Research Square

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The Stability, Structural, Electronic, and Optical Properties of Hydrogenated Silicene Under Hydrostatic Pressures: A First-principle Study

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Research Article

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Abstract

The structural, electronic, and optical properties of hydrogenated silicene have been studied under different hydrostatic pressures using first-principle calculations. The binding energy and band structure have been calculated for Chair (C-) and Boat (B-) structures, which are having good stability at 0 GPa, 3 GPa, 6 GPa, 9 GPa, 12 GPa, 15 GPa, and 18 GPa hydrostatic pressures. Stability has been verified using binding energy and phonon calculations. The C- and B- structures have become metallic and unstable at 21 GPa. The optical properties of B-configuration have been studied in the energy range of 0-20 eV. Five optical parameters such as conductivity threshold (σ_{th}), dielectric constant $\varepsilon(0)$, refractive index $n(0)$, birefringence $\Delta n(0)$ and plasmon energy ($\hbar\omega_p$) have been calculated for the first time under different hydrostatic pressures. The calculated values are in good agreement with the reported values at 0 GPa.

Full Text

Due to technical limitations, full-text HTML conversion of this manuscript could not be completed. However, the manuscript can be downloaded and accessed as a PDF.

Tables

Table 1. Lattice constants (a, b and c), Si-Si bond length (d_{Si-Si}), Si-H bond length (d_{Si-H}), Si-Si-Si bond angle ($\theta_{Si-Si-Si}$), Si-Si-H bond angle ($\theta_{Si-Si-H}$), total energy (E_T), unit cell volume (V), band gap energy (E_g), and binding energy (E_b) of B- configuration of hydrogenated silicene under different pressures.

Parameters	Pressure (GPa)								
	0		3	6	9	12	15	18	21
	This work	Rep. [33]	This work						
a (Å)	6.40	6.32	6.29	6.10	5.91	5.82	5.65	5.68	5.74
b (Å)	3.85	3.82	3.78	3.79	3.71	3.59	3.61	3.50	3.611
c (Å)	6.20		5.75	4.95	4.93	4.90	4.07	4.01	3.98
d_{Si-Si} (Å)	2.36, 2.36	2.36	2.34, 2.33	2.35, 2.32	2.30, 2.29	2.27, 2.30	2.30, 2.24	2.28, 2.32	2.32, 2.29
d_{Si-H} (Å)	1.51	1.5	1.52	1.496	1.49	1.48	1.45	1.44	1.41
$\Theta_{Si-Si-Si}$ (degree)	110.80, 109.68	110	110.22, 108.47	109.37, 107.60	106.60, 107.29	105.40, 104.49	104.71, 103.27	103.20, 99.94	102.36, 98.19
$\Theta_{Si-Si-H}$ (degree)	107.66		108.18	109.07	110.26	112.70	113.12	114.81	115.54
E_T (eV)	-744.33		-741.74	-739.81	-737.75	-735.67	-734.30	-732.56	-731.18
V ($Å^3$)	152.97		136.89	114.46	107.92	102.45	83.10	83.05	78.98
E_g (eV)	1.663	1.6	1.557	1.01	0.60	0.13	0.04	0.01	0.00
E_b (eV)	2.992		2.345	1.86	1.346	0.827	0.46	0.05	-0.29

Table 2. The structural parameters of C- configuration of hydrogenated silicene under different pressures.

Parameter			Pressure (GPa)						
	0		3	6	9	12	15	18	21
	This work	Rep. [33]	This work						
a = b (A)	3.83	3.82	3.81	3.77	3.75	3.72	3.70	3.64	3.61
c (A)	4.96		4.32	4.097	3.942	3.836	3.75	3.23	3.20
d_{Si-Si} (A)	2.32	2.16	2.31	2.289	2.274	2.26	2.25	2.22	2.18
d_{Si-H} (A)	1.50	1.50	1.49	1.491	1.486	1.483	1.48	1.47	1.47
$\Theta_{Si-Si-Si}$ (degree)	111.15	112.00	112.10	113.09	114.97	115.82	116.73	118	119.99
$\Theta_{Si-Si-H}$ (degree)	107.72		106.75	105.79	107.92	108.07	108.18	89.99	89.84
E_T (eV)	-247.30		-247.30	-247.20	-247.1	-246.9	-246.8	-246.5	-245.90
V ($Å^3$)	69.40		54.26	50.42	47.95	46.025	44.4	41.29	40.11
E_g (eV)	1.96	2.00	1.54	1.38	0.94	0.59	0.29	0.02	00
E_b (eV)	3.036		2.332	1.854	1.390	0.921	0.479	0.094	-0.29

Table 3 The conductivity threshold (E_{th}), static dielectric constant ε(0), static refractive index n(0), birefringence Δn(0) and plasmon energy ($\hbar\omega_p$) of B- configuration of hydrogenated silicene under 0 GPa, 6 GPa and 12 GPa external pressures.

