Dozen predicated SiGe alloys with low enthalpies and strong absorption to sunlight for photovoltaic applications

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Discussion of RG^2:

The principle of RG2 can be described as follows: the crystal structure can be represented as an infinitely large graph, with the top set used to record atoms and the edge sets describing chemical bonding relationships; The periodic part can be described as a labeled quotient graph. The steps for calculating RG^2 are as follows: the first step is to generate an initial quotient graph, sort all atomic pairs by distance, and form bonds (establish a quotient graph based on the principle of proximity). The second step is to optimize the atomic coordinates and lattice based on the error between the bond length, bond angle determined by the quotient diagram and the reference value. Step three, filter based on the set geometric features. Step 4: Conduct structural optimization, stability assessment, and property research.

Discussion of HSE hybrid function:

Hybrid functionals which include a portion of Hartree-Fock exchange have been successfully applied in the calculation of thermochemical properties of molecules, in addition to yielding good structural properties. The Heyd-Scuseria-Ernzerhof (HSE) hybrid functional originated as an alternative approach that can be efficiently applied to solids. HSE employs screened short-range Hartree-Fock exchange instead of the full exact exchange, drastically reducing the computational requirements and, at the same time, overcoming the known problems of Hartree-Fock exchange. The expression for the HSE exchange-correlation energy is:

$$E_{xc}^{Hse} = aE_x^{HF,\mathrm{SR}} + (1-a)aE_x^{PBE,\mathrm{SR}} + E_x^{PBE,\mathrm{LR}} + E_c^{PBE} \quad (1)$$

where $E_x^{HF,\mathrm{SR}}$ is the short-range Hartree-Fock exchange, $E_x^{\mathrm{PBE,SR}}$ and $E_x^{\mathrm{PBE,LR}}$ are the short-range and long-range components of the Perdew-Burke-Ernzerhof (PBE) exchange functional, respectively, and a=1/4 is the Hartree-Fock exchange mixing parameter determined via perturbation theory. In HSE, the short-range and long-range partition in Eq. 1 is carried out splitting the Coulomb operator as:

$$\frac{1}{r} = \frac{erfc(\omega \mathrm{r})}{r}(SR) + \frac{erfc(\omega \mathrm{r})}{r}(LR)$$

where erf and erfc are the error and complementary error functions, respectively, and ω is the screening parameter.

