Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C
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Supporting Information

Controllable Modulation of Electronic Properties of Graphene and Silicene by Interface Engineering and Pressure

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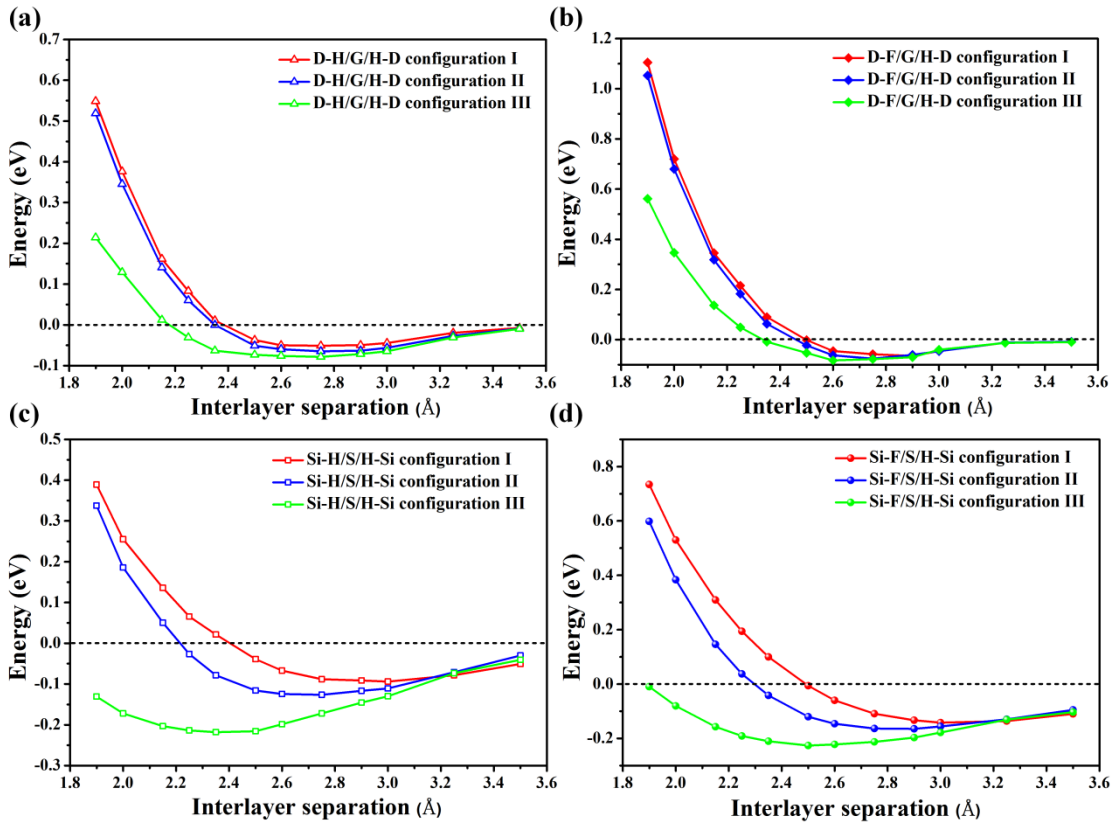

Fig. S1 The evolution of the binding energy (BE) per unit cell of (a) D-H/G/H-D, (b) D-F/G/H-D, (c) Si-H/S/H-Si, and (d) Si-F/S/H-Si as a function of the interlayer spacing. The red color presents configuration I, the blue color presents configuration II and the green color presents configuration III. The hollow triangles present D-H/G/H-D. Rhombuses present D-F/G/H-D. Hollow squares present Si-H/S/H-Si. Spheres present Si-F/S/H-Si.