Parameter	0 GPa		6 GPa		12 GPa	
	E⊥c	E||c	E⊥c	E||c	E⊥c	E||c
E_{th} (eV)	2.205	3.646	1.243	2.498	0.88	1.549
ε(0)	6.115	3.851	8.140	5.373	9.750	6.157
n	2.472	1.962	2.853	2.318	3.122	2.481
Δn	0.510		0.534		0.641	
	15.223	15.104	16.962	16.842	17.713	17.395

Figures

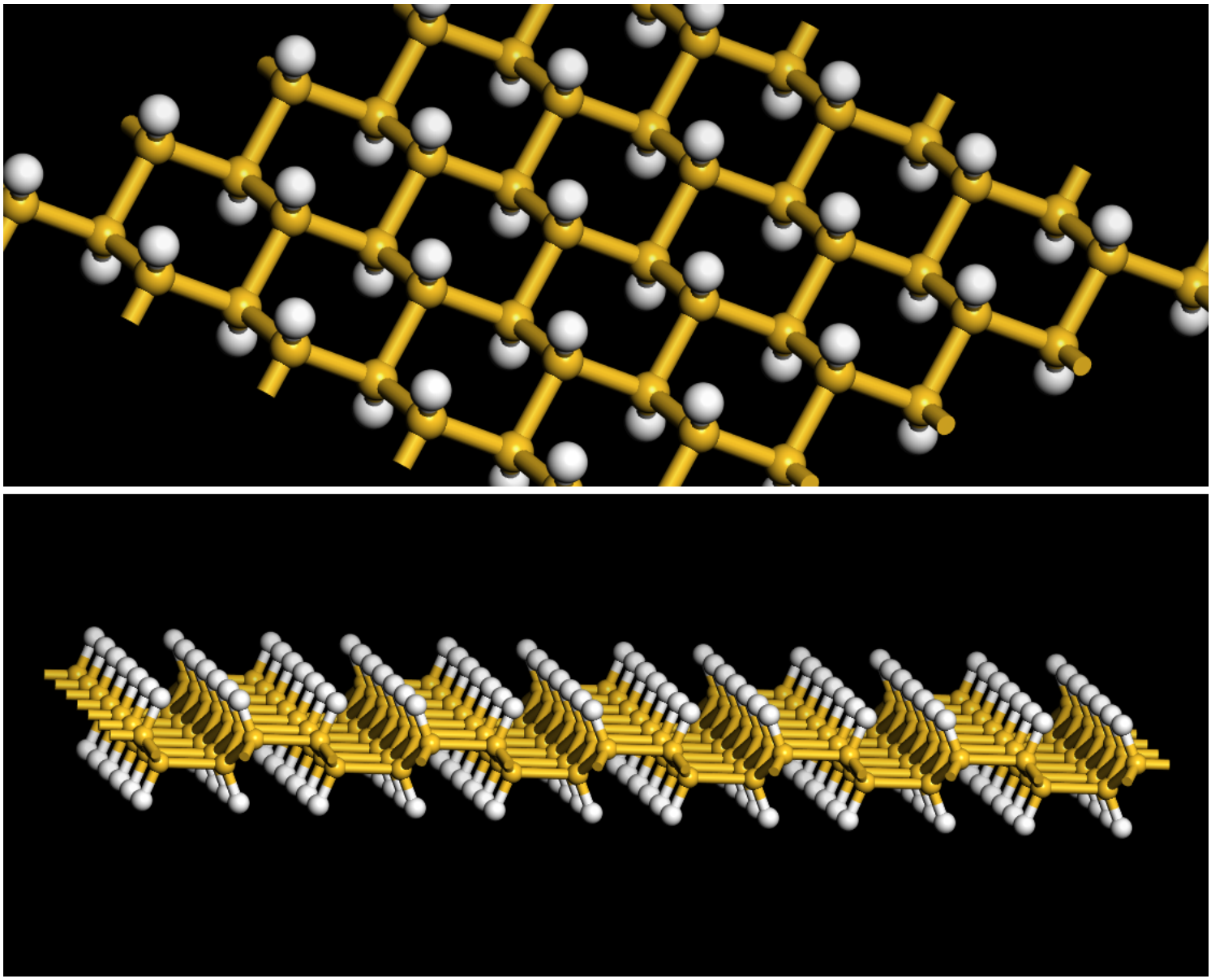

Figure 1

The pictorial representation of (a) C-configuration (b) B-configuration hydrogenated silicene in which white circles are indicated by hydrogen atoms and yellow circles by silicon atoms.

