Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Theoretical investigation of the role of hydrogenation-induced strain in single-layer h10-Si

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TABLE S1: Bader analysis of fully hydrogenated SL h10-Si. The values of δ show the charge transfer between silicon and hydrogen atoms.

Atom	Number	Charge (e)	$\delta(e)$
Si1	6	3.98	0.02
Si2	4	3.47	0.53
H	4	1.56	-0.56

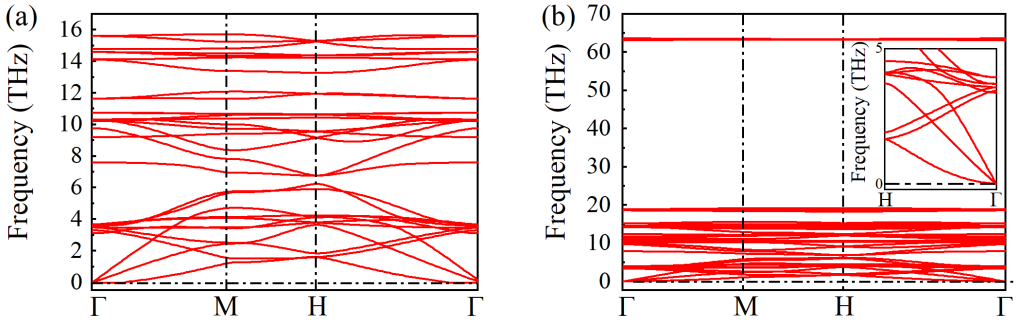

FIG. S1: Phonon spectrum of pristine (a) and fully hydrogenated (b) single-layer (SL) h10-Si. The inset shows the low-frequency modes of fully hydrogenated SL h10-Si aroud Γ point.

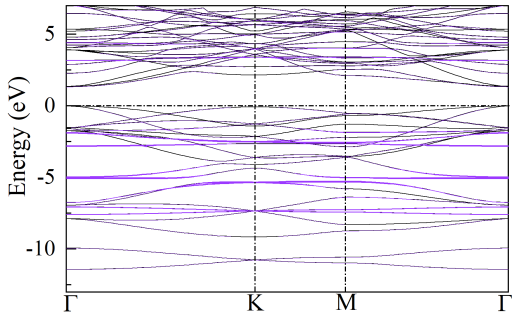

FIG. S2: The orbital projected electronic band structures of fully hydrogenated SL h10-Si. The s states of hydrogen atoms are represented by purple lines.

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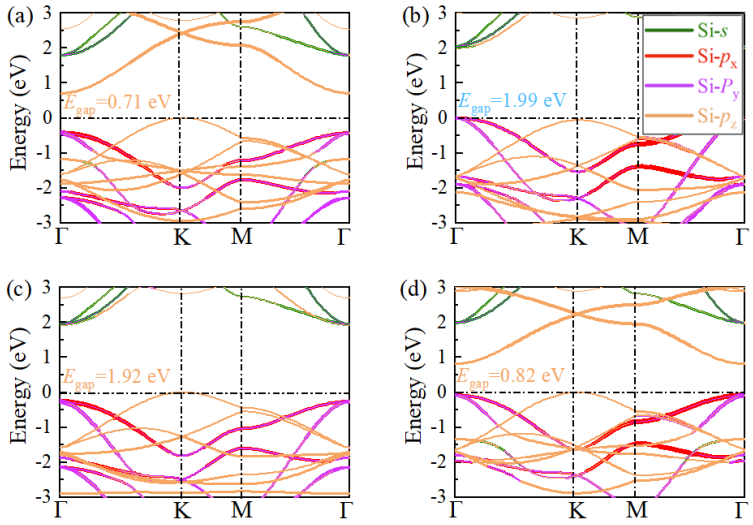

FIG. S3: The orbital projected electronic band structures of SL h10-Si in the (a) pristine structure, (b) fully hydrogenated structure, (c) pristine structure after hydrogen atoms attached, and (d) fully hydrogenated structure after hydrogen atoms removal calculated by using HSE06 functional. The values of indirect and direct band gaps are exhibited by orange and blue texts, respectively.

