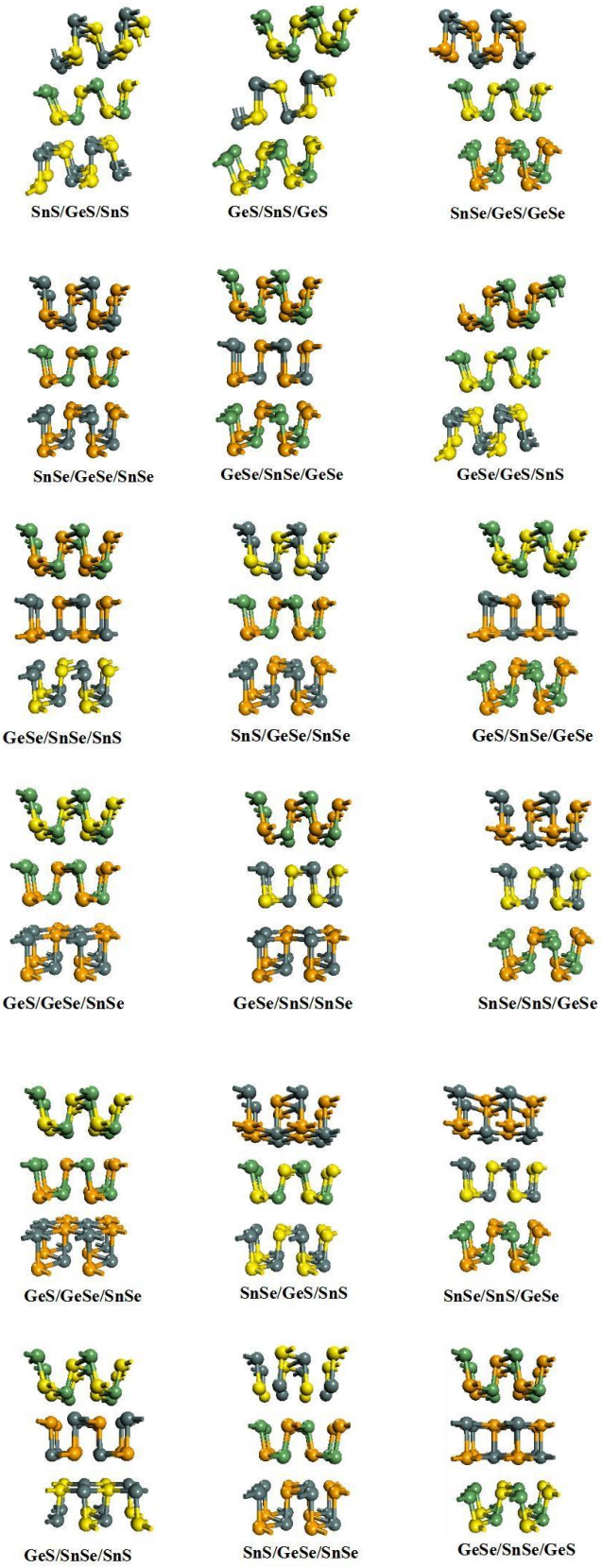

Figure S1. Optimized crystal structure of the eighteen heterojunctions. Among them, yellow, green, orange, and gray balls represent S, Ge, Se, and Sn atoms, respectively.