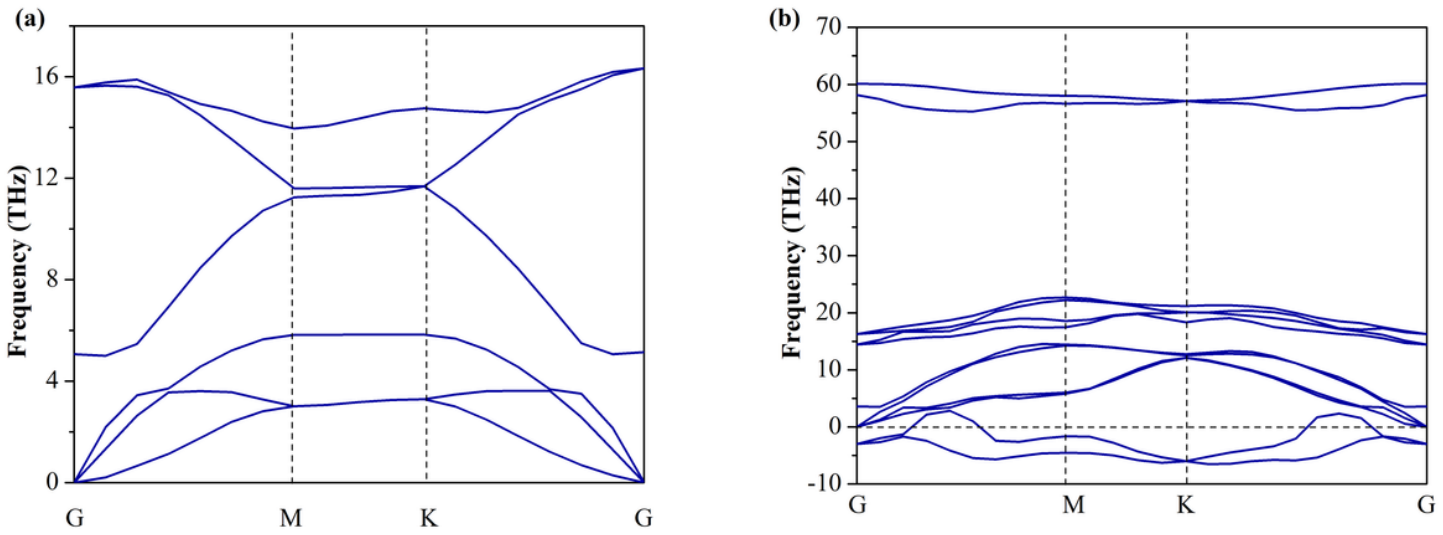

Figure 2

The phonon dispersion of C-configuration at (a) 0 GPa (b) 21 GPa hydrostatic pressures.

