Supplementary Material for

Strain-Engineering Tunable Electron Mobility of Monolayer IV-V Group Compounds

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1. *Kinetic stability calculations*

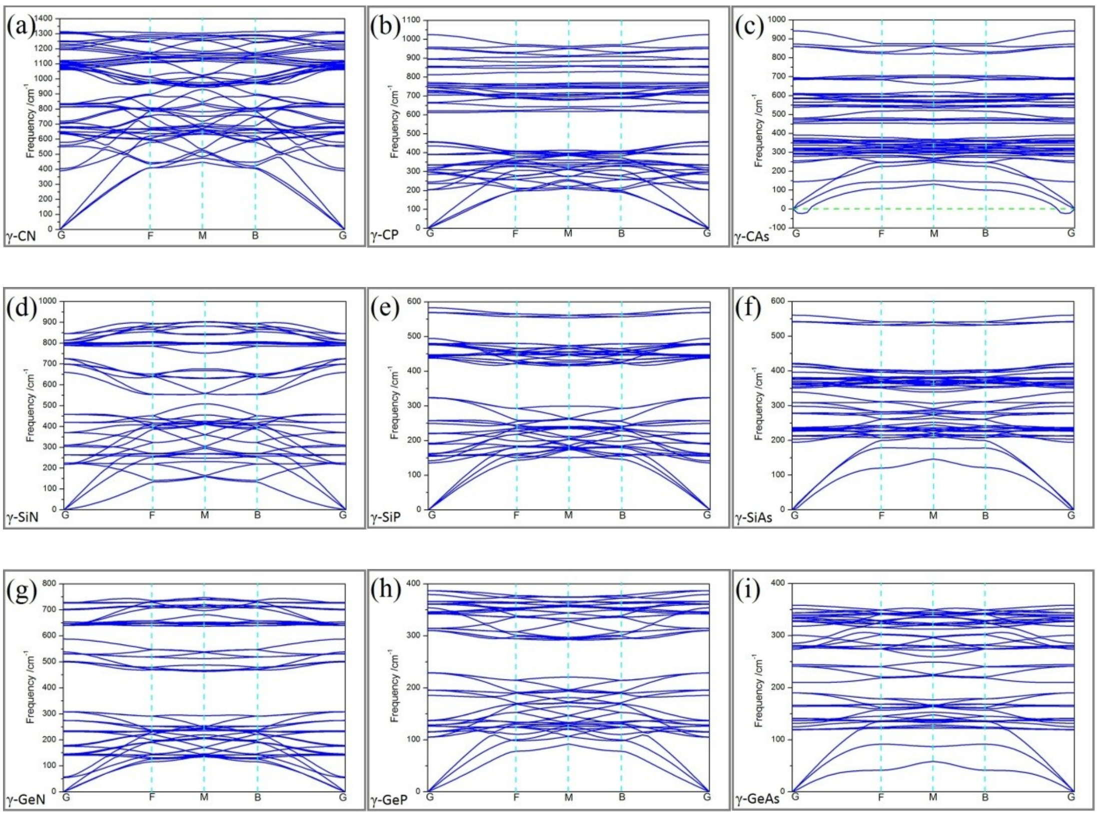


Figure s1. The phonon dispersion curves of monolayer IV-V materials.

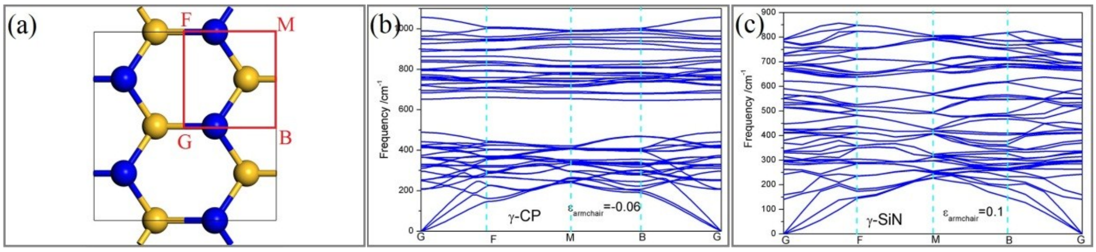


Figure s2. The phonon dispersion curves of monolayer γ-CP and γ-SiN at armchair strains of -0.06 and 0.1, respectively.