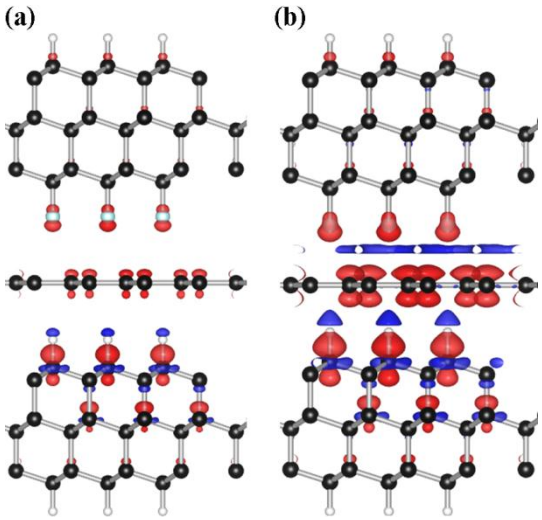

Fig. S2 Charge density difference (CDD) in D-F/G/H-D configuration III with separations of 2.42Å, 1.98Å. Red and blue areas represent electron accumulation and depletion, respectively. Iso-values are 0.004 in Panel a and Panel b.

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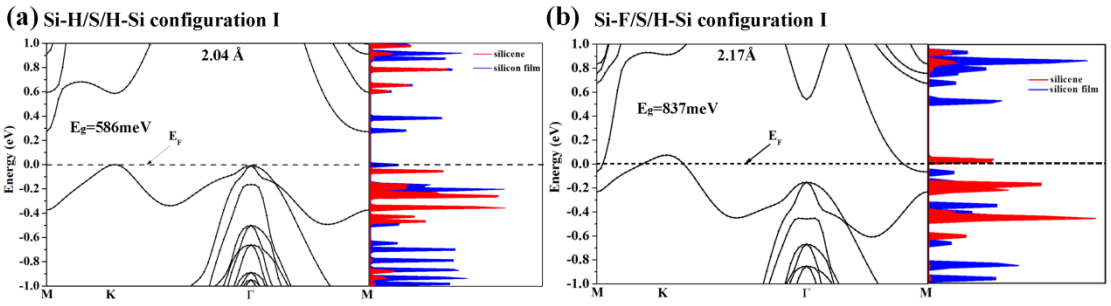

Fig. S3 Band structure and density of states of Si-H/S/H-Si configuration I and Si-F/S/H-Si configuration I with a separation of 2.04Å (a), and 2.17Å (b). The red and blue areas in the density of states correspond to the states that come from silicene and silicon film, respectively.