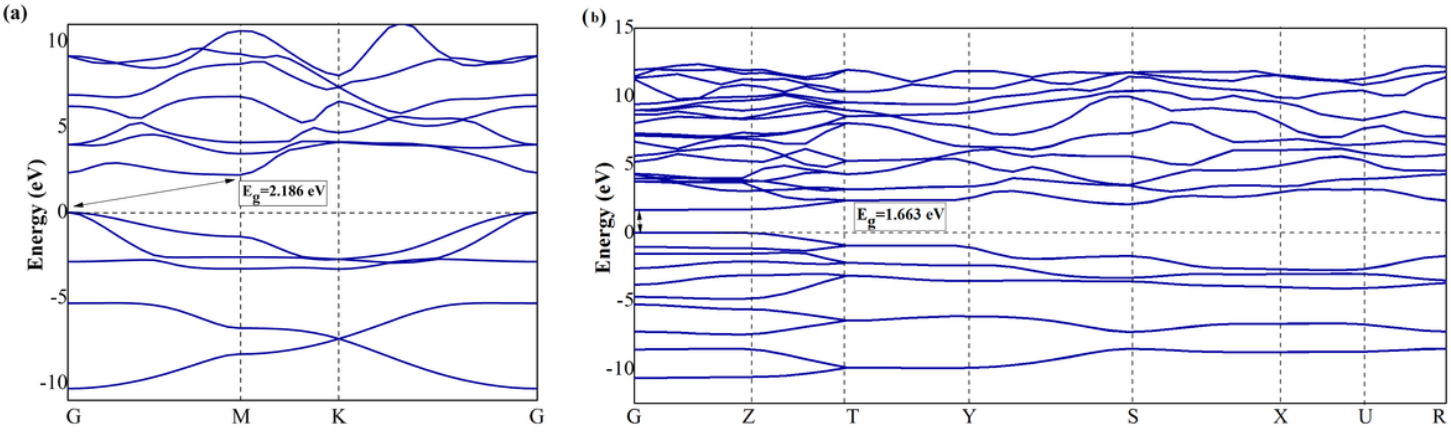

Figure 3

(a) The band structure of C- configuration (b) B-configuration of hydrogenated silicene.

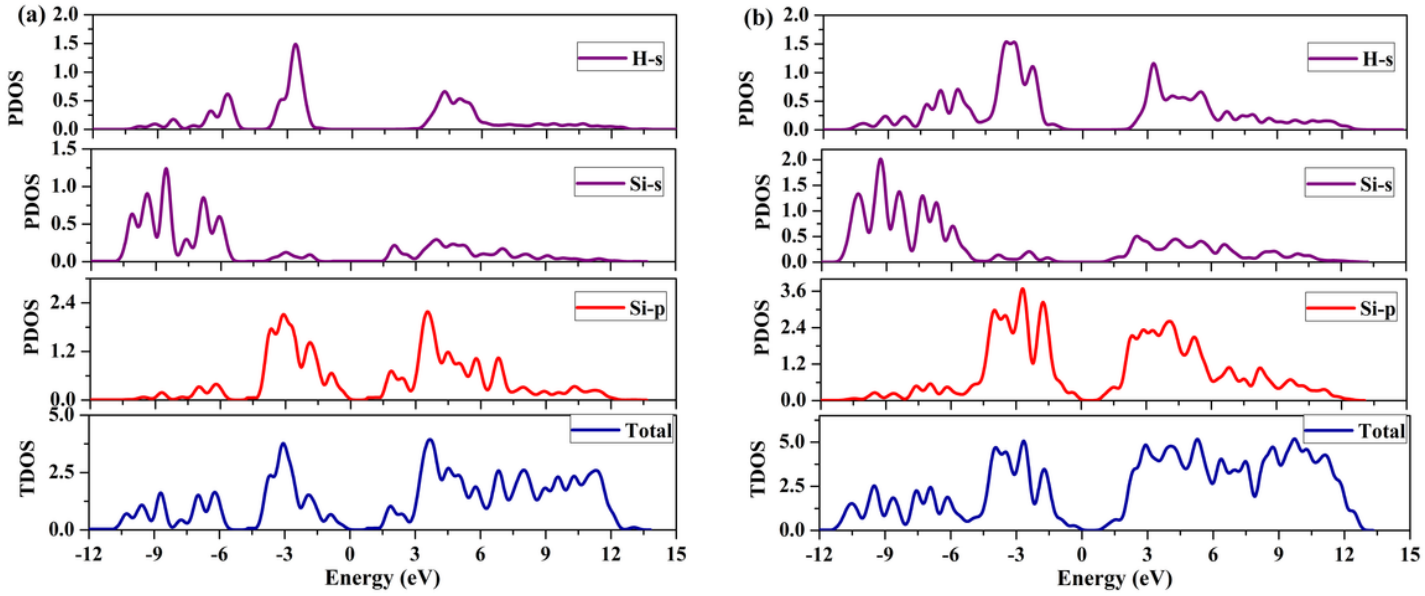

Figure 4

The total density of states (TDOS) and partial density of states (PDOS) for (a) B- and (b) C- configurations of hydrogenated silicene.