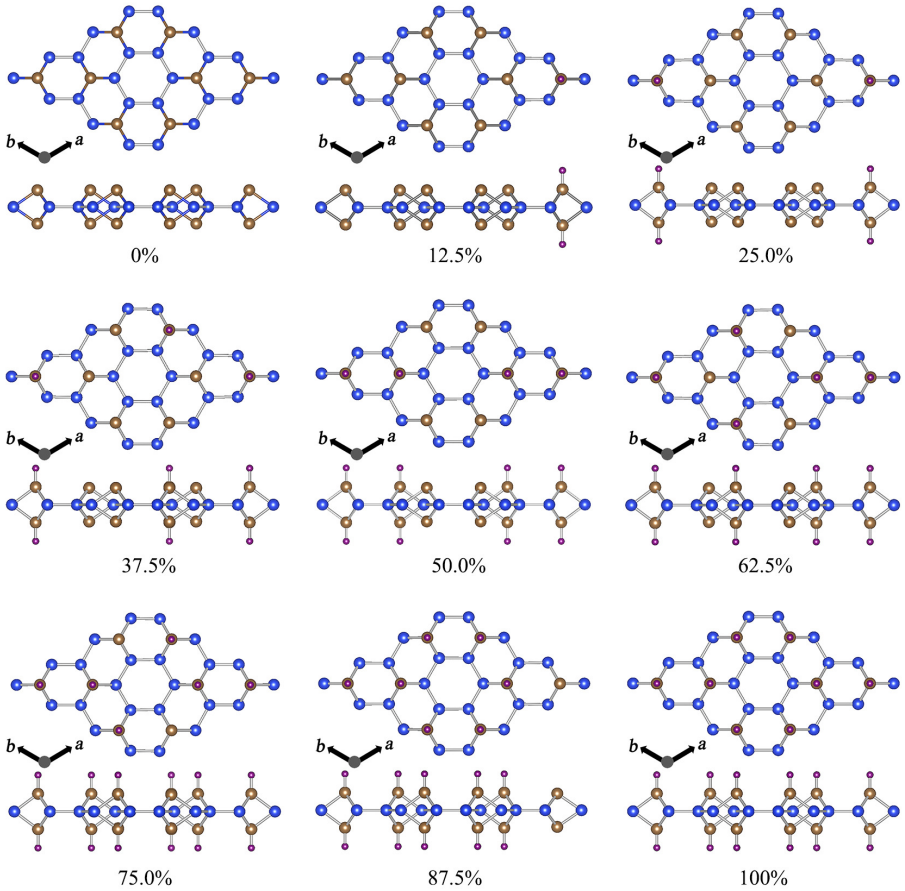

FIG. S4: The structures of hydrogenated SL h10-Si with the hydrogenation concentrations of 0%, 12.5%, 25.0%, 37.5%, 50.0%, 62.5%, 75.0%, 87.5% and 100%, respectively.