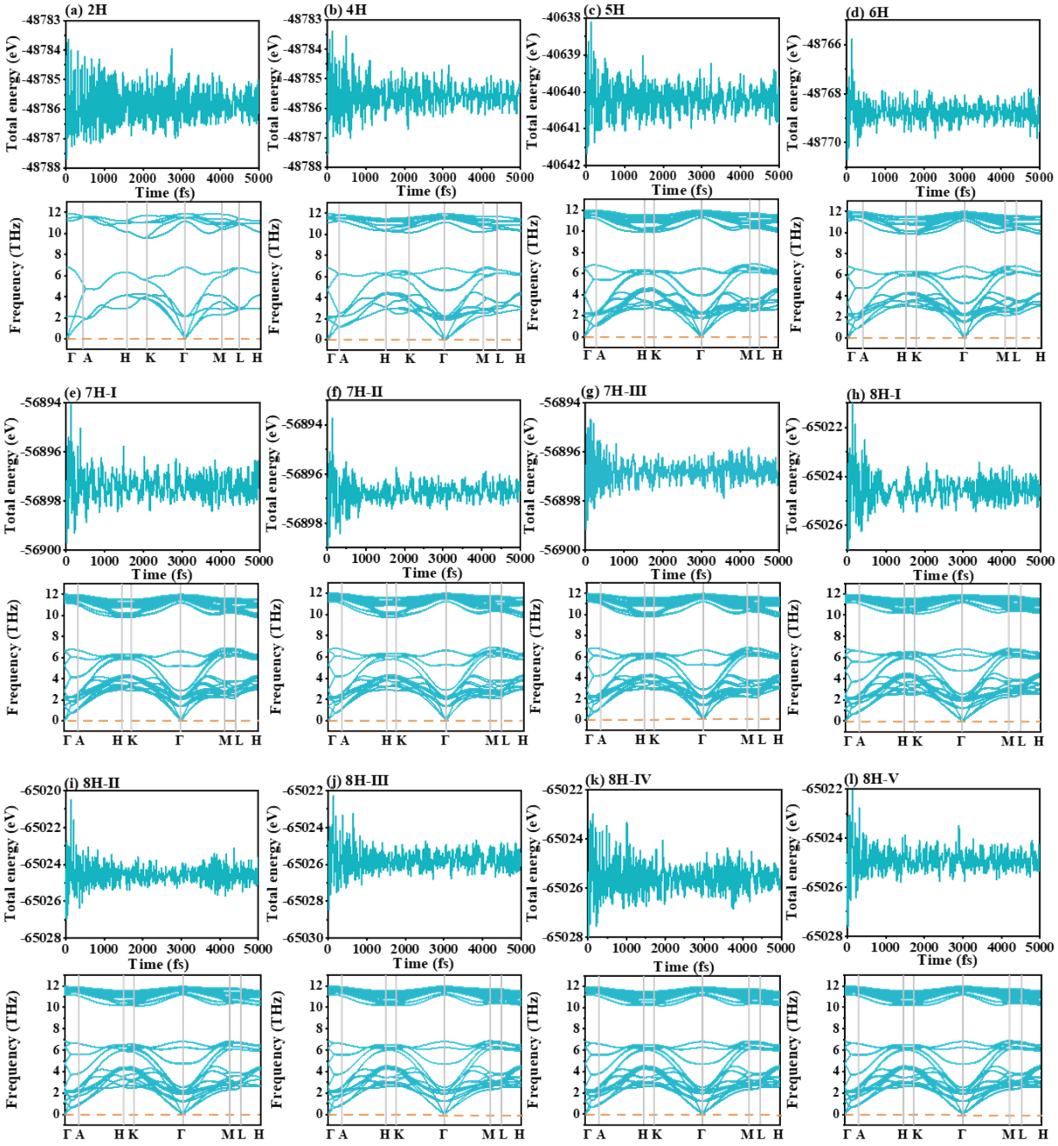

FIG. S1 Total energy fluctuations and phonon spectra of nH SiGe.