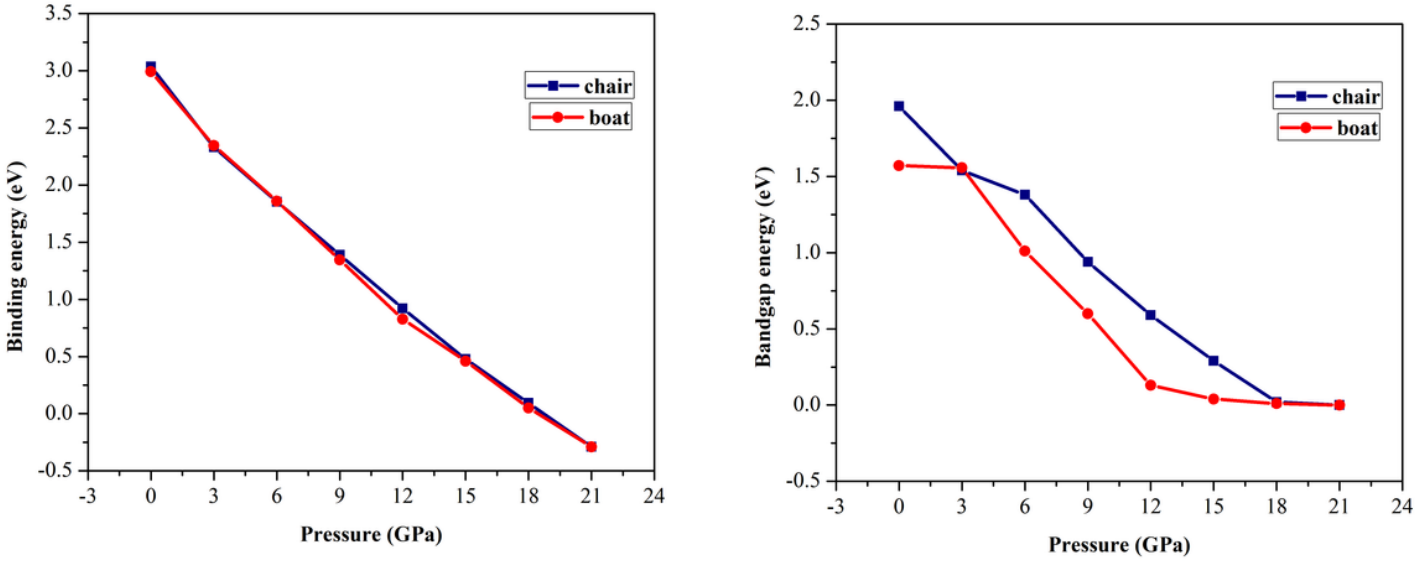

Figure 5

Behavior of (a) binding energy (b) energy band gap under different pressures.