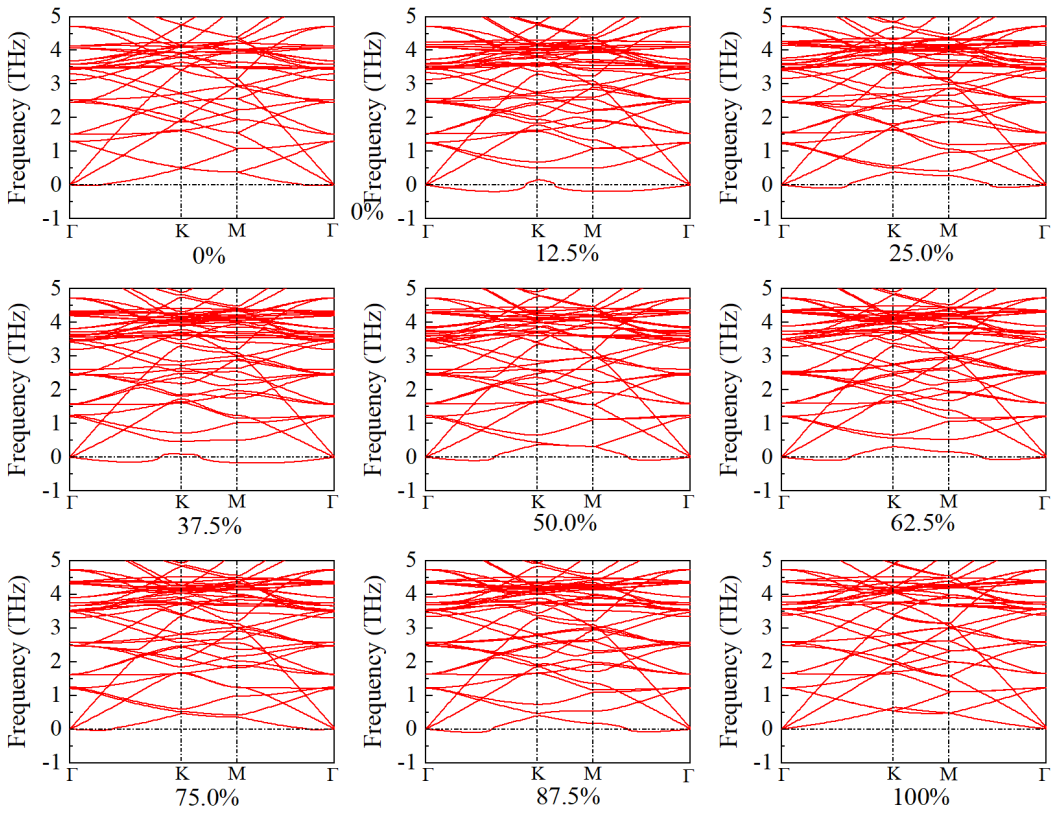

FIG. S5: The phonon spectra of hydrogenated SL h10-Si with the hydrogenation concentrations of 0%, 12.5%, 25.0%, 37.5%, 50.0%, 62.5%, 75.0%, 87.5% and 100%, respectively.

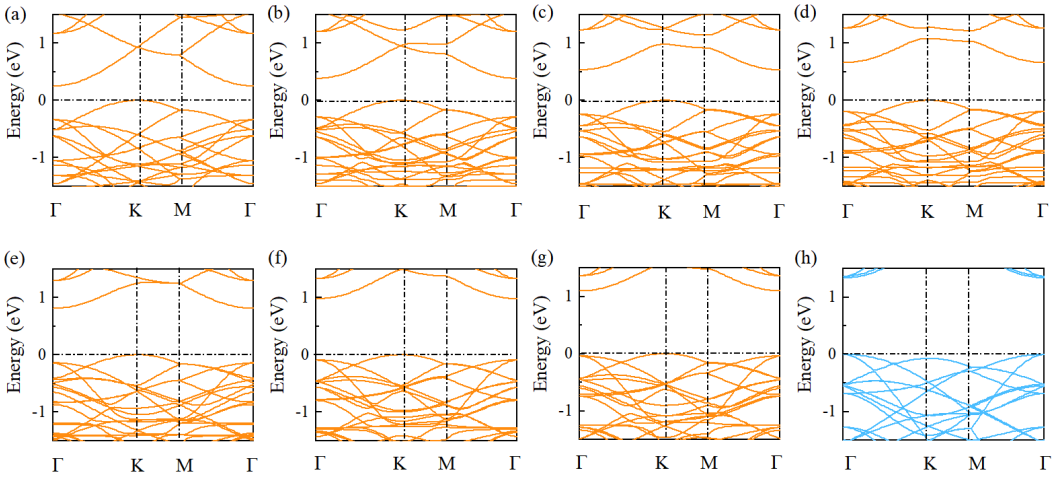

FIG. S6: The electronic band structures of (a) pristine and (b)-(h) hydrogenated SL h10-Si with the hydrogenation concentrations of 12.5%, 25.0%, 37.5%, 50.0%, 62.5%, 75.0%, and 100%, respectively.

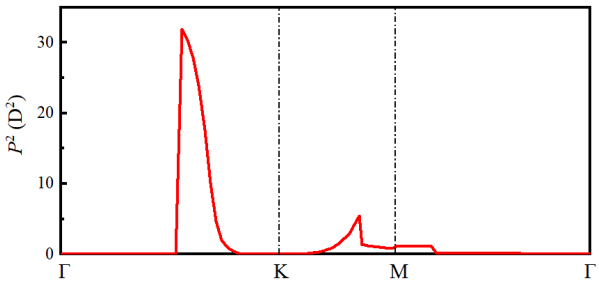

FIG. S7: The transition matrix elements between the top valence and the lowest conduction bands for fully hydrogenated SL h10-Si.