Supplementary Information

First-principles study of hydrogen storage capacity based on Li-Na-decorated silicene†

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†Electronic Supplementary Information (ESI): The optimized structure of Li-Na-decorated silicene with sites information of Li and Na atoms (Fig. S1), the energy band structure of Li-Na-decorated silicene based on HSE06 functional (Fig. S2), the molecular dynamics simulation analysis of Li-Na-decorated silicene (Fig. S3), the optimized structures of Li-Na-decorated silicene with much more H_2 molecules around Li or Na atom (Fig. S4), the optimized structures of Li-decorated and Na-decorated silicene with corresponding maximum H_2 molecules (Fig. S5), and the calculated parameters for Li-Na-decorated silicene (Table S1).

‡Both authors contributed equally to this work.

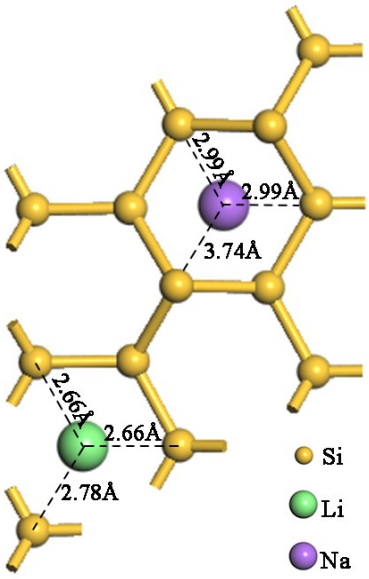


Fig. S1 The optimized structure of Li-Na-decorated silicene with sites information of Li and Na atoms. The distances between the Li atom and the three neighboring Si atoms are 2.66 Å, 2.66 Å, and 2.78 Å, respectively, and 2.99 Å, 2.99 Å, and 3.74 Å for the Na atom. The distance of Li-Li and Na-Na is as large as 7.54 Å.

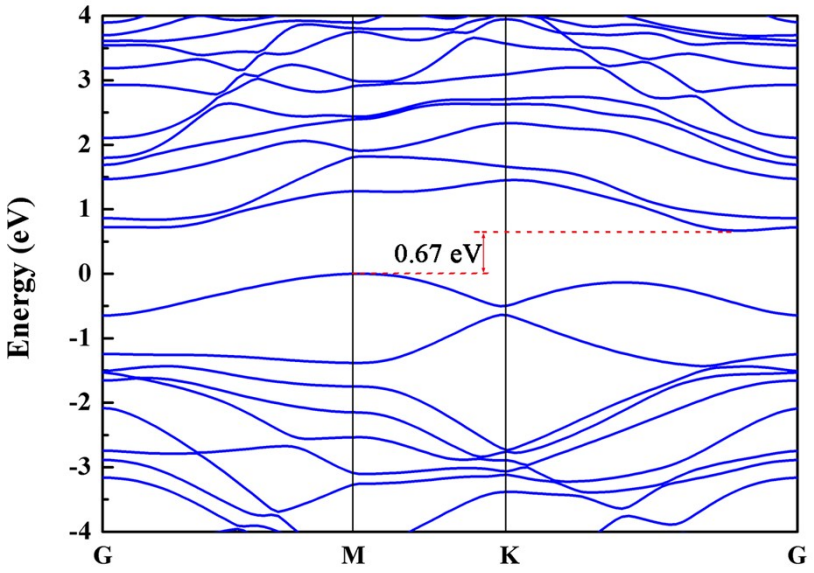


Fig. S2 The energy band structure of Li-Na-decorated silicene based on HSE06 functional.

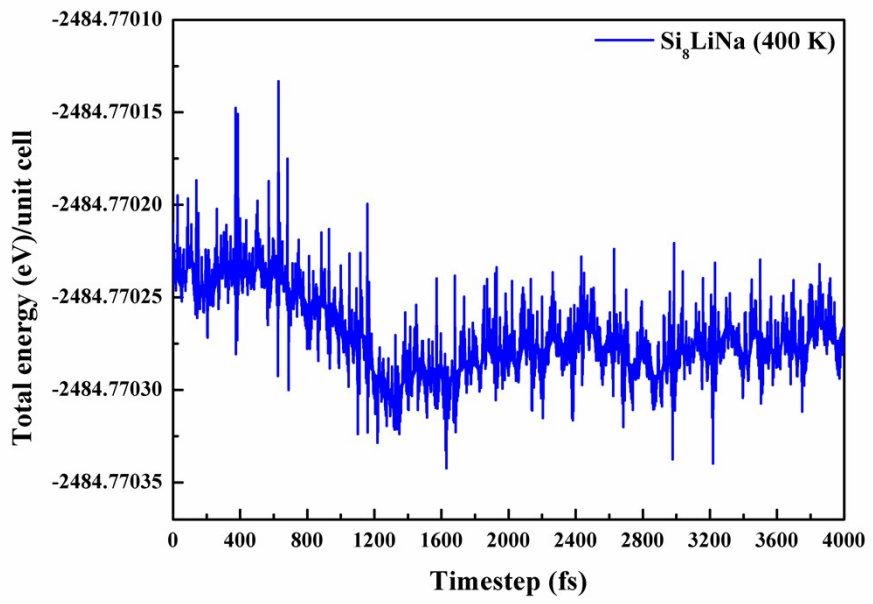
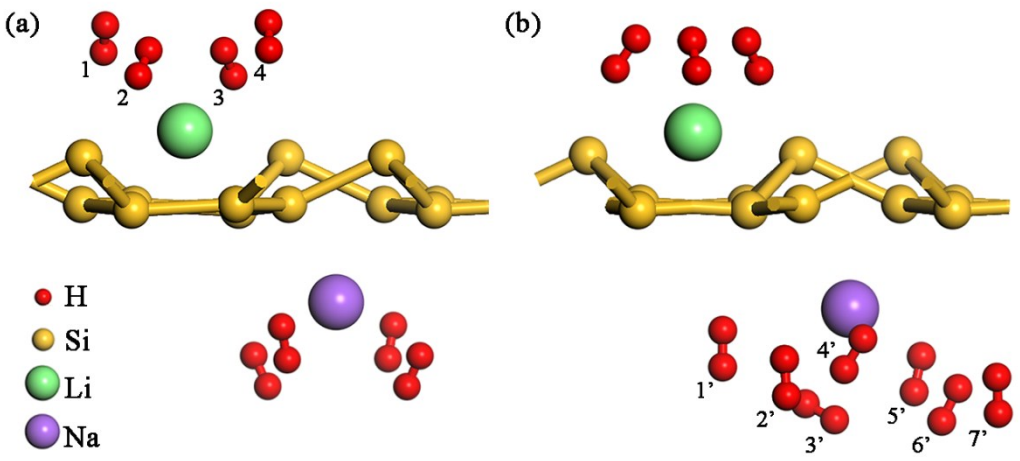


