Supplementary Information of

Study on $Si_{1-x}Ge_x$ gradual buffer layer of III-V/Si multi-junction solar cells based on first-principles calculations

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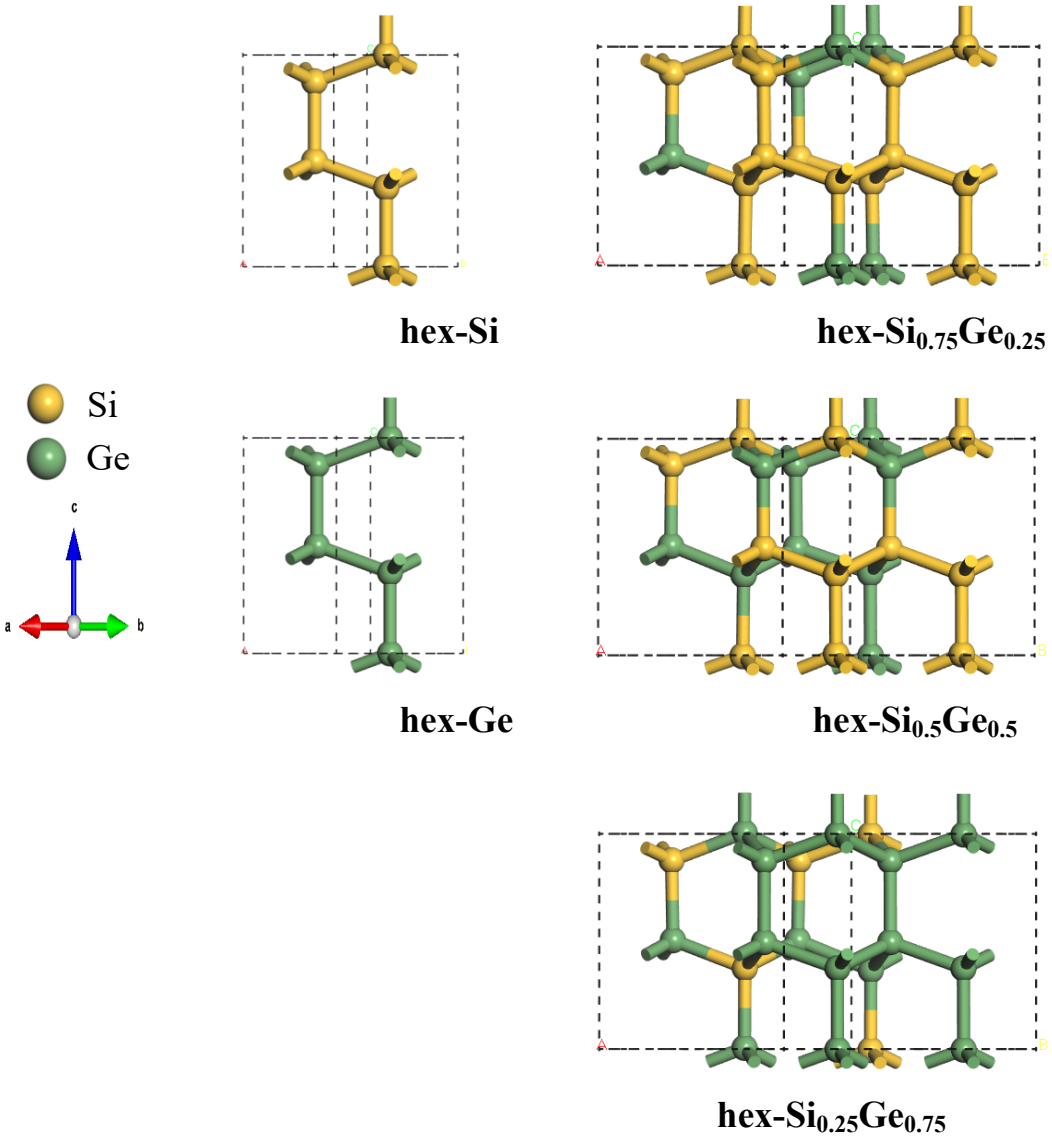

Fig.S1 The atomic structure of hex-Si and hex-Ge primitive cell and the disordered hex-$Si_{1-x}Ge_x$ (0.25, 0.5, 0.75) alloys.