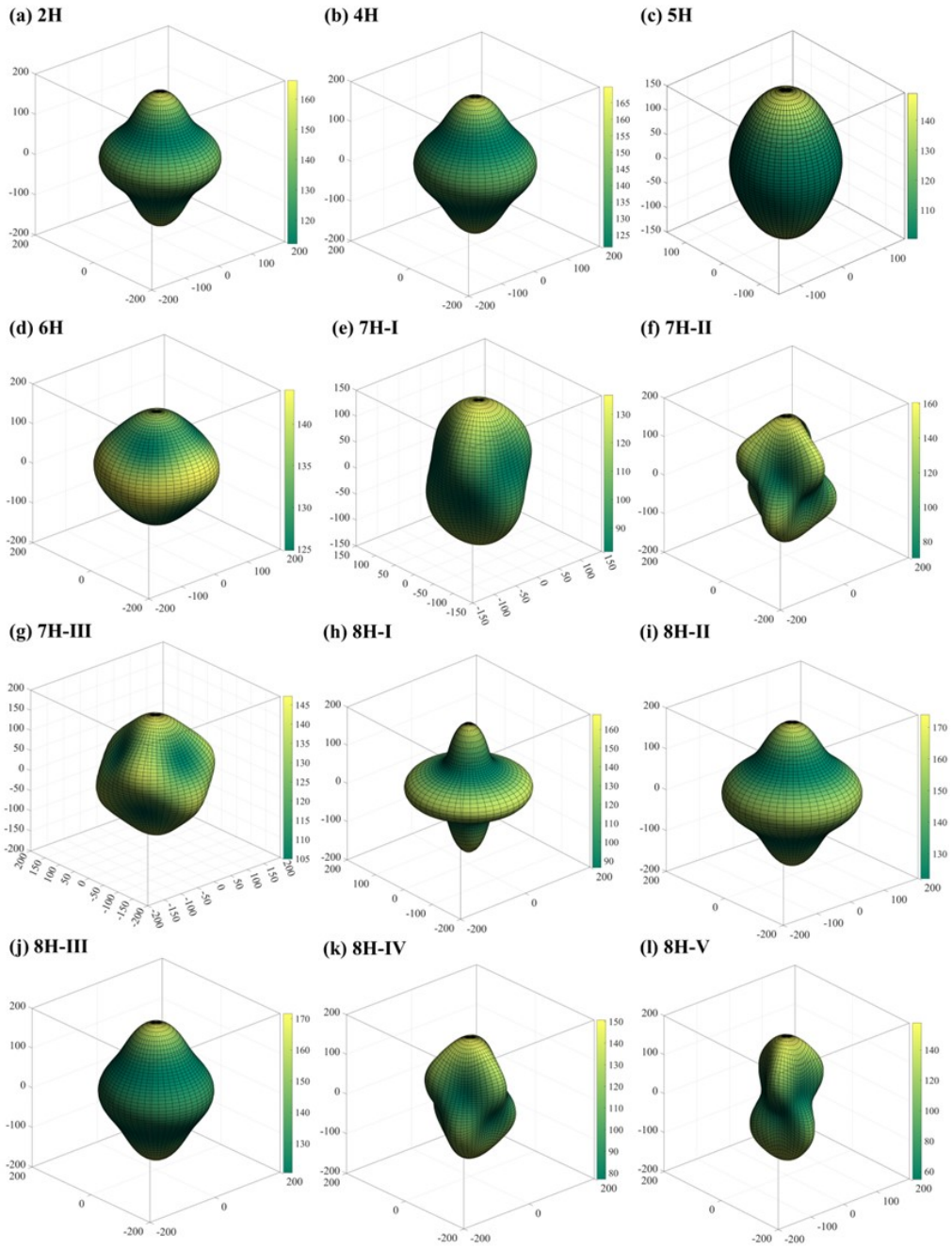

FIG. S2 Directional dependence of the Young's modulus for nH SiGe.