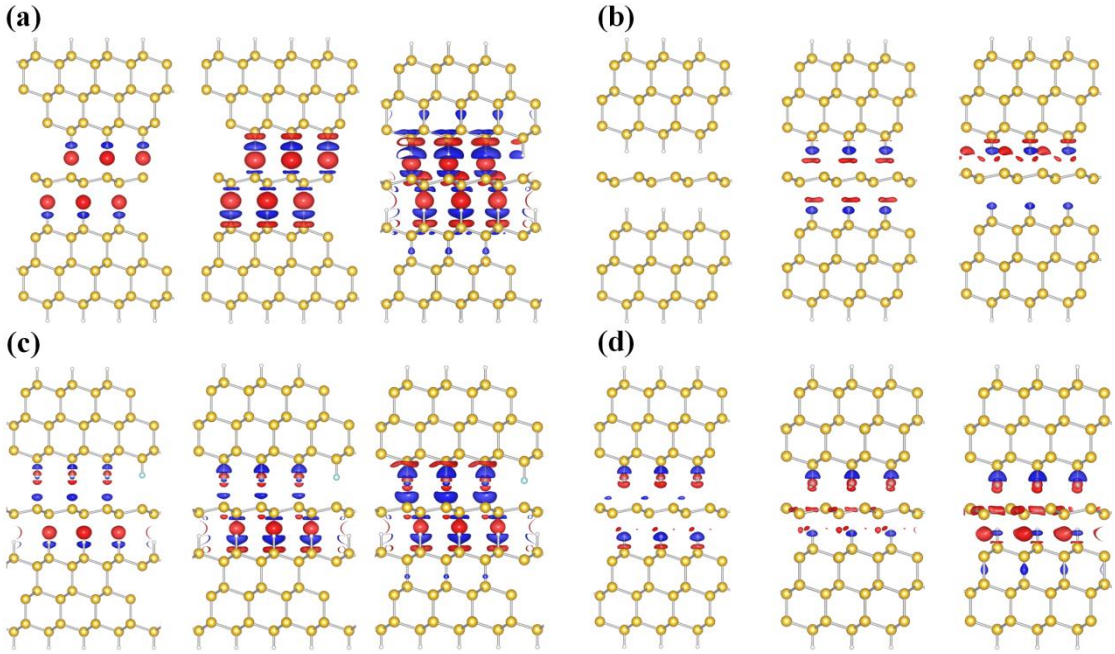

Fig. S4 (a) Charge density difference (CDD) in Si-H/S/H-Si configuration II with separations of 2.77Å, 2.17Å, and 2Å. (b) CDD in Si-H/S/H-Si configuration III with separations of 2.81Å, 2.21 Å and 2.01 Å. (c) CDD in Si-F/S/H-Si configuration II with separations of 3.2Å, 2.33 Å, and 2.1 Å (d) CDD in Si-F/S/H-Si configuration III with separations of 2.8 Å, 2.2 Å,1.86 Å. Iso-values are 0.007 in Panel a, 0.005 in Panel b, 0.01 in Panel c, and 0.007 in Panel d.

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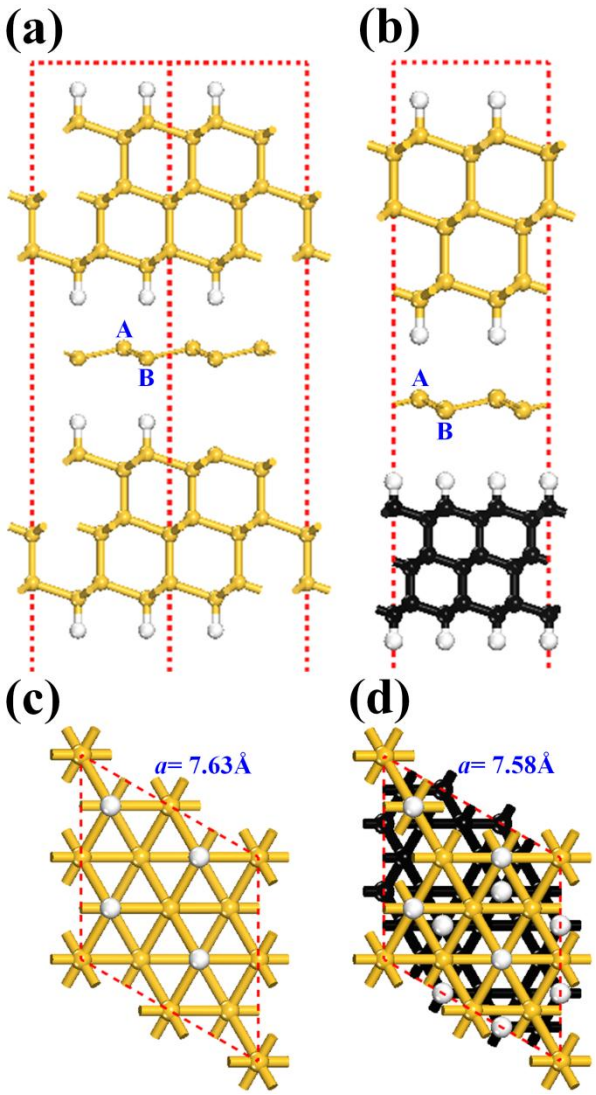

Fig. S5 Structure diagram of 75% hydrogenated Si-H/S/H-Si configuration I and D-H/S/H-Si. Red dashed rectangles and rhombuses represent the supercells adopted in the calculations. (a) and (b) are the side views of 75% hydrogenated Si-H/S/H-Si configuration I and D-H/S/H-Si. (c) and (d) are the top views of 75% hydrogenated Si-H/S/H-Si configuration I and D-H/S/H-Si.

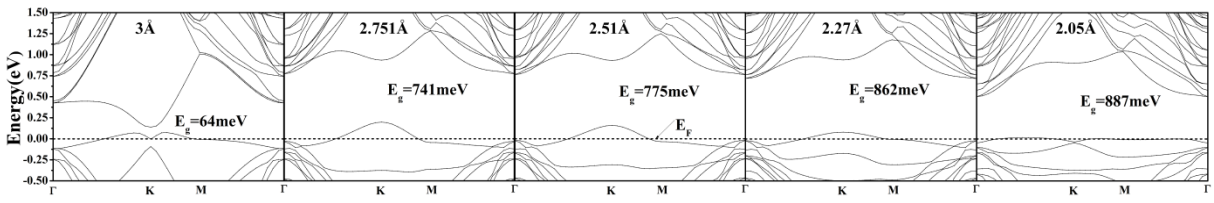

Fig. S6 The band structures of 75% hydrogenated Si-H/S/H-Si configuration I with different interlayer spacings.