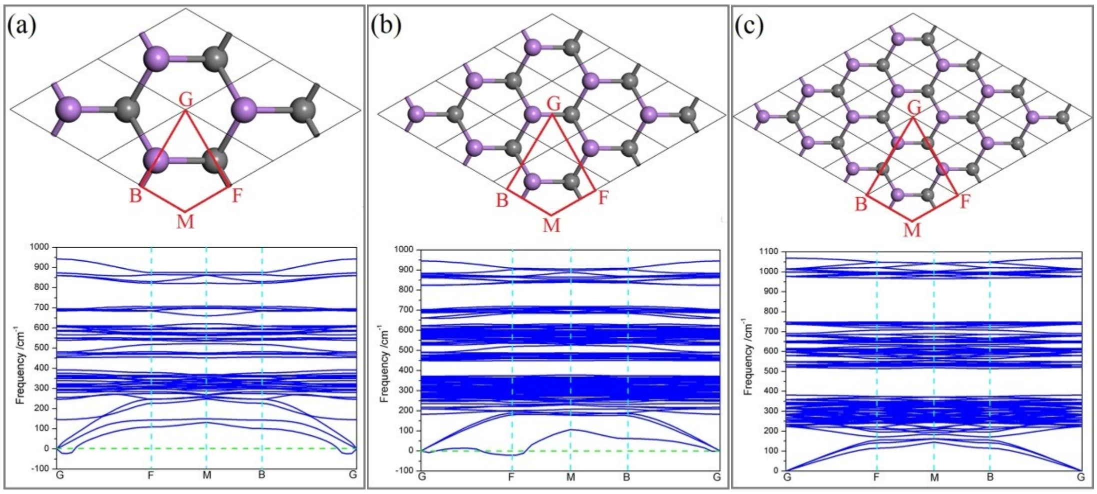
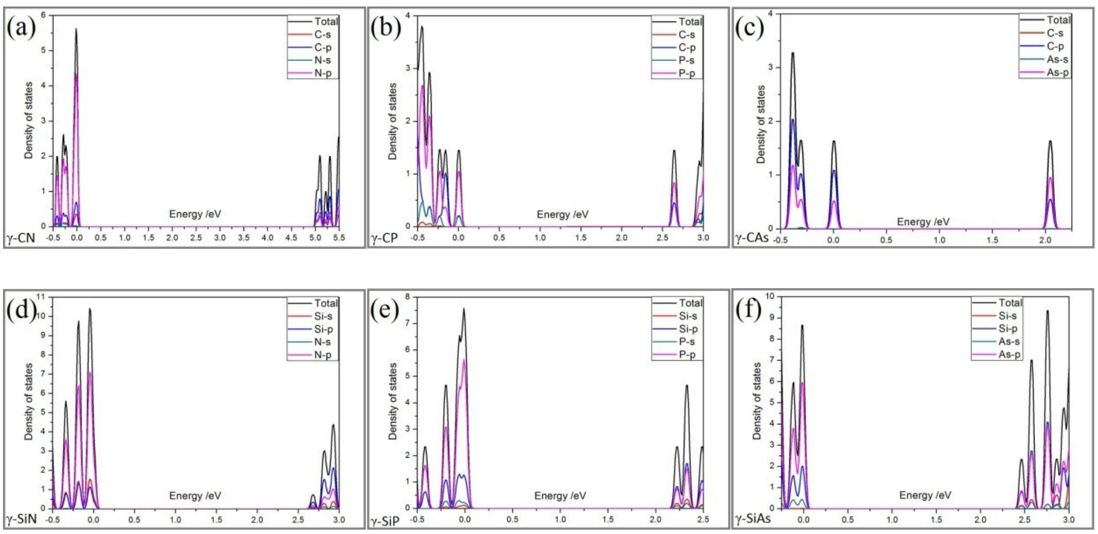


Figure s3. The phonon dispersion curves of 2×2×1, 3×3×1 and 4×4×1 supercells of monolayer γ-CAs.