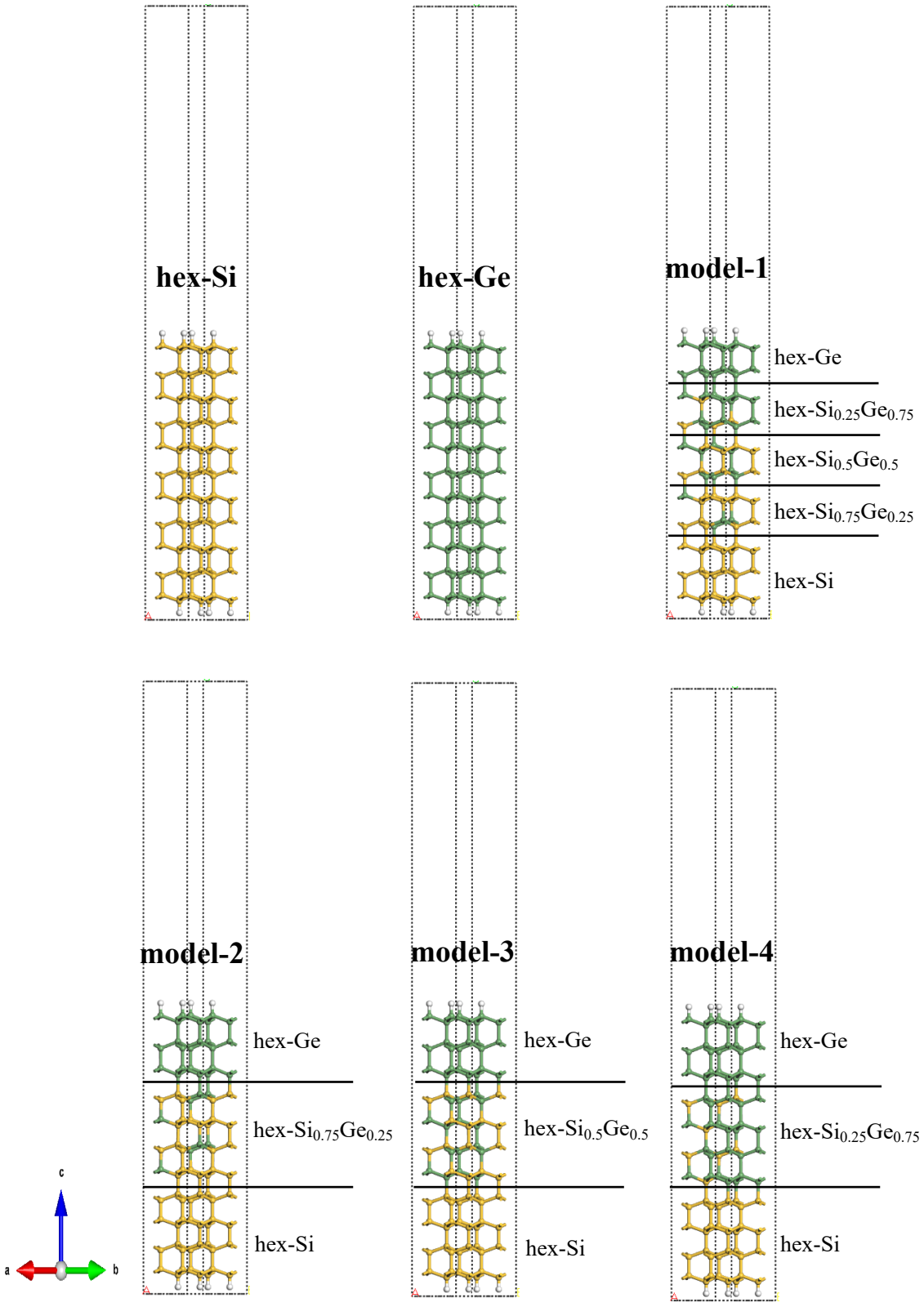

Fig.S2 The atomic structure of hex-Si, hex-Ge slab and model-1, 2, 3, 4.