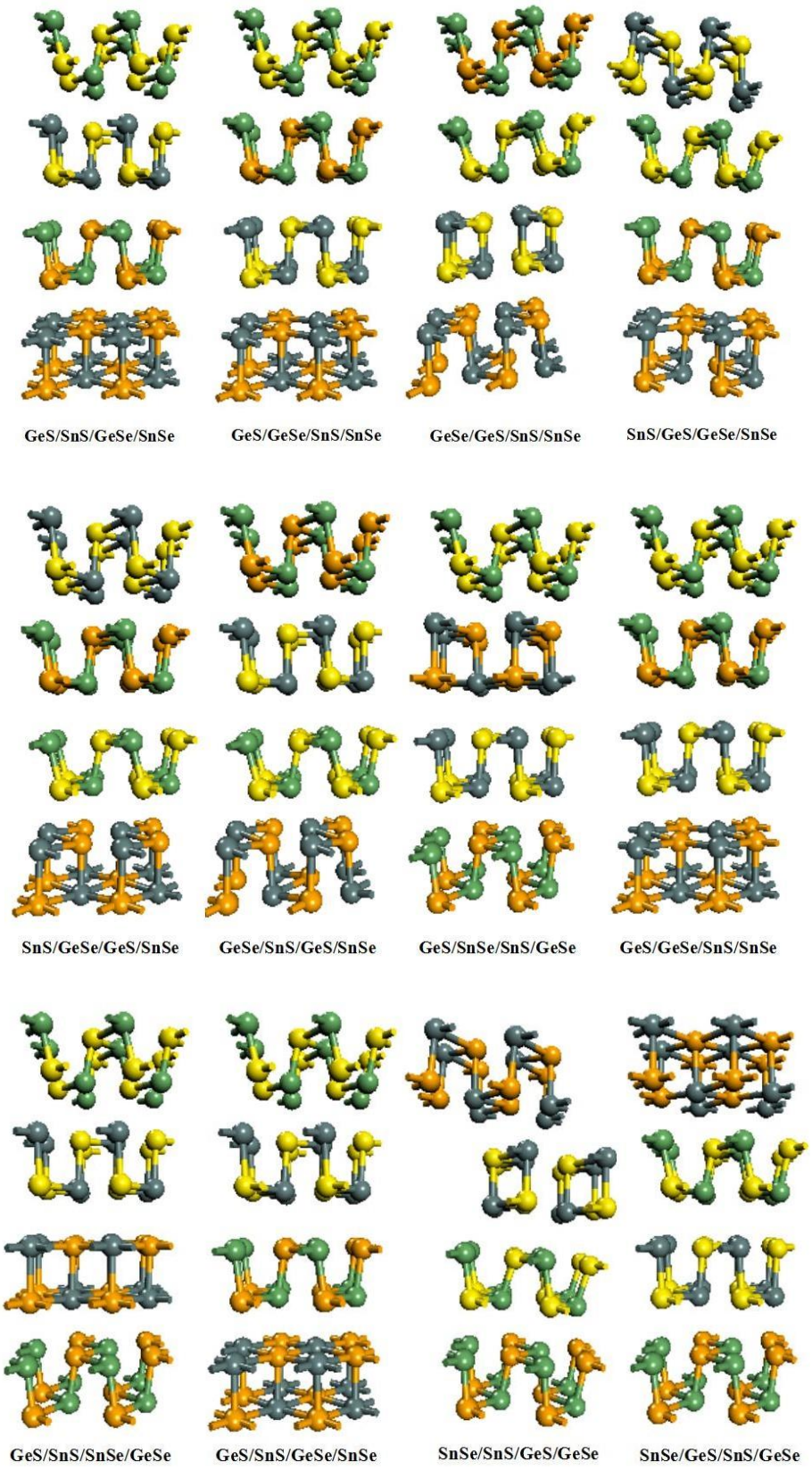

Figure S2. Optimized crystal structure of the twelve heterojunctions. Among them, yellow, green, orange, and gray balls represent S, Ge, Se, and Sn atoms, respectively.