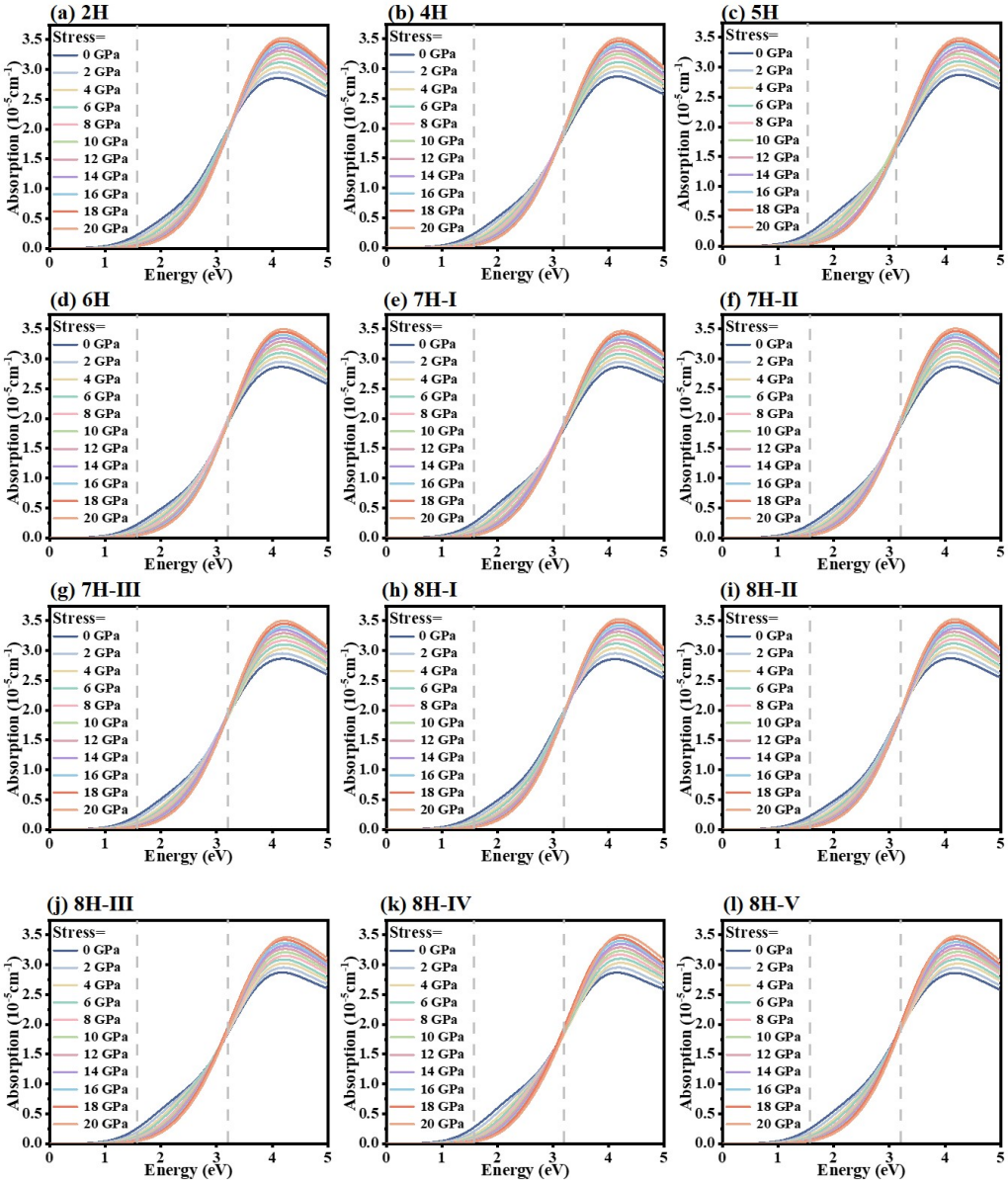

FIG. S3 The relationship between absorption and stress of nH SiGe.