In order to obtain the strain of hex-$Si_{1-x}Ge_x$ induced by lattice mismatch when stacking in between the hex-Ge and hex-Si, the strain in different directions was defined as:

$$x = \frac{A - B}{B} * 100\%$$

where A represents the lattice constants of hex-$Si_{1-x}Ge_x$ staking in the buffer layer, and B represents lattice constants of the hex-$Si_{1-x}Ge_x$ itself in relaxed form. A and B value of component of each model were listed in Table 1 in the main text. The lattice constants along ab direction was the average distance between all the adjacent atoms in each atomic layers as shown in the Fig. S3. The calculation of the strain in the c direction is also the same.

Eg: model-1 (hex-$Si_{1-x}Ge_x$(x=0, 0.25, 0.5, 0.75, 1))

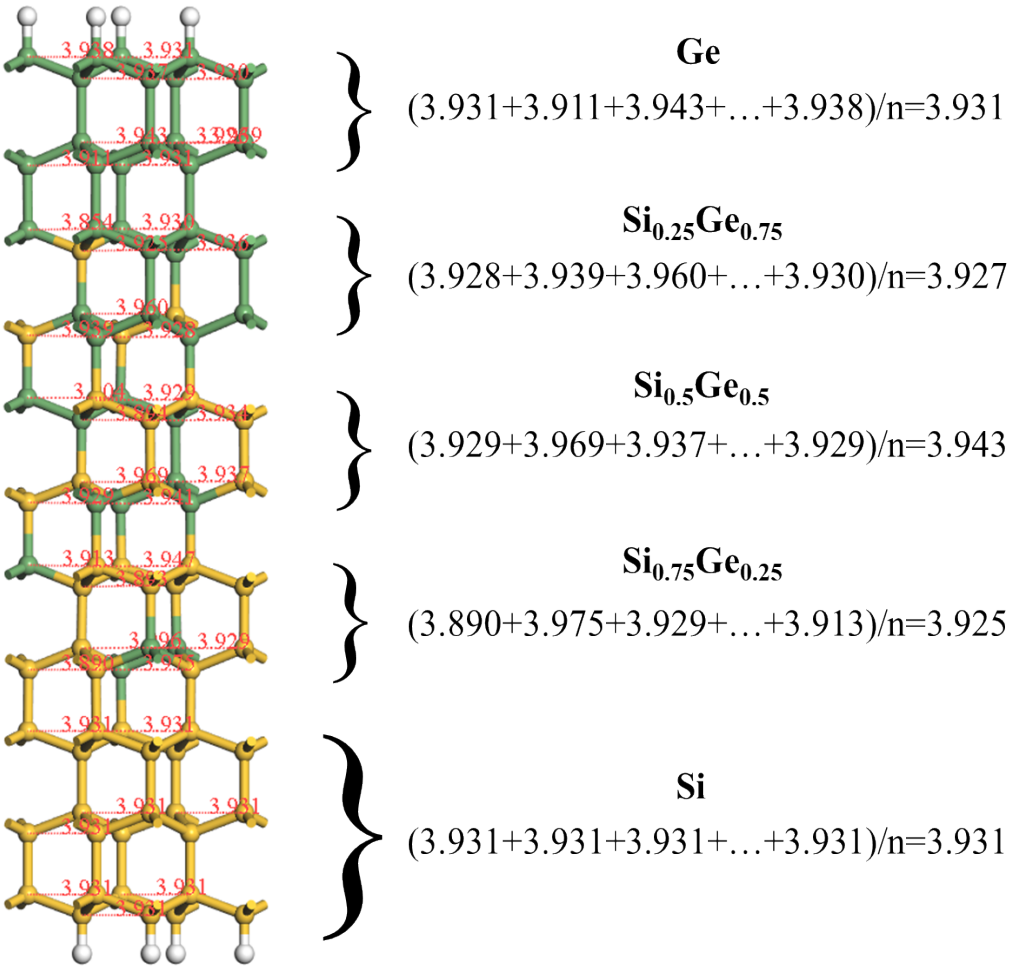

Fig.S3 The calculation method for strain of hex-$Si_{1-x}Ge_x$ (0, 0.25, 0.5, 0.75, 1) buffer layer