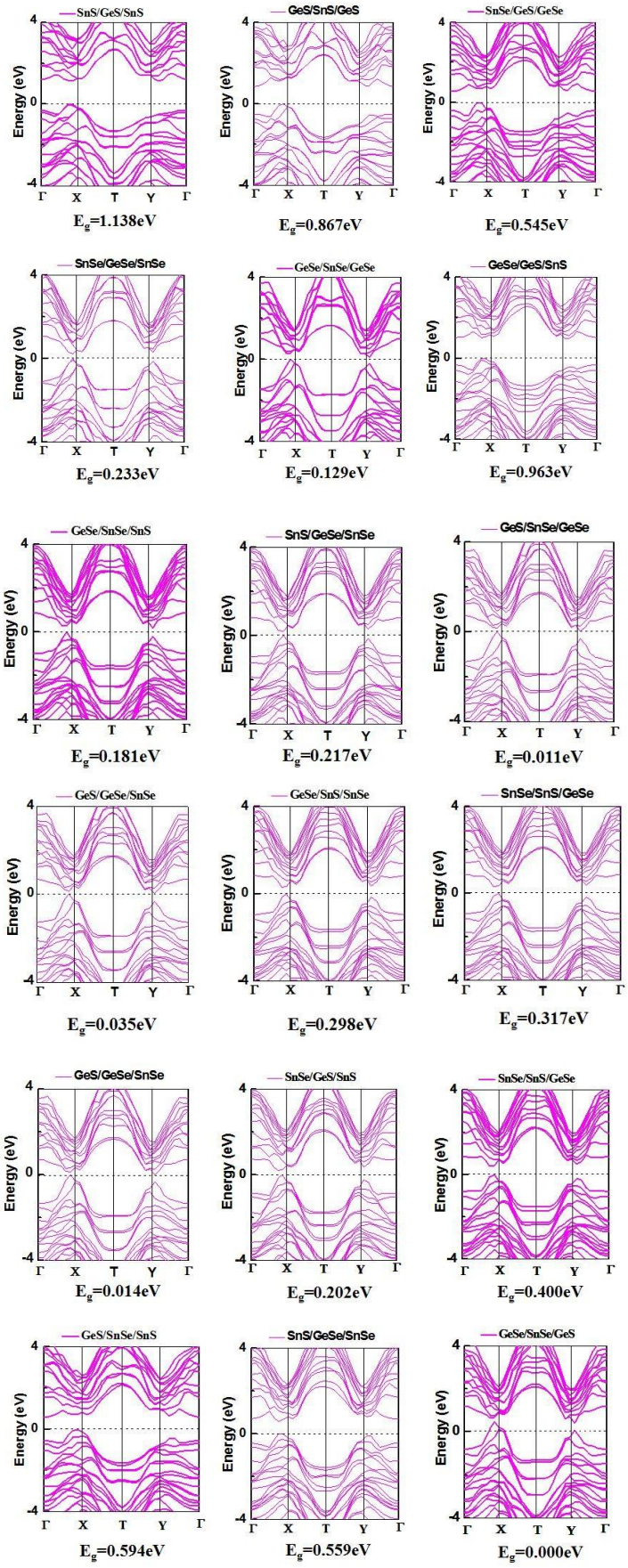

Figure S3. The energy band structures for the eighteen trilayer heterojunctions.