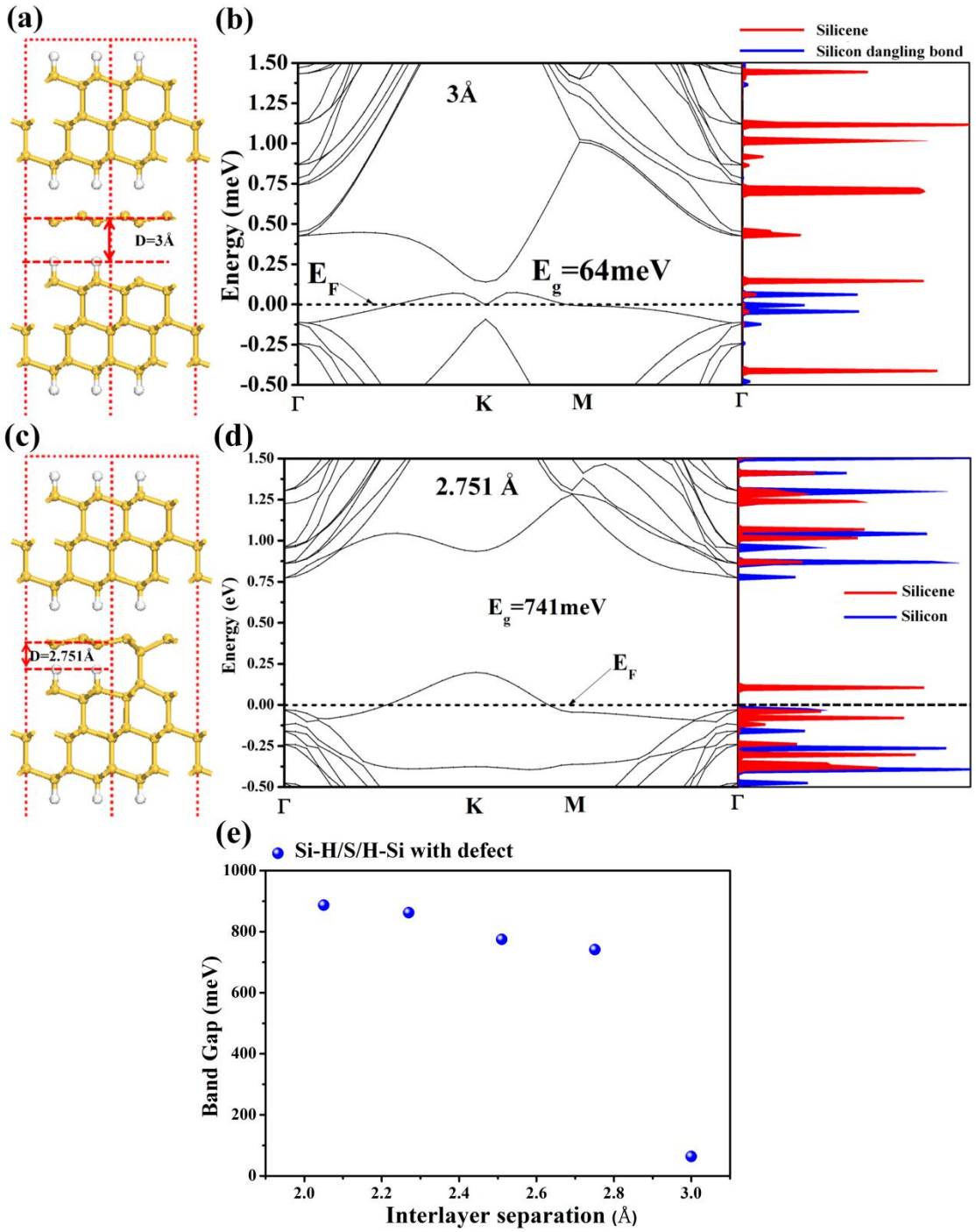

Fig. S7 (a) The side views of 75% hydrogenated Si-H/S/H-Si configuration I with a separation of 3Å. (b) Band structure and density of states of 75% hydrogenated Si-H/S/H-Si configuration I with a separation of 3Å. The red and blue areas in the density of states correspond to the states that come from silicene and silicon dangling bond, respectively. (c) The side views of 75% hydrogenated Si-H/S/H-Si configuration I with a separation of 2.751Å. (d) Band structure and density of states of 75% hydrogenated Si-H/S/H-Si configuration I with a separation of 2.751Å. The red and blue areas in the density of states correspond to the states that come from silicene and silicon films, respectively. (e) The

variation in the energy gap of 75% hydrogenated Si-H/S/H-Si configuration I, as a function of interlayer spacing.

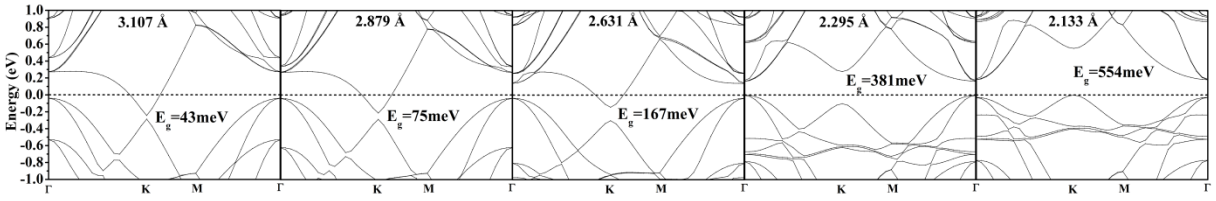

Fig. S8 The band structures of D-H/S/H-Si with different interlayer spacings.

