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

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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 ($\sigma_{th}$), 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 | 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}  | 2.36 | 2.36 | 2.34, 2.35, 2.33, 2.32 | 2.30, 2.29, 2.30 | 2.27, 2.30, 2.24, 2.32 | 2.28, 2.32, 2.29 |
| d_{Si-H}   | 1.51 | 1.5  | 1.52 | 1.496 | 1.49 | 1.48 | 1.45 | 1.44 | 1.41 |
| θ_{Si-Si-Si} (degree) | 110.80, 109.68 | 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 |
| θ_{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 (Å³)     | 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 (Å) | 3.83          | 3.82 | 3.81 | 3.77 | 3.75 | 3.72 | 3.70 | 3.64 | 3.61 |
| c (Å)     | 4.96          | 4.32 | 4.097| 3.942| 3.836| 3.75 | 3.23 | 3.20 |
| d_{Si-Si} (Å) | 2.32       | 2.16 | 2.31 | 2.289| 2.274| 2.26 | 2.25 | 2.22 | 2.18 |
| d_{Si-H} (Å) | 1.50        | 1.50 | 1.49 | 1.491| 1.486| 1.483| 1.48 | 1.47 | 1.47 |
| Θ_{Si-Si-Si} (degree) | 111.15 | 112.00 | 112.10 | 113.09 | 114.97 | 115.82 | 116.73 | 118 | 119.99 |
| Θ_{Si-Si-H} (degree) | 107.72 | 106.75 | 105.79 | 107.92 | 108.07 | 108.18 | 89.99 | 89.84 |
| E_⊥ (eV)  | -247.30       | -247.30 | -247.20 | -247.1 | -246.9 | -246.8 | -246.5 | -245.90 |
| V (Å³)    | 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  | 0.00 |
| 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 $\varepsilon(0)$, static refractive index $n(0)$, birefringence $\Delta n(0)$ and plasmon energy ($\hbar\omega_p$) of B-configuration of hydrogenated silicene under 0 GPa, 6 GPa and 12 GPa external pressures.

**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 $\varepsilon_2(\omega)$ 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 $\varepsilon_1(\omega)$ under different pressures: (a) parallel polarization and (b) perpendicular polarization of electric field for B- configuration of hydrogenated silicene.
Figure 8

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