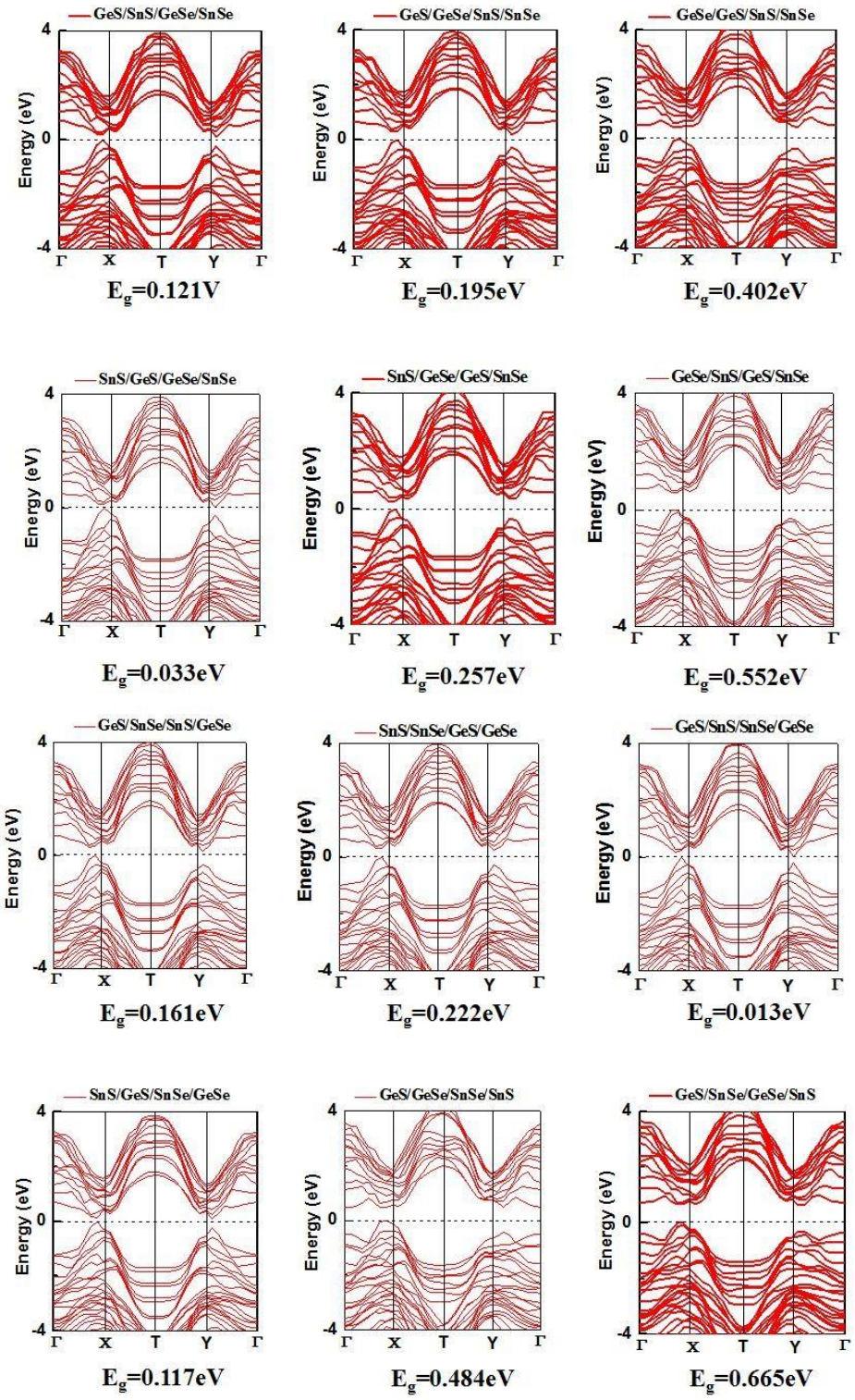

Figure S4. The energy band structures for the twelve four-layer heterojunctions.