Fig. S3 The molecular dynamics simulation analysis to confirm the structural stability of the Li-Na-decorated silicene (Si_8LiNa).



hydrogen	1	2	3	4
adsorption distance(Å)	3.10	2.03	2.03	3.19

hydrogen	1'	2'	3'	4'	5'	6'	7'
adsorption distance(Å)	3.49	2.56	2.55	2.42	2.47	2.48	3.74

Fig. S4 The optimized structures of Li-Na-decorated silicene with (a) four H_2 molecules adsorbed around the Li atom and (b) seven H_2 molecules adsorbed around the Na atom. The tables listed below present the adsorption distance of each H_2 molecule for the above structure. It is clear to see that the adsorption distance of two H_2 molecules adsorbed around the Li atom (marked as 1 and 4) is obviously larger than the other two (marked as 2 and 3) in Fig. S4(a). Similarly, in the terms of Na atom, the adsorption distance of the H_2 molecules marked as 1' and 7' is larger than the others in Fig. S4(b).

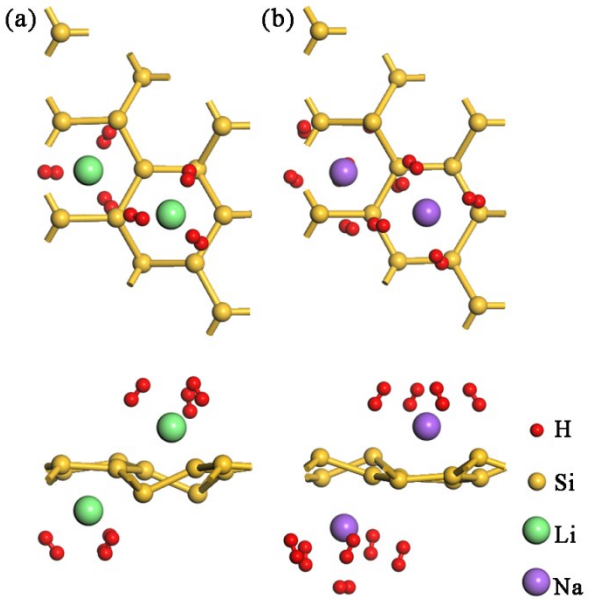


Fig. S5 The optimized structures of (a) Li-decorated and (b) Na-decorated silicene with corresponding maximum H_2 molecules. Up to six and ten H_2 molecules can be absorbed on Li-decorated and Na-decorated silicene, respectively, leading to the maximum storage capacities of 4.82% and 6.93 wt%, as well as the average E_{ads} of 0.39 eV/H_2 and 0.27 eV/H_2, respectively.

Table S1 Calculated parameters with n (n = 0-9) absorbed H_2 molecules for Li-Na-decorated silicene (Si_8LiNa). The listed parameters are average lattice parameter (a); Si-Si bond length (d); average buckled value (h); average adsorption energy (E_{ads}), and hydrogen storage capacity, respectively.

System	n	a (Å)	d (Å)	h (Å)	E_{ads} (eV/H_2)		Storage capacity (wt%)
					GGA	GGA+vdW	
Si_8LiNa	0	7.585	2.272-2.351	1.106	None	None	None
	1	7.538	2.262-2.345	1.099	0.11	1.67	0.79
	2	7.537	2.262-2.346	1.098	0.08	0.91	1.58
	3	7.536	2.261-2.344	1.099	0.06	0.64	2.32
	4	7.521	2.255-2.338	1.098	0.05	0.52	3.07
	5	7.517	2.255-2.340	1.097	0.04	0.45	3.81
	6	7.509	2.253-2.337	1.099	0.04	0.40	4.53
	7	7.504	2.252-2.336	1.098	0.02	0.35	5.25
	8	7.502	2.251-2.336	1.098	0.01	0.31	6.33
	9	7.497	2.250-2.334	1.097	0.01	0.29	6.65