2. *Density of states calculations*



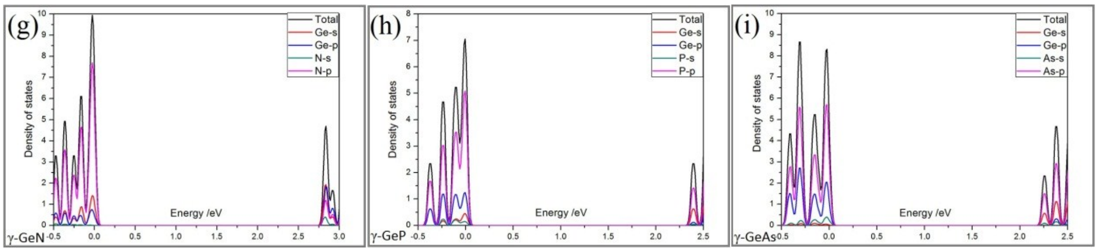


Figure s4. The total and partial densities of states for monolayer IV-V materials.

3. *Intrinsic mobility calculations*

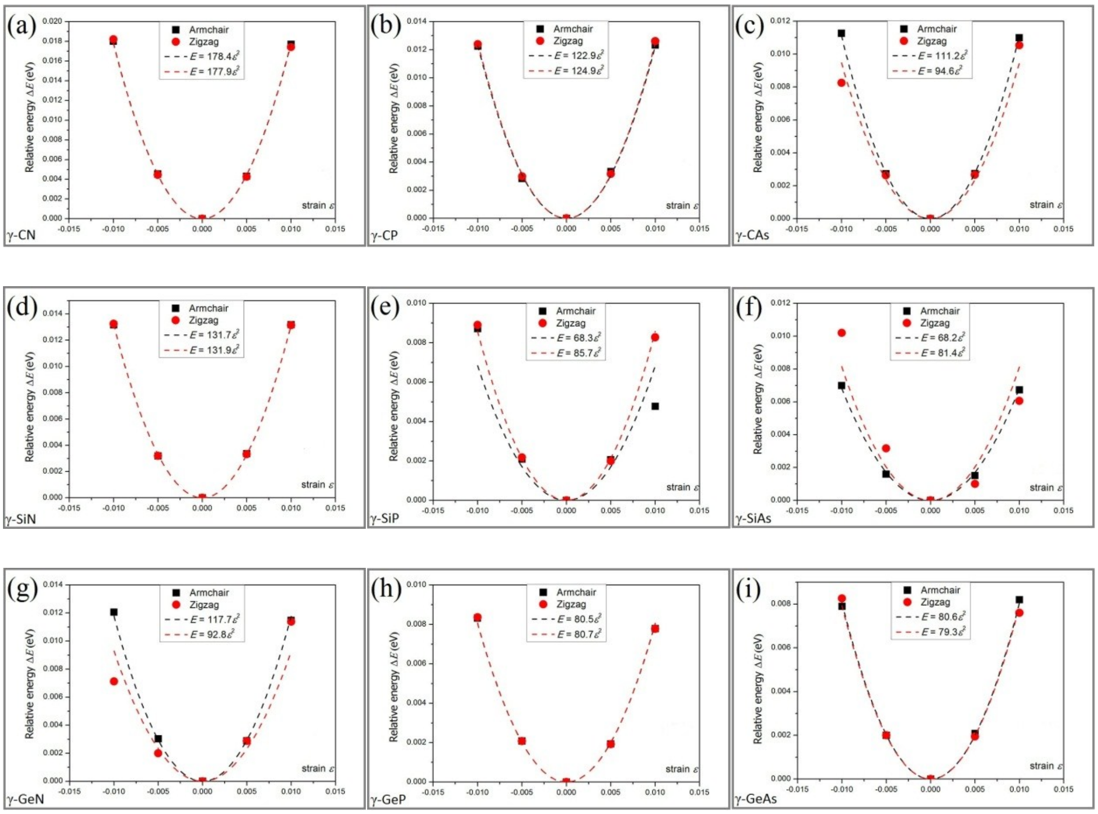
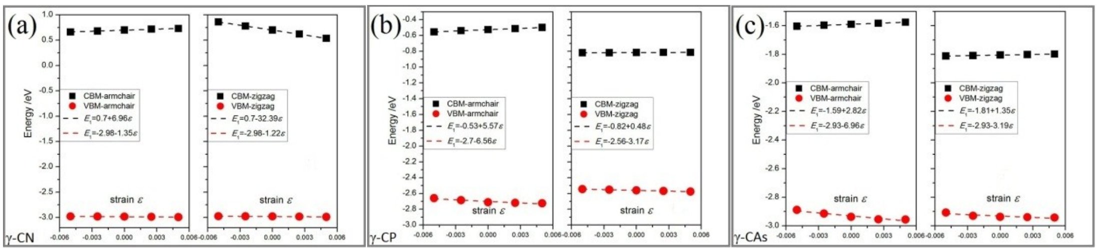