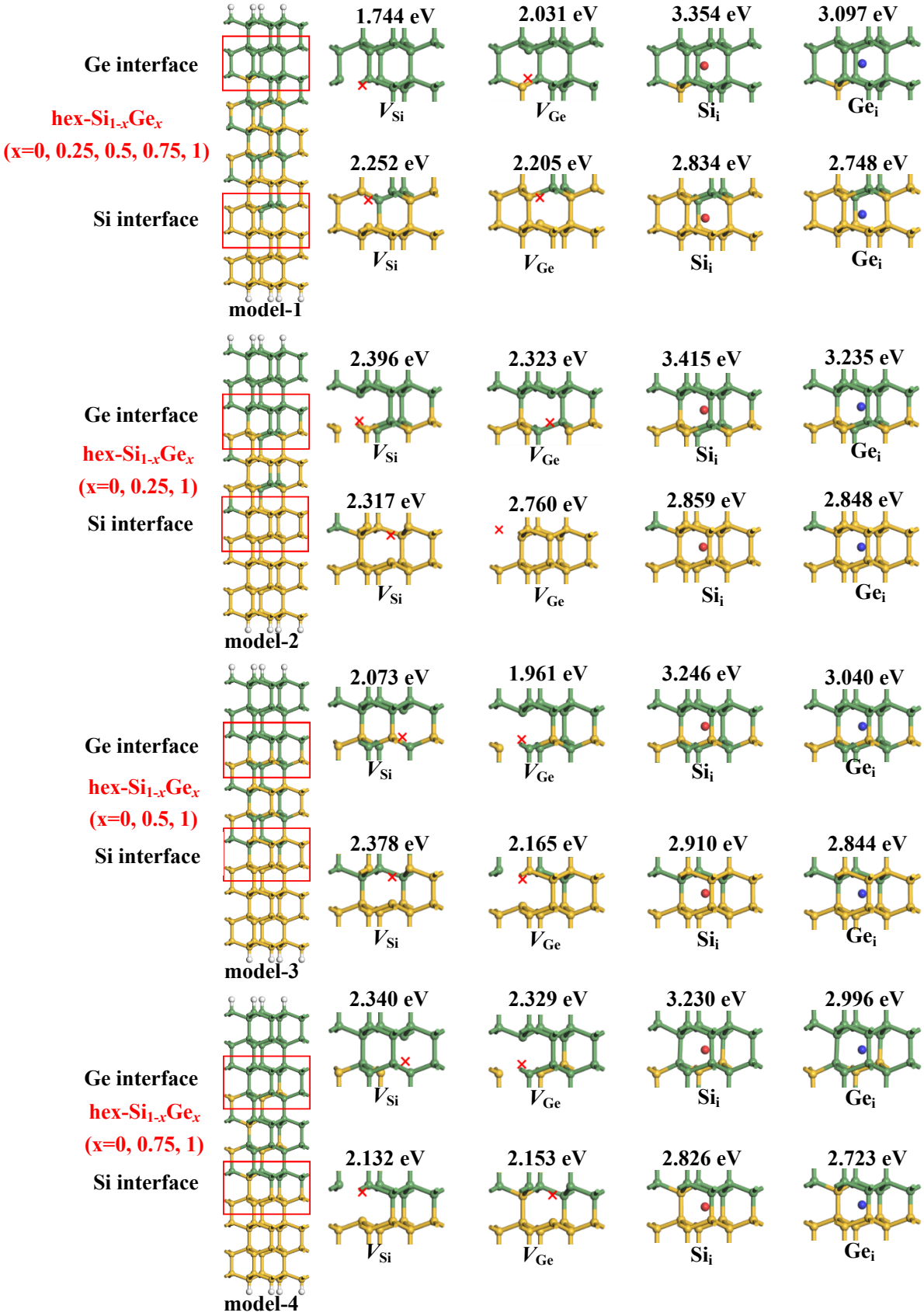

Fig.S4 The atomic structure of different vacancy and interstitial at Si interface and Ge interface of model-1, 2, 3, 4. For clarity, only the two atom layers concerned with defects are displayed. The corresponding defect formation energies are also indicated in the figure.