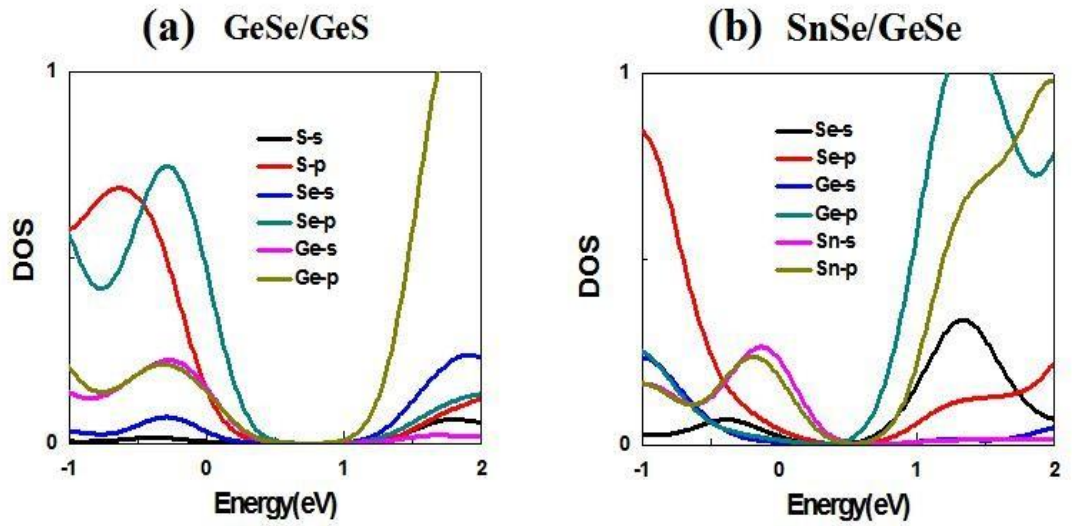

Figure S5. PDOS diagrams of GeSe/GeS (a) and SnSe/GeSe (b) heterojunctions. It's found from Fig. S5(a) that P orbitals of S and Se atoms contribute the VBM most and p orbital of Ge atom contribute the CBM most. It's found from Fig. S5(b) that P orbital of Se atom contribute the VBM most and p orbitals of Ge and Sn atoms contribute the CBM most.

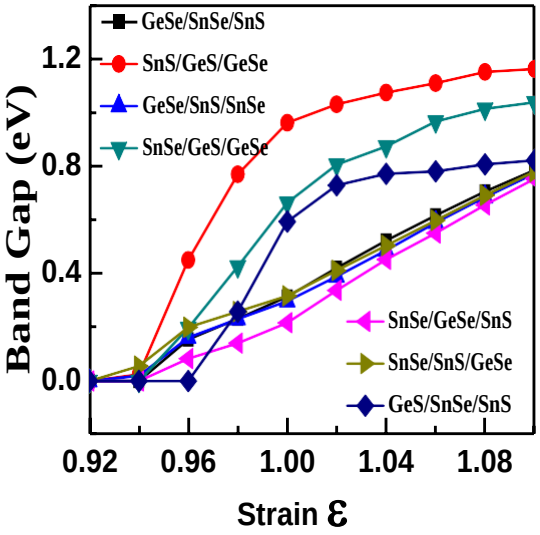

Figure S6. Band gaps variations of the seven trilayer heterojunctions with biaxial strain.

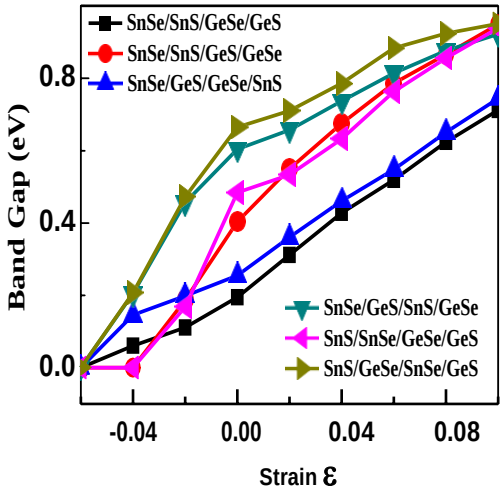

Figure S7. Band gaps variations of the six four-layer heterojunctions with biaxial strain.

Tab. S1 The lattice constants (a and b), the average bond length ($\bar{l}$), and the band gap value (E_g) of the group-IVA monochalcogenides monolayers. In the table, "I " represent indirect gap, and "D "represents direct gap.

Monolayers	a (Å)	b (Å)	$\bar{l}$ (Å)	E_g (eV)
GeS	3.72	4.25	2.45	1.64 I
GeSe	3.97	4.12	2.59	1.20 D
SnS	4.10	4.17	2.71	1.50 I
SnSe	4.25	4.31	2.82	1.10 I

Tab. S2 Lattice constants (a and b), average bond length ($\bar{l}$), average distance between the three monolayers ($\bar{d}$), binding energy (E_b), and band gap (E_g) of the trilayer vdW heterojunction crystals of group-IVA monochalcogenides. In the table, "I " represent indirect gap, and "D "represents direct gap.