Figure s5. Energy difference between the total energy of relaxed and strained monolayer IV-V materials along zigzag and armchair directions.



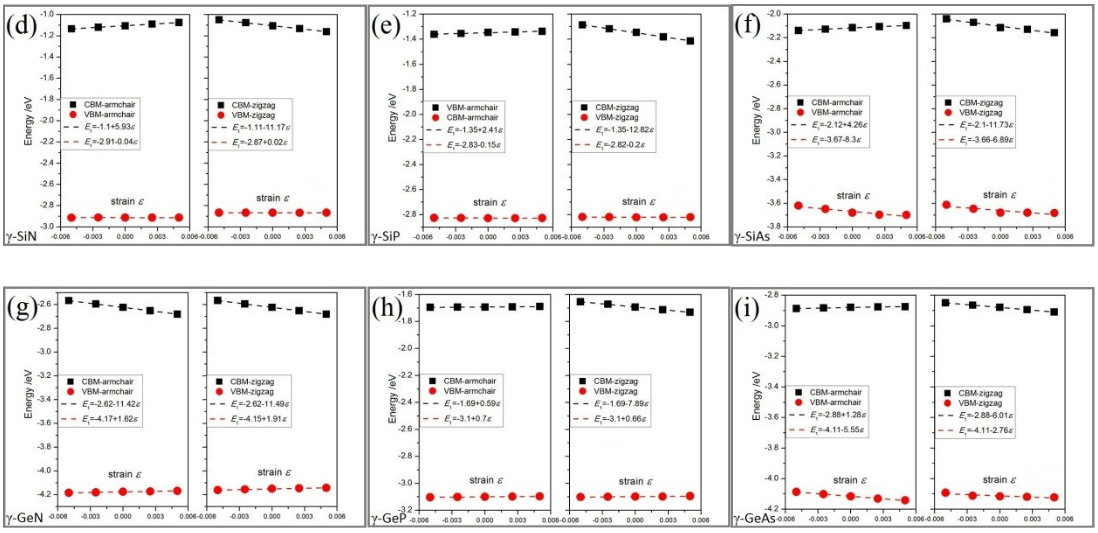


Figure s6. Energy shift of CBM and VBM for monolayer IV-V materials with respect to the lattice dilation and compression along the zigzag and armchair directions, respectively.