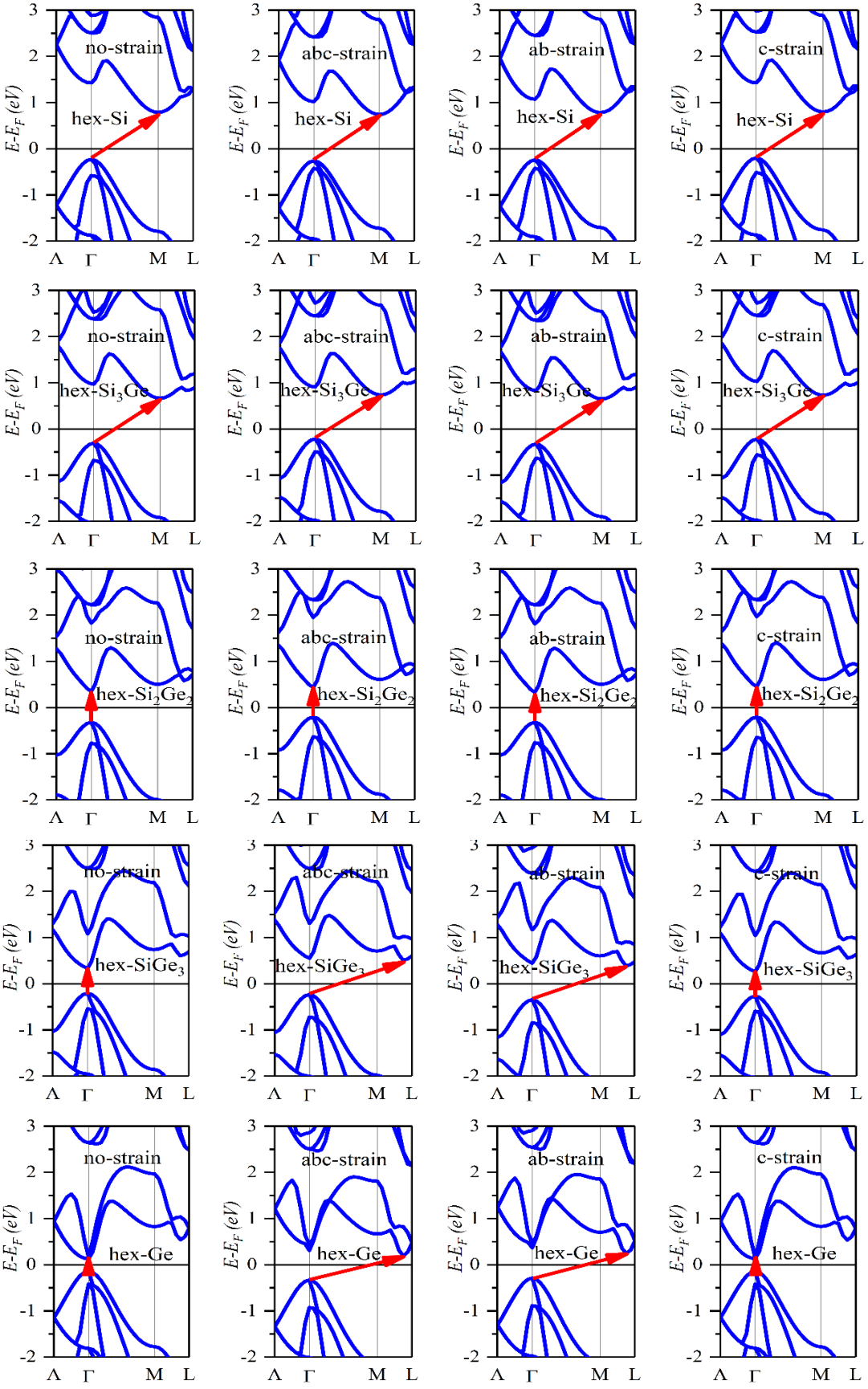

Fig.S5 The band structure of each component of the model-1 buffer layer calculated by using the HSE06 hybrid functional, i.e. hex-$Si_{1-x}Ge_x$ (x= 0, 0.25, 0.5, 0.75, 1) alloys without strain and strain on abc directions, ab directions and c direction, respectively.