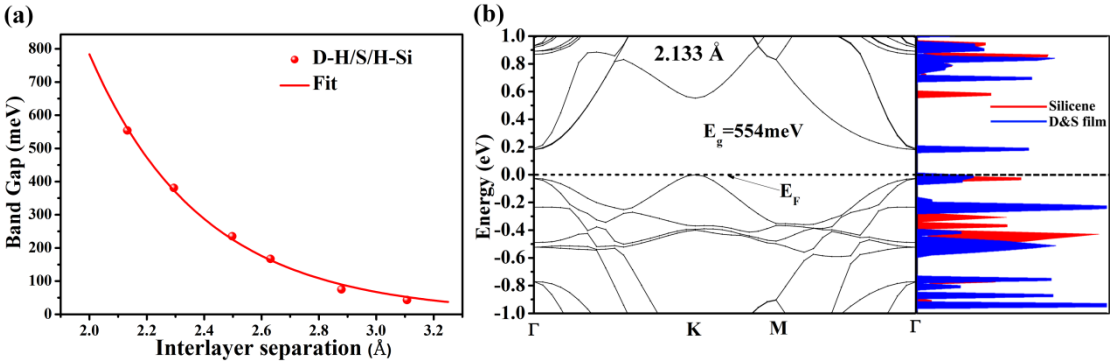

Fig. S9 (a) The variation in the energy gap of D-H/S/H-Si, as a function of interlayer spacing. (b) Band structure and density of states of D-H/S/H-Si with a separation of 2.133Å. The red and blue areas in the density of states correspond to the states that come from silicene and diamond & silicon films (D&S film), respectively.

Table S1. Summary of electronic properties of D-X/G/H-D (X = Hydrogen (H) or Fluorine (F), D=diamond layer, and G=graphene,)

D-H/G/H-D configuration I						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3	-0.112	-0.112	0	-0.01	-0.01	0
2.75	-0.212	-0.212	0	-0.02	-0.02	0
2.52	-0.449	-0.470	21	-0.03	-0.01	0.0033
2.3	-0.657	-0.737	80	-0.03	-0.01	0.0072
2.1	-0.773	-0.956	183	-0.04	-0.01	0.0161
1.92	-0.700	-1.077	377	-0.05	-0.01	0.0595
1.83	-0.577	-1.073	496	-0.06	-0.01	0.0790
D-H/G/H-D configuration II						
Interlayer	CBM at K	VBM at K	Band gap	Charge of	Charge of	Effective