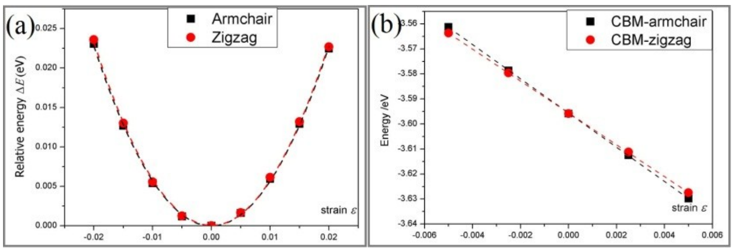


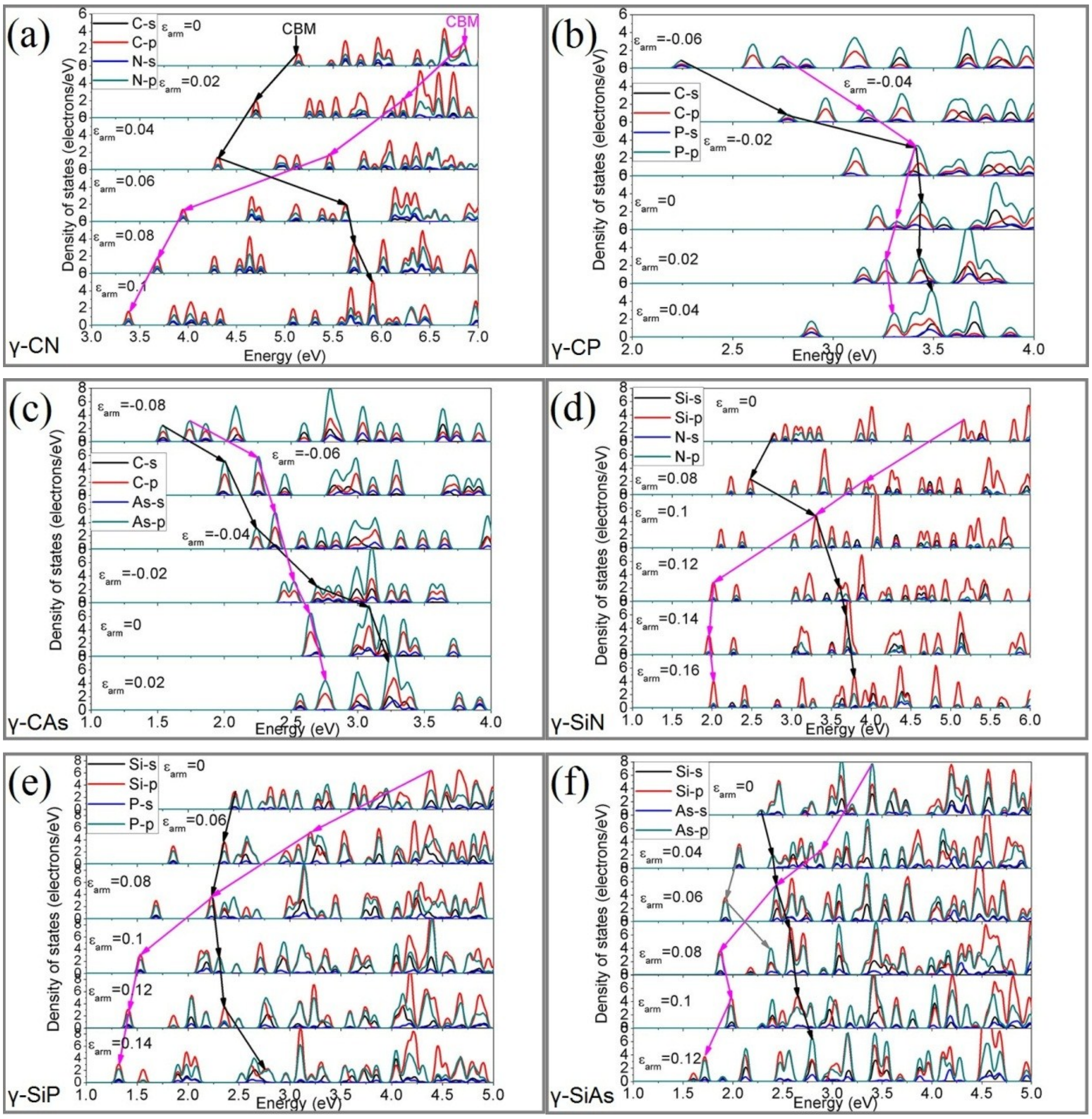
Figure s7. (a) Energy difference between the total energy of relaxed and strained monolayer γ-InSe along zigzag and armchair directions. (b) Energy shift of CBM for monolayer γ-InSe with respect to the lattice dilation and compression along the zigzag and armchair directions, respectively.