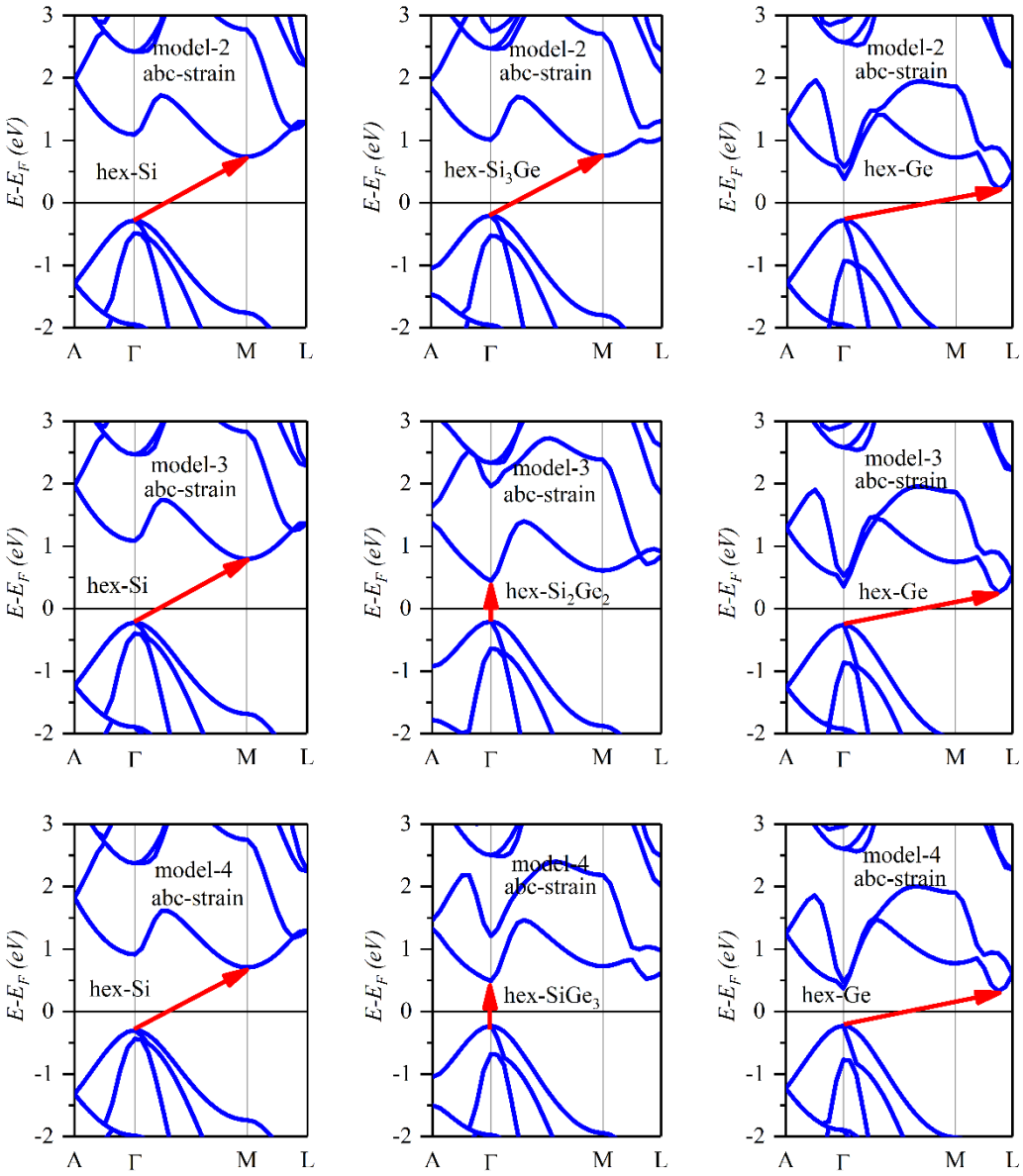

Fig.S6 The band structure of each component of the model-2, 3, 4 buffer layer calculated by using the HSE06 hybrid functional, i.e. hex-$Si_{1-x}Ge_x$ (x = 0, 0.25, 1) (x = 0, 0.5, 1) (x = 0, 0.75, 1) alloys with strain in the abc directions.