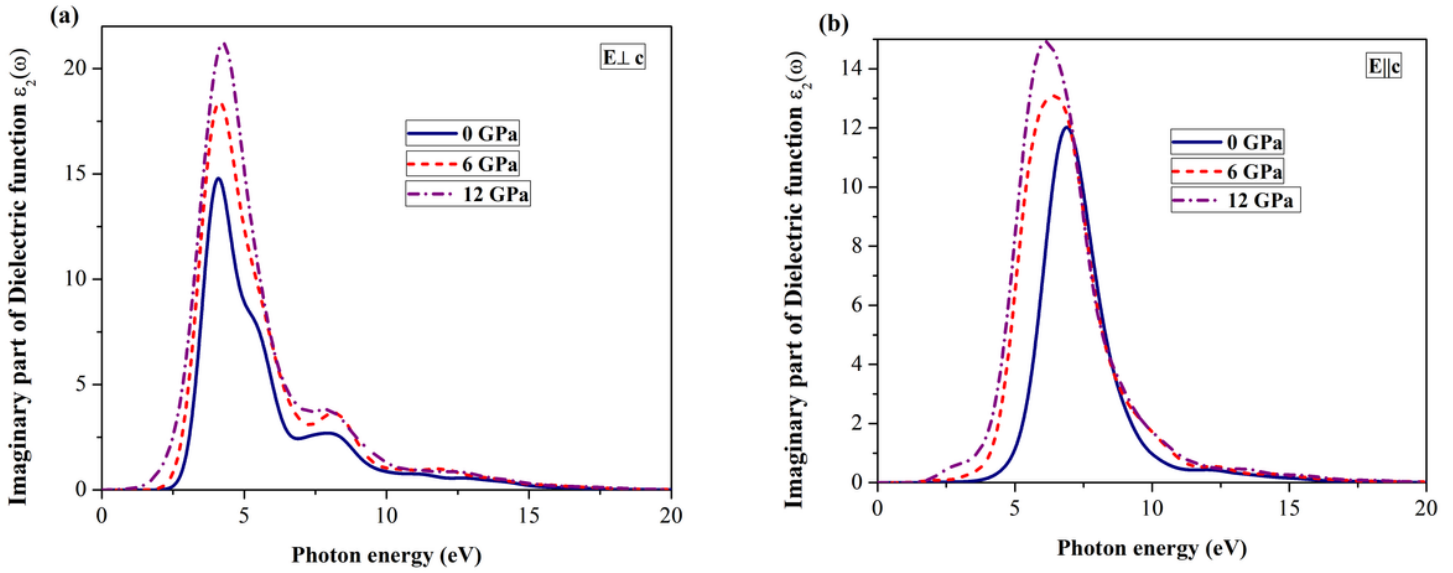

Figure 6

The calculated imaginary part of dielectric function ε2(ω) under different pressures (a) parallel polarization (b) perpendicular polarization of electric field for B- configuration of hydrogenated silicene.

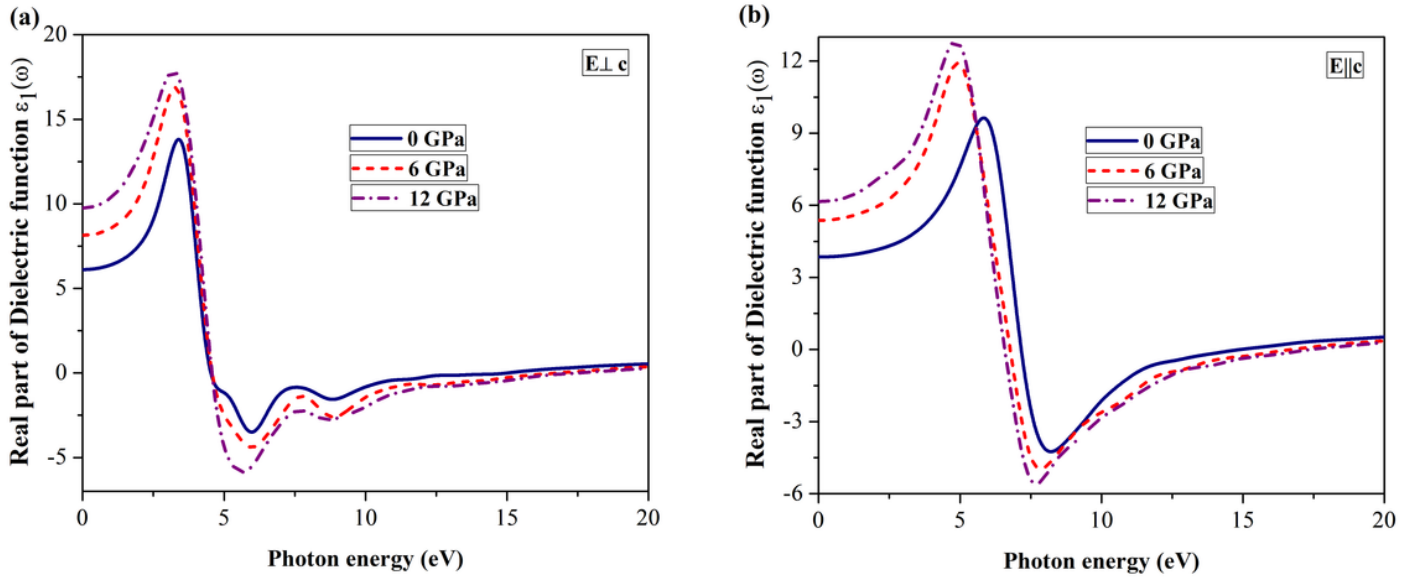

Figure 7

The real part of dielectric function ε1(ω) under different pressures: (a) parallel polarization and (b) perpendicular polarization of electric field for B- configuration of hydrogenated silicene.