Table s1. Calculated free electrons effective masses, DP constant, in-plane stiffness and mobility along armchair and zigzag directions in InSe.

	Effective mass m^*		DP constant ǀE1ǀ(eV)		Stiffness C2d(N/m)		Mobility T(cm^{2}s^{-1}v^{-1})	
	Armchair	Zigzag	Armchair	Zigzag	Armchair	Zigzag	Armchair	Zigzag

Work1[1]	0.197	0.186	5.380	5.222	40.470	49.733	789.615	1090.872
Work2[2]	0.234	0.245	8.90	8.75	73.6	74.5	240	230
Our work	0.196	0.200	6.840	6.370	63.730	64.930	502.970	567.450

4. *Strained electronic and geometric structures*



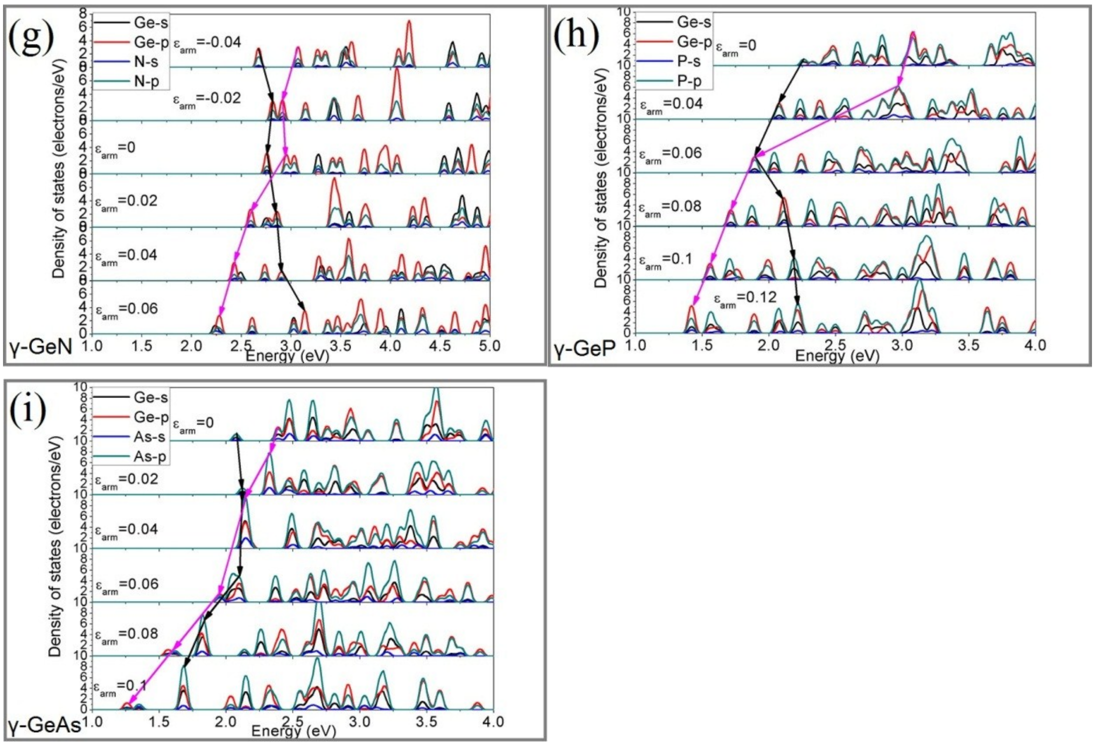


Figure s8. The partial densities of states (conduction bands) for monolayer IV-V materials under strain engineering.

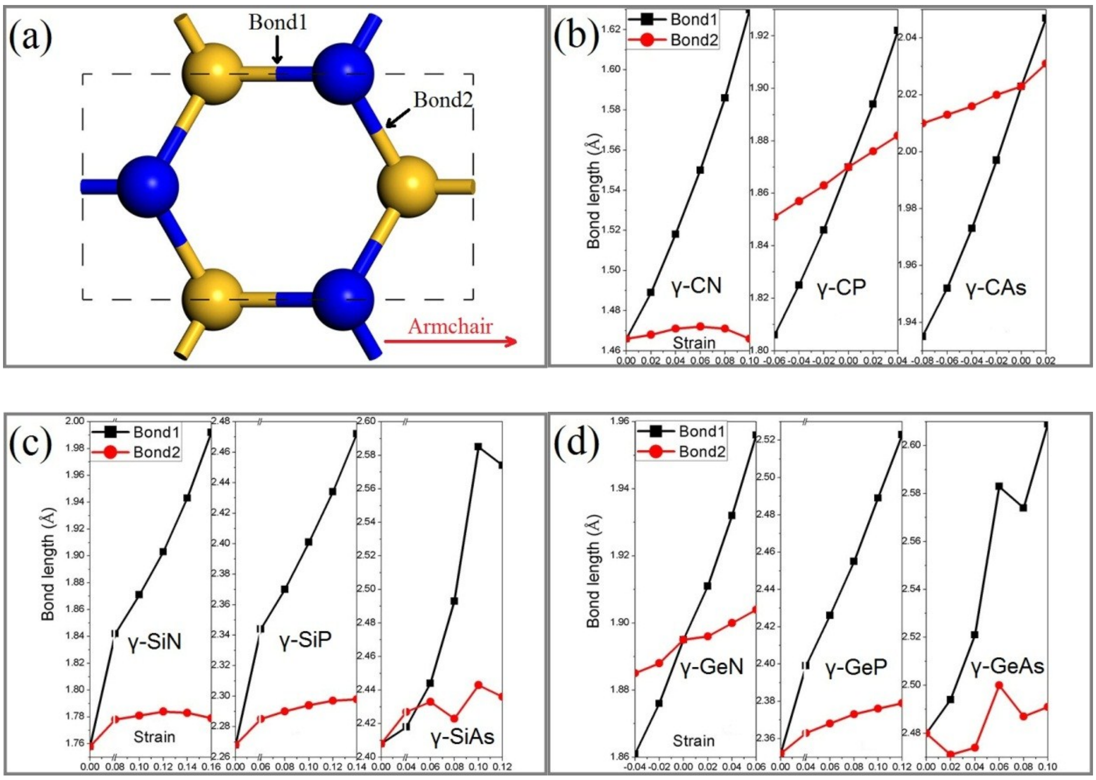


Figure s9. Changes of IV-V bonds under armchair strain engineering progress.

5. *Strained mobility calculations*

Table s2. The stiffness C2d, DP constant E1 and mobility T at 300K of monolayer IV-V materials when a certain armchair uniaxial stain is applied.