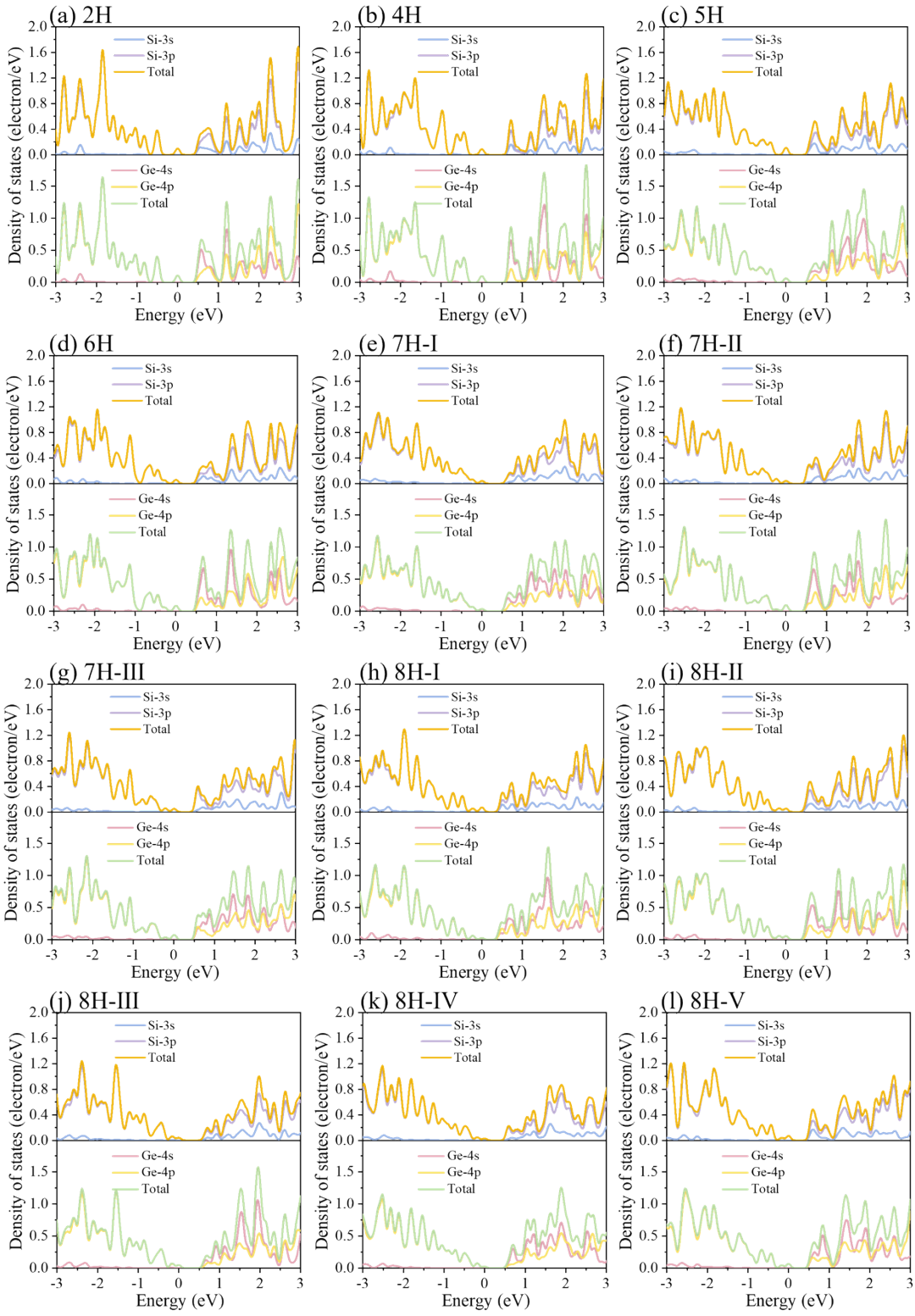

FIG. S4 The PDOS of nH SiGe.