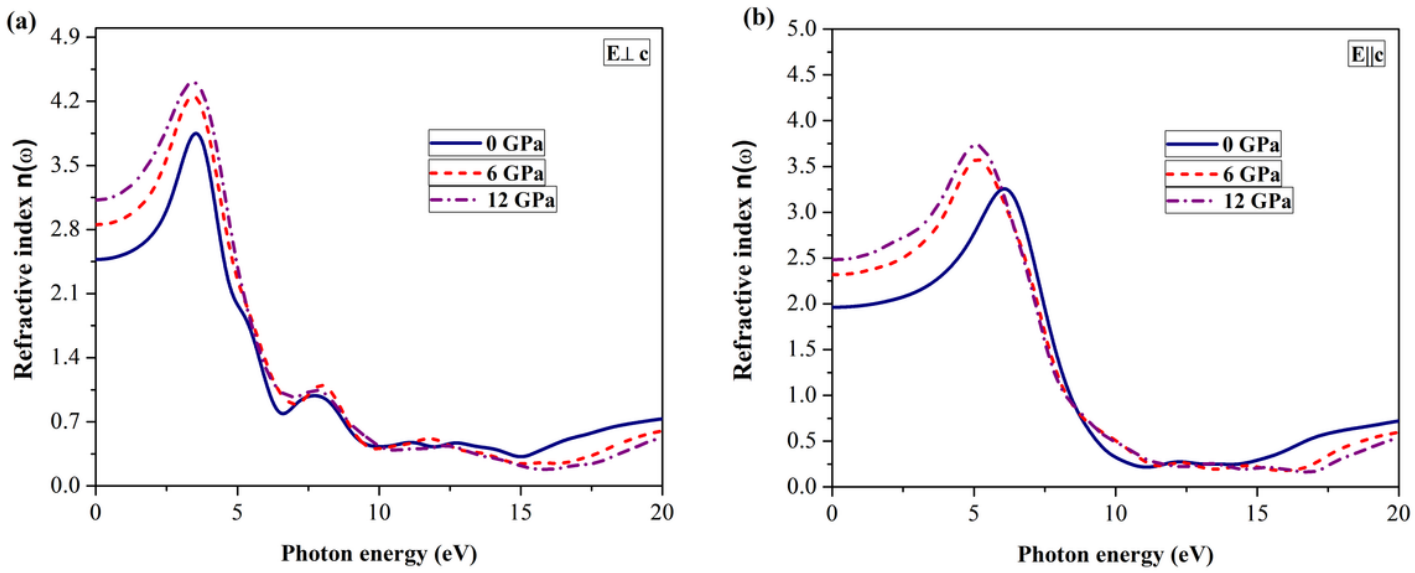

Figure 8

The refractive index n(ω) under different pressures: (a) parallel polarization (b) perpendicular polarization of electric field for B- configuration of hydrogenated silicene.