Models	a (Å)	b (Å)	$\bar{l}$ (Å)	$\bar{d}$ (Å)	E_b (meV)	E_g (eV)
SnS/GeS/SnS	3.94	4.29	2.60	3.17	-80.8	1.138 I
GeS/SnS/GeS	3.83	4.25	2.51	3.39	-79.7	0.867 I
SnSe/GeS/GeSe	3.96	4.28	2.62	2.92	-56.1	0.545 I
SnSe/GeSe/SnSe	4.14	4.26	2.76	3.14	-72.1	0.233 D
GeSe/SnSe/GeSe	4.04	4.21	2.70	3.12	-74.9	0.129 I
GeSe/GeS/SnS	3.90	4.21	2.56	3.07	-69.7	0.963 I
GeSe/SnSe/SnS	4.10	4.21	2.72	3.15	-74.0	0.181 I
SnS/GeSe/SnSe	4.10	4.22	2.71	3.25	-66.2	0.217 D
GeS/SnSe/GeSe	3.98	4.24	2.63	3.13	-59.5	0.011 I
GeS/GeSe/SnSe	3.99	4.23	2.64	3.18	-53.0	0.035 I
GeSe/SnS/SnSe	4.10	4.22	2.70	3.25	-64.8	0.298 I
SnSe/SnS/GeSe	4.10	4.22	2.71	3.21	-68.9	0.317 I
GeS/GeSe/SnSe	4.00	4.22	2.63	3.19	-53.0	0.014 I
SnSe/GeS/SnS	4.05	4.23	2.64	3.14	-49.0	0.202 I
SnSe/SnS/GeSe	4.10	4.22	2.70	3.22	-68.6	0.400 I
GeS/SnSe/SnS	4.00	4.23	2.64	2.74	-74.4	0.594 I
SnS/GeSe/SnSe	4.10	4.22	2.57	3.06	-50.0	0.559 D
GeSe/SnSe/GeS	4.04	4.21	2.69	3.09	-74.9	0.000

Tab. S3 Lattice constants (a and b), average bond length ($\bar{l}$), average distance between the four monolayers ($\bar{d}$), binding energy (E_b), and band gap (E_g) of the four-layer vdW heterojunction crystals of group-IVA monochalcogenides. In the table, “I ” represent indirect gap, and “D ”represents direct gap.

Models	a (Å)	b (Å)	$\bar{l}$ (Å)	$\bar{d}$ (Å)	E_b (meV)	E_g (eV)
GeS/SnS/GeSe/SnSe	4.02	4.20	2.629	3.19	-67.2	0.121 I
GeS/GeSe/SnS/SnSe	4.01	4.22	2.651	3.20	-67.4	0.195 I
GeSe/GeS/SnS/SnSe	4.01	4.23	2.628	3.42	-72.1	0.402 I
SnS/GeS/GeSe/SnSe	4.01	4.22	2.652	3.08	-69.8	0.033 I
SnS/GeSe/GeS/SnSe	4.01	4.22	2.640	3.14	-63.5	0.257 I
GeSe/SnS/GeS/SnSe	4.01	4.22	2.649	3.07	-69.4	0.552 I
GeS/SnSe/SnS/GeSe	4.01	4.22	2.648	3.06	-73.9	0.161 I
GeS/GeSe/SnS/SnSe	4.01	4.22	2.649	3.17	-66.9	0.222 I
GeS/SnS/SnSe/GeSe	4.02	4.20	2.655	3.09	-74.2	0.013 I
GeS/SnS/GeSe/SnSe	4.02	4.20	2.654	3.13	-68.5	0.117 I
SnSe/SnS/GeS/GeSe	4.00	4.25	2.632	2.98	-75.1	0.484 I
SnSe/GeS/SnS/GeSe	4.00	4.23	2.645	3.11	-69.7	0.625 I

Table S4. Band structure variations with biaxial stress for the six bilayer heterojunctions. In this table, “I ” represent indirect gap, and “D ”represents direct gap.