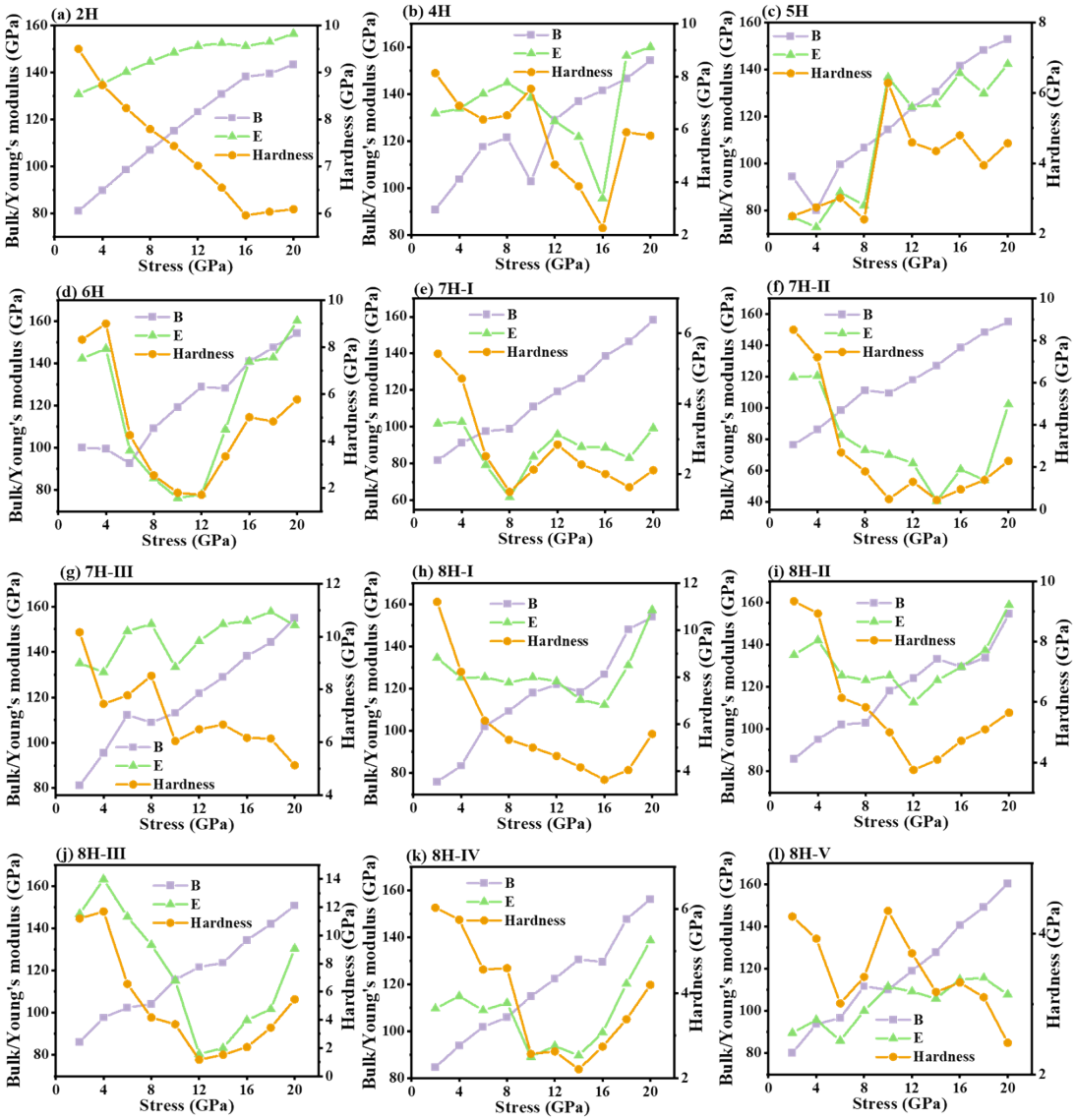

FIG. S5 The relationship between elastic moduli and stress of nH SiGe.