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separation (Å)	point (eV)	point (eV)	at K point (meV)	sublattice A (e)	sublattice B (e)	mass (m_e)
3.15	-0.087	-0.083	4	-0.01	-0.01	0.00063
2.9	-0.128	-0.134	6	-0.02	-0.02	0.00079
2.65	-0.336	-0.343	7	-0.02	-0.02	0.00094
2.43	-0.573	-0.584	11	-0.02	-0.02	0.0017
2.21	-0.840	-0.852	12	-0.02	-0.02	0.0019
2.02	-0.885	-0.899	14	-0.02	-0.02	0.0022
1.88	-0.936	0.954	18	-0.03	-0.03	0.0028
1.79	-0.803	-0.833	30	-0.03	-0.03	0.0047
D-F/G/H-D configuration I						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
2.99	0	0	0	0	0	0
2.76	0.004	-0.001	5	-0.01	0	0.00078
2.53	-0.027	-0.050	23	-0.01	0	0.0036
2.32	-0.018	-0.092	74	-0.02	0	0.0095
2.12	-0.009	-0.200	191	-0.02	0	0.0258
1.91	0.126	-0.329	455	-0.03	0	0.0679
D-F/G/H-D configuration II						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3	0	0	0	0	0	0
2.75	-0.012	-0.017	5	-0.01	0	0.00078
2.53	-0.033	-0.040	7	-0.01	0	0.0011
2.32	-0.038	-0.071	33	-0.01	0	0.0052
2.13	-0.032	-0.112	70	-0.02	0	0.0077
1.91	0.042	-0.192	150	-0.03	0	0.0306
D-F/G/H-D configuration III						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3	0	0	0	0	0	0
2.75	-0.012	-0.017	5	-0.01	0	0.00078
2.53	-0.033	-0.040	7	-0.01	0	0.0011

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2.32	-0.038	-0.071	33	-0.01	0	0.0052
2.13	-0.032	-0.112	70	-0.02	0	0.0077
1.91	0.042	-0.192	150	-0.03	0	0.0306

Table S2. Summary of electronic properties of Si-X/S/H-Si (Si=silicon layer and S=silicene)

Si-H/S/H-Si configuration I						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3	0.085	-0.024	92	0.02	0	0.032
2.94	0.102	-0.008	110	0.02	0	0.0333
2.55	0.228	-0.004	232	0.04	-0.01	0.0893
2.26	0.316	-0.078	394	0.08	-0.04	0.2294
2.04	0.588	0.002	586	0.11	-0.07	0.5780
1.94	0.588	-0.11	590	0.14	-0.09	1.0724
Si-H/S/H-Si configuration II						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
2.77	0.005	0.005	0	0.01	0.01	0
2.4	0.007	0.007	0	0.02	0.02	0
2.17	0.045	0.001	44	0.04	0.02	0.0126
2	0.047	0.001	46	0.06	0.03	0.0142
1.87	0.144	0.113	31	0.07	0.05	0.0099
Si-H/S/H-Si configuration III						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
2.81	0	0	0	0	0	0
2.51	-0.220	-0.220	0	-0.01	-0.01	0
2.21	-0.226	-0.226	0	-0.01	-0.01	0
2.01	-0.287	-0.280	8	-0.02	-0.01	0.0025
1.79	-0.252	-0.231	21	-0.02	-0.01	0.0065
Si-F/S/H-Si configuration I						
Interlayer separation	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point	Charge of sublattice	Charge of sublattice	Effective mass (m_e)