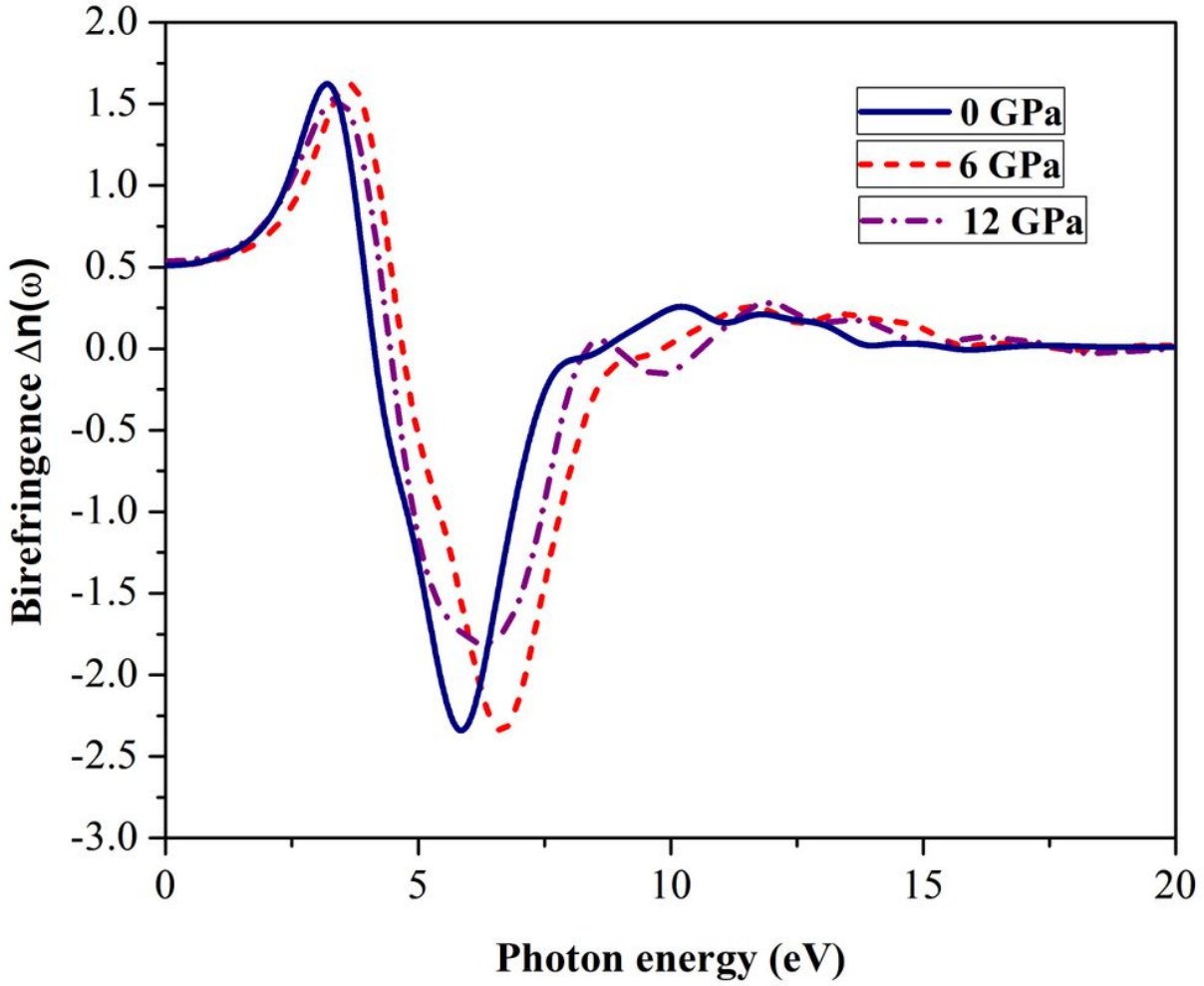

Figure 9

The birefringence for B- configuration of hydrogenated silicene under different pressures.

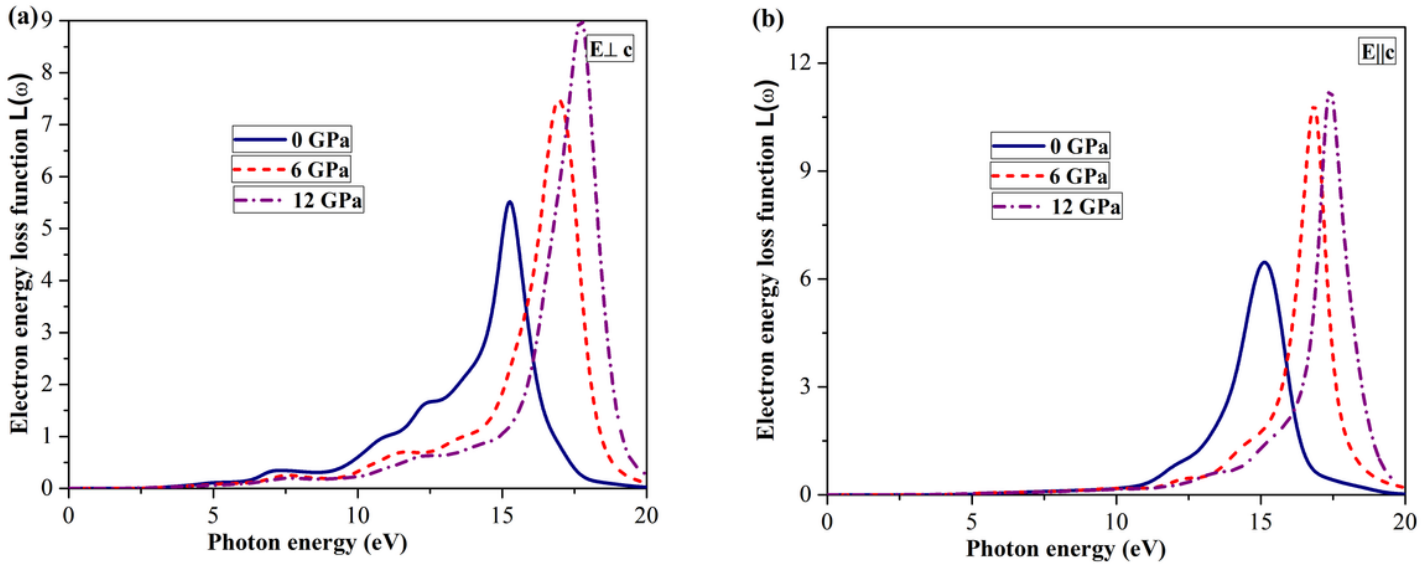

Figure 10

The electron energy loss function L(ω) of hydrogenated silicene under different pressures:(a) parallel polarization (b) perpendicular polarization of the electric field for B- configuration.