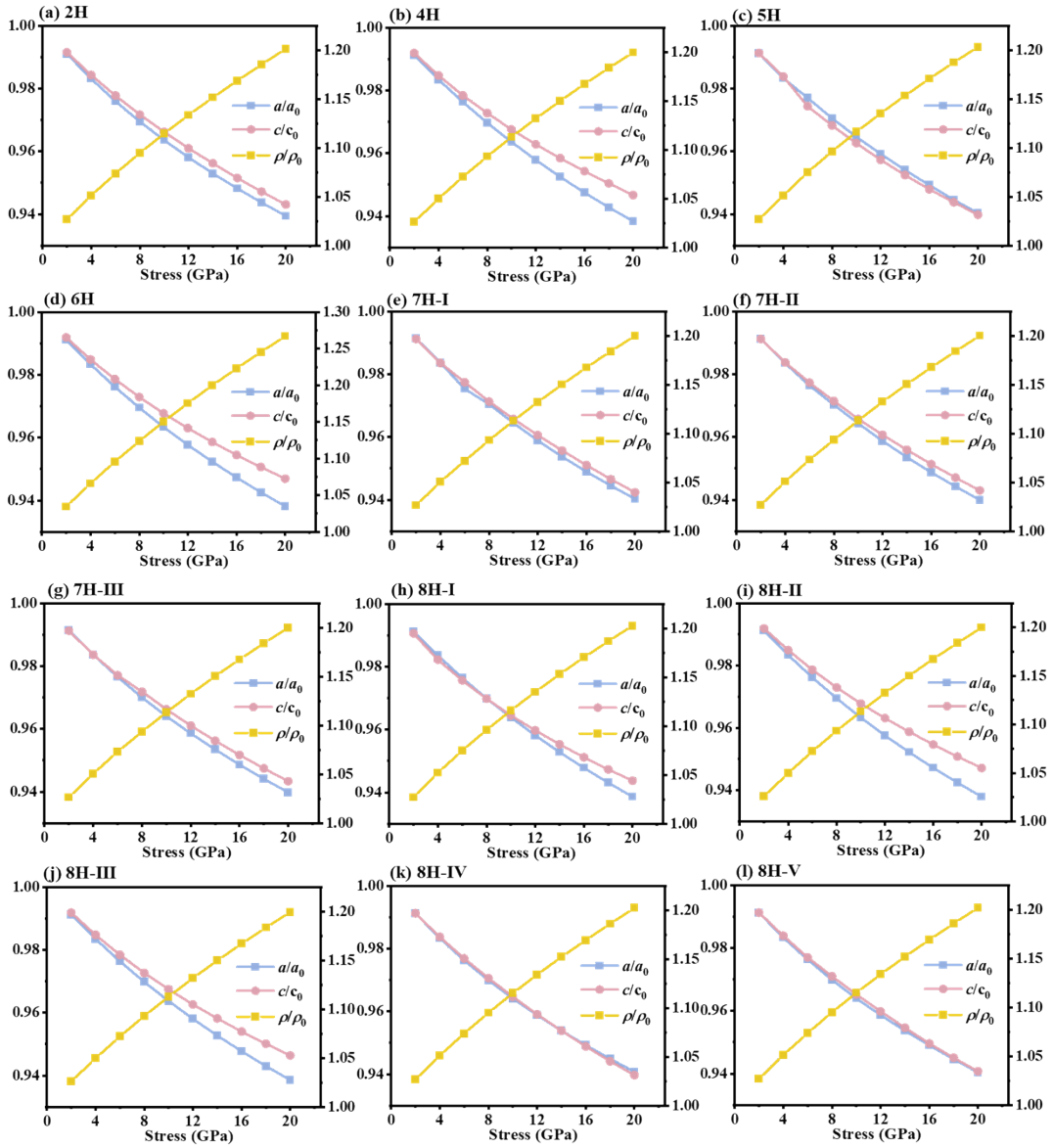

FIG. S6 The parameters as a function of stress of nH SiGe.

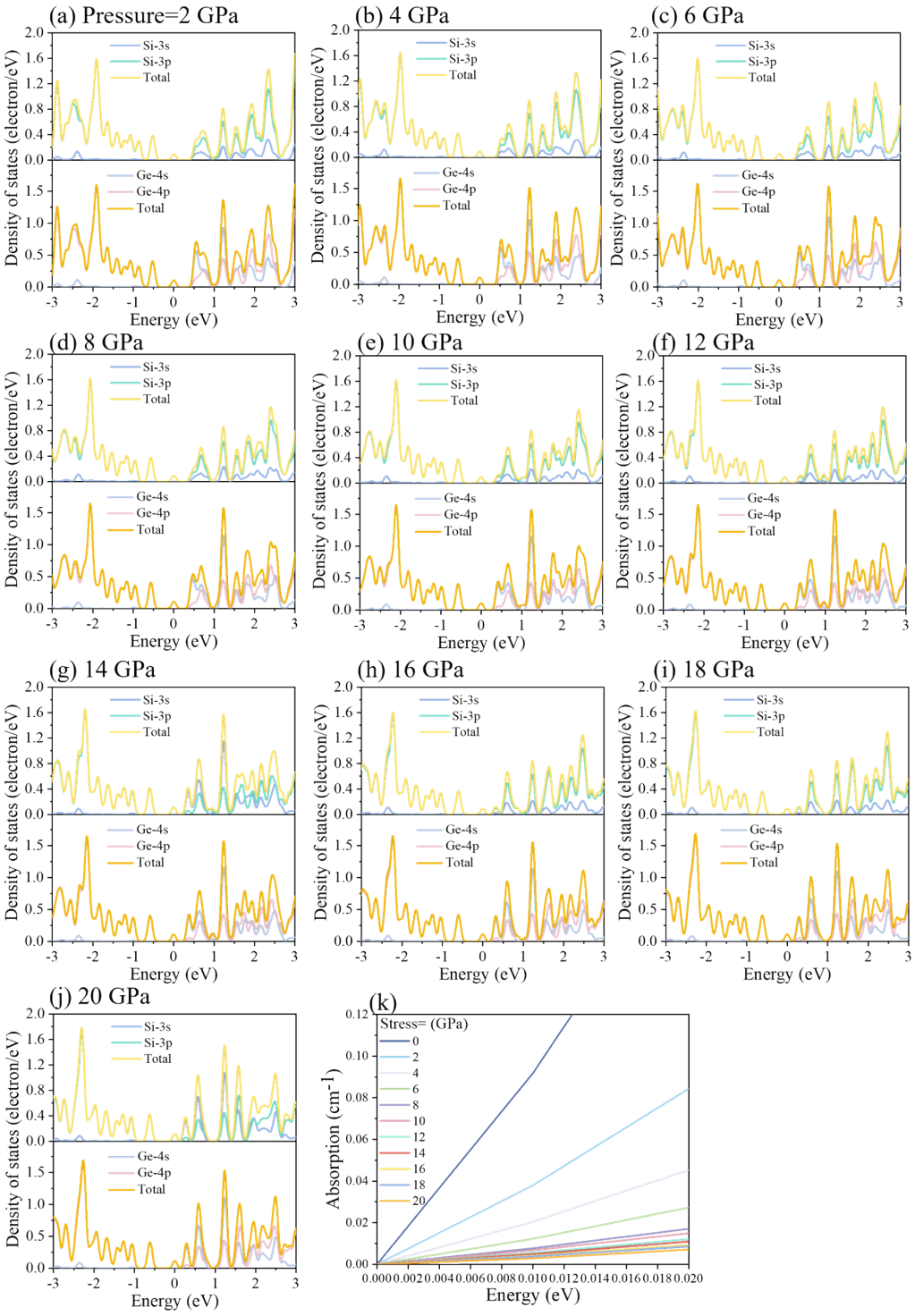

FIG. S7 The PDOS of 6H SiGe under increasing stress and the detailed absorption of nH SiGe at CBM.