(Å)			(meV)	A (e)	B (e)	
3.17	0.375	0.270	105	0.05	-0.02	0.0281
2.94	0.407	0.229	178	0.06	-0.02	0.0495
2.61	0.536	0.147	389	0.1	-0.04	0.1377
2.33	0.773	0.092	681	0.17	-0.07	0.3689
2.17	0.911	0.074	837	0.21	-0.10	0.7554
1.98	1.036	0.012	1024	0.3	-0.14	3.0384
Si-F/S/H-Si configuration II						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3.2	0.355	0.309	46	-0.01	0.03	0.0166
2.92	0.337	0.315	21	0	0.04	0.008
2.5	0.309	0.291	18	0.01	0.05	0.0059
2.33	0.306	0.289	17	0	0.04	0.0055
2.18	0.304	0.288	16	0.03	0.08	0.0049
2.1	0.371	0.294	77	0.04	0.12	0.0415
1.95	0.491	0.139	352	0.12	0.02	0.2083
Si-F/S/H-Si configuration III						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3.05	0.345	0.314	31	-0.01	0.03	0.0096
2.8	0.323	0.262	61	-0.03	0.05	0.0188
2.67	0.250	0.191	59	-0.02	0.05	0.0182
2.58	0.241	0.184	57	-0.02	0.05	0.0176
2.2	0.244	0.195	49	-0.02	0.07	0.0151
2.01	0.223	0.213	10	-0.01	0.07	0.0034
1.86	0.250	0.194	56	-0.01	0.08	0.0173
1.71	0.296	0.176	120	0.04	0.12	0.0490

Table S3. Summary of electronic properties of D-X/S/H-D

D-H/S/H-D						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
2.75	-0.281	-0.281	0	-0.0175	-0.0175	0

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2.45	-0.219	-0.219	0	-0.01	-0.01	0
2.26	-0.145	-0.145	0	-0.005	-0.005	0
2.13	0	0	0	0	0	0
1.94	0	0	0	0	0	0
D-F/S/H-D						
Interlayer separation (Å)	CBM at K point (eV)	VBM at K point (eV)	Band gap at K point (meV)	Charge of sublattice A (e)	Charge of sublattice B (e)	Effective mass (m_e)
3.03	0.064	0.003	61	0.05	-0.05	0.0069
2.75	0.198	0.139	59	0.0525	-0.0475	0.0070
2.57	0.268	0.212	56	0.065	-0.0325	0.0078
2.36	0.285	0.238	47	0.08	-0.015	0.0097
2.01	0.274	0.247	27	0.1	0.08	0.0140

Table S4. Coefficient values of fitting curves for Figure 2

$P(D)=a\exp(-bD)/D$	a (Å GPa)	b ($Å^{-1}$)
D-H/G/H-D configuration I	14332.03	2.403
D-H/G/H-D configuration II	176217.15	3.503
D-F/G/H-D configuration I	43481.59	2.584
D-F/G/H-D configuration II	199879.95	3.257
D-F/G/H-D configuration III	36394.81	2.806
Si-H/S/H-Si configuration I	94895.18	3.857
Si-H/S/H-Si configuration II	9200.53	3.247
Si-H/S/H-Si configuration III	26537.10	4.126
Si-F/S/H-Si configuration I	973.51	1.499
Si-F/S/H-Si configuration II	192100.03	3.749
Si-F/S/H-Si configuration III	1783.42	2.192
D-H/S/H-D	77784.54	3.009
D-F/S/H-D	14231.23	2.139

Table S5. Coefficient values of fitting curves for Figure 4

Figure 4 a $E_g=\alpha e^{-\beta(D+\mu)^2}$	α ($Å^{-1}$ meV)	β ($Å^{-1}$)	μ (Å)
D-H/G/H-D configuration I	1.874	0.477	-2.012
D-H/G/H-D configuration II	0.5	0.137	1.008
D-F/G/H-D configuration I	2.657	0.472	-1.881

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D-F/G/H-D configuration II	0.602	0.422	-1.946
D-F/G/H-D configuration III	51.269	0.160	2.768
Figure 4 c $E_g = \alpha e^{-\beta(D+\mu)^2}$	α (Å^{-1} meV)	β (Å^{-1})	μ (Å)
Si-H/S/H-Si configuration I	267.776	0.032	9.747
Si-F/S/H-Si configuration I	3.744	0.088	-0.112
Si-F/S/H-Si configuration II	509.782	0.447	2.594
Figure 4 d $E_g = \lambda e^{(-P/\varepsilon)} + \tau$	λ (meV)	ε (GPa)	τ (meV)
Si-H/S/H-Si configuration I	-1501.1039	19.171	1429.179
Si-F/S/H-Si configuration I	-517.592	5.976	597.539
Figure 4 g $E_g = \lambda e^{(-D/\varepsilon)} + \tau$	λ (meV)	ε (Å)	τ (meV)
D-F/S/H-D	-3302.696	0.45293	66.155