γ-CN	ε	0	0.02	0.04	0.06	0.08	0.1
	C2d (N/m)	291.9	283.88	231.43	182.35	106.4	18.32
	E1(eV)	6.96	5.73	7.63	38.7	43.23	43.24
	T($cm^2s^{-1}v^{-1}$)	15.83	105.15	14.46	12.62	3.59	3.15
γ-CP	ε	-0.06	-0.04	-0.02	0	0.02	0.04
	C2d (N/m)	220.62	199.7	179.42	137.45	138.45	117.83
	E1(eV)	6.43	3.17	2.37	5.57	1.69	1.78
	T($cm^2s^{-1}v^{-1}$)	14.77	55	186.43	570.02	8176.11	5670.74
γ-CAs	ε	-0.08	-0.06	-0.04	-0.02	0	0.02
	C2d (N/m)	119.61	164.41	187.10	140.11	108.04	100.01
	E1(eV)	23.64	15.1	16.3	0.9	2.82	0.86
	T($cm^2s^{-1}v^{-1}$)	0	0.18	0.99	17826.23	1418.57	16208.87
γ-SiN	ε	0	0.08	0.1	0.12	0.14	0.16
	C2d (N/m)	145.62	107.55	105.82	60.22	38.97	20.17
	E1(eV)	5.93	6.36	6.5	21.85	22.32	21.9
	T($cm^2s^{-1}v^{-1}$)	58.7	27.74	24.07	48.03	34.63	21.39
γ-SiP	ε	0	0.06	0.08	0.1	0.12	0.14
	C2d (N/m)	50.93	52.23	45.28	37.32	28.09	18.07
	E1(eV)	2.41	2.97	3.02	16.79	15.13	13.4
	T($cm^2s^{-1}v^{-1}$)	46.88	23.46	20.03	126.17	122.91	99.13
γ-SiAs	ε	0	0.04	0.06	0.08	0.1	0.12
	C2d (N/m)	46.48	50.12	42.78	6.65	27.77	25.06
	E1(eV)	4.26	4.67	16.41	6.82	14.23	13.83
	T($cm^2s^{-1}v^{-1}$)	3.58	0.92	189.67	187.5	211.08	201.66
γ-GeN	ε	-0.04	-0.02	0	0.02	0.04	0.06
	C2d (N/m)	136.9	130.63	114.84	110.64	99.09	73.31
	E1(eV)	7.51	7.13	7.2	12.67	14.34	15.56
	T($cm^2s^{-1}v^{-1}$)	31.05	21.97	228.63	213.48	199.72	137.09
γ-GeP	ε	0	0.04	0.06	0.08	0.1	0.12

	C2d (N/m)	56.26	49.49	44.8	36.34	28.59	19.27
	E1(eV)	0.59	1.21	1.7	16.5	14.91	12.73
	T($cm^2s^{-1}v^{-1}$)	6731.33	1829.07	893.8	189.34	189.95	172.1
γ-GeAs	ε	0	0.02	0.04	0.06	0.08	0.1
	C2d (N/m)	51.79	46.26	38.41	35.05	29.82	25.29
	E1(eV)	1.27	2.48	1.88	10.34	13.34	12.35
	T($cm^2s^{-1}v^{-1}$)	1404.25	225.4	604.46	465.02	306.94	318.01

5. ***Reference***

1. Xia, C.; Du, J.; Huang, X.; Xiao, W.; Xiong, W.; Wang, T.; Wei, Z.; Jia, Y.; Shi, J.; Li, J., Two-dimensional n-InSe/p-GeSe(SnS) van der Waals heterojunctions: High carrier mobility and broadband performance. *Physical Review B* 2018, 97, 115416.
2. Chong, S.; Hui, X.; Bo, X.; Yidong, X.; Jiang, Y.; Zhiguo, L., Ab initio study of carrier mobility of few-layer InSe. *Applied Physics Express* 2016, 9, 035203.