TABLE S1. The crystal lattice parameters (a, c in Å), density ρ (g/cm^3) and cell volume/atom V (Å^3) of nH SiGe.

Name	Space group	a	c	ρ	V
2H	$P6_3mc$	3.939	6.524	3.815	21.911
4H	$P6_3mc$	3.951	12.913	3.831	21.818
5H	$P3m1$	3.948	16.246	3.812	21.927
6H	$P3m1$	3.948	19.398	3.831	21.821
7H-I	$P3m1$	3.951	22.645	3.823	21.866
7H-II	$P3m1$	3.946	22.700	3.822	21.869
7H-III	$P3m1$	3.946	22.700	3.823	21.864
8H- I	$P3m1$	3.945	25.973	3.821	21.875
8H-II	$P6_3mc$	3.947	25.880	3.830	21.822
8H-III	$P6_3mc$	3.955	25.778	3.829	21.829
8H-IV	$P3m1$	3.950	25.968	3.811	21.935
8H-V	$P3m1$	3.946	26.002	3.814	21.915
Diamond Si [b]	$Fd\bar{3}m$	5.442		2.267	

[a] Reference [1].

[1]S. Adachi, Springer **1** (2004).

TABLE S2. The elastic constants (GPa), bulk, shear, Young's moduli (GPa), hardness (H) and anisotropy index (U) for nH SiGe.

Name	C_{11}	C_{12}	C_{13}	C_{14}	C_{33}	C_{44}	C_{66}	B	G	E	H	U
2H	151	39	24	0	172	42	56	72	53	127	11	0.220
4H	153	40	26	0	177	47	57	74	55	133	12	0.141
5H	140	72	39	0	163	46	34	83	43	111	6	0.282
6H	164	19	60	2	179	46	72	86	56	138	10	0.297
7H-I	119	60	32	-5	148	45	30	71	40	100	7	0.422
7H-II	125	56	21	16	165	52	34	68	44	109	8	1.202
7H-III	152	48	39	-8	162	47	52	80	51	126	9	0.164
8H-I	156	28	-13	-1	170	31	64	54	52	118	14	1.093
8H-II	165	29	24	0	180	45	68	74	59	140	13	0.250
8H-III	146	43	15	0	174	49	51	68	55	130	12	0.168
8H-IV	127	63	32	10	161	47	32	74	42	106	7	0.697
8H-V	119	79	28	-9	166	45	20	75	35	90	5	1.903
4H Si [a]	180	50	36		197	52		63	40	99		
Diamond Si [b]	166	64				80		88	64	155		

[a] Reference [1].

[b] Reference [2].

[1]S. Adachi, Springer **1** (2004).

[2]Y. L. Wei, J. X. Li, X. Z. Shi, J. Li and C. Y He, Scripta Mater. **219**, 114843 (2022)

TABLE S3. The absorption strength of nH SiGe and their multiple absorption intensity compared to diamond Si in different regions.

Name	absorption strength in the whole region	Multiple	absorption strength in the visible region	Multiple
2H	621471.65	3.09	120282.59	14.15
4H	621792.55	3.09	124579.69	14.65
5H	616851.51	3.07	124993.53	14.70
6H	621251.20	3.09	127525.76	15.00
7H-I	619926.73	3.08	127172.40	15.00
7H-II	617616.92	3.07	122022.44	14.35
7H-III	620217.38	3.08	123187.99	14.49
8H-I	624660.98	3.10	124087.82	14.60
8H-II	621480.66	3.09	120481.49	14.17
8H-III	622943.13	3.10	128502.16	15.11
8H-IV	628205.84	3.12	131932.58	15.52
8H-V	626667.62	3.12	128651.01	15.13
Diamond Si	201028.92	1	8501.79	1