Band gap (eV)		strain ε										
		-0.10	-0.08	-0.06	-0.04	-0.02	0.00	0.02	0.04	0.06	0.08	0.10
Materials	GeSe/GeS	0	0.008	0.318	0.495	0.683	0.846	0.944	1.030	1.092	1.140	1.186
		-	I	I	I	I	I	I	I	I	I	I
	SnSe/GeSe	0	0	0	0.048	0.173	0.289	0.405	0.521	0.619	0.729	0.829
		-	-	-	I	I	D	D	D	D	D	D
	SnS/GeSe	0	0.162	0.399	0.626	0.651	0.689	0.740	0.796	0.855	0.917	0.978
		-	I	I	I	D	I	D	I	I	D	D
	GeS/SnS	0	0.126	0.276	0.472	0.649	0.725	0.779	0.837	0.898	0.966	1.026
		-	I	I	I	I	D	D	D	D	I	I
	GeS/SnSe	0	0	0.007	0.270	0.513	0.637	0.728	0.811	0.880	0.957	1.022
		-	-	I	I	I	I	D	D	D	I	I
	SnS/SnSe	0	0.020	0.261	0.484	0.610	0.732	0.850	0.962	1.050	1.139	1.216
		-	I	I	I	I	I	I	I	I	I	I

Table S5. Band structure variations with biaxial stress for the seven trilayer heterojunctions. In this table, “I ” represent indirect gap, and “D ”represents direct gap.

Band gap (eV)		strain ε										
		-0.10	-0.08	-0.06	-0.04	-0.02	0.00	0.02	0.04	0.06	0.08	0.10
Materials	GeSe/SnSe/SnS	0	0	0	0.155	0.232	0.314	0.421	0.523	0.617	0.706	0.786
		-	-	-	D	D	D	D	D	D	D	D
	GeSe/GeS/SnS	0	0	0.025	0.451	0.770	0.963	1.031	1.075	1.110	1.152	1.163
		-	-	I	I	I	I	I	I	I	I	I
	GeSe/SnS/SnSe	0	0	0.019	0.162	0.231	0.298	0.390	0.487	0.590	0.685	0.773
		-	-	I	I	I	I	I	I	D	D	D
	SnSe/SnS/GeSe	0	0	0.055	0.200	0.259	0.317	0.412	0.505	0.599	0.692	0.781
		-	-	I	I	I	I	I	I	D	D	D
	SnSe/GeS/GeSe	0	0	0	0.197	0.427	0.665	0.807	0.874	0.967	1.015	1.039
		-	-	-	I	I	D	D	D	I	D	D
	SnS/GeSe/SnSe	0	0	0	0.083	0.141	0.217	0.338	0.453	0.551	0.656	0.754
		-	-	-	I	D	D	D	D	D	D	D
	GeS/SnSe/SnS	0	0	0	0	0.259	0.594	0.730	0.772	0.782	0.808	0.822
		-	-	-	-	I	I	I	I	I	I	I

Table S6. Band structure variations with biaxial stress for the six four-layer heterojunctions. In this table, “I ” represent indirect gap, and “D ”represents direct gap.

Band gap (eV)		strain $\mathcal{E}$										
		-0.10	-0.08	-0.06	-0.04	-0.02	0.00	0.02	0.04	0.06	0.08	0.10
Materials	GeS/GeSe/SnS/SnSe	0	0	0	0.061	0.111	0.195	0.312	0.428	0.519	0.624	0.712
		-	-	-	I	I	I	I	I	I	I	I
	GeSe/GeS/SnS/SnSe	0	0	0	0	0.187	0.404	0.550	0.675	0.786	0.866	0.949
		-	-	-	-	I	I	I	I	I	D	D
	SnS/GeSe/GeS/SnSe	0	0	0	0.146	0.199	0.255	0.361	0.461	0.548	0.651	0.744
		-	-	-	I	I	I	I	I	D	D	D
	GeSe/SnS/GeS/SnSe	0	0	0	0.205	0.457	0.604	0.657	0.737	0.814	0.876	0.922
		-	-	-	I	I	I	D	D	D	D	D
	GeS/GeSe/SnSe/SnS	0	0	0	0	0.168	0.484	0.533	0.632	0.763	0.856	0.939
		-	-	-	-	I	I	I	I	I	I	I
	GeS/SnSe/GeSe/SnS	0	0	0	0.207	0.472	0.625	0.710	0.786	0.883	0.924	0.951
		-	-	-	I	D	I	D	D	I	I	D