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Ultra high capacity of hydrogen storage in Li decorated two-dimensional C_2N layer

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Adsorption Energies of H_2 on a single layer C_2N

The total energy of Vacancy site (V) is set to zero as a reference energy.

TABLE SI: Calculated Energy difference and adsorption energies (in eV) of H_2 at Pristine C_2N.

System (Different sites)	Vacancy (V)	N-top (N)	Hollow-I (H_1)	Hollow-II (H_2)	C-top (C)
Energy difference	0	0.02	0.06	0.05	0.07
Adsorption energy	0.12	0.1	0.06	0.07	0.05

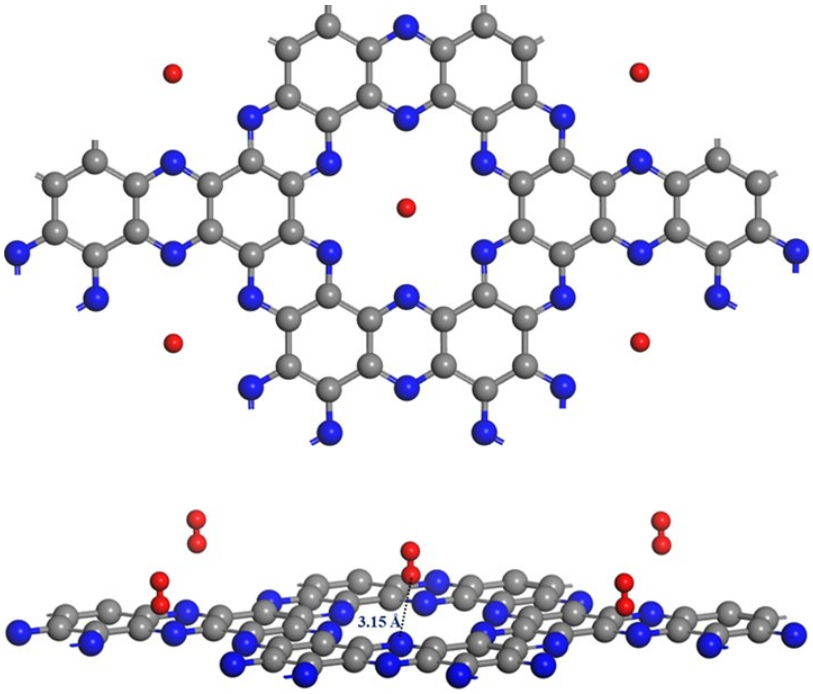

Fig. S1 Top and side view of most stable optimized geometry of one hydrogen molecule absorbed on the holey C2N. The gray, blue and red balls represent carbon, nitrogen and hydrogen atoms respectively.

Binding Energies of Li at single layer C_2N-h2D

Different adsorption sites for single Li has been checked to find out the most stable site. This corresponds to C_2N single side Li adsorption.

The total energy of Vacancy site (V) is set to zero as a reference energy.

TABLE S2: Calculated Energy difference (in eV) of single Li decorated C_2N.

System (Different sites)	Vacancy (V)	N-top (N)	Hollow-I (H_1)	Hollow-II (H_2)	C-top (C)
Energy difference	0	moved to V-site	3.04	2.85	moved to V-site

Different adsorption sites for 2 Li atoms has been checked to find out the most stable site. This corresponds to C_2N double side Li adsorption.

The total energy of Vacancy site (V up & dn) is set to zero as a reference energy.

TABLE S3: Calculated Energy difference (in eV) of 2-Li decorated C_2N.

System	V (up & dn)	C+N-top	C-top	H_2+H_2	N-top	H_1+V
Energy difference	0	Not-seen	Not-seen	4.80	Not-seen	1.34

Different adsorption sites for various Li concentrations is checked. It was found that Li atom always prefers to the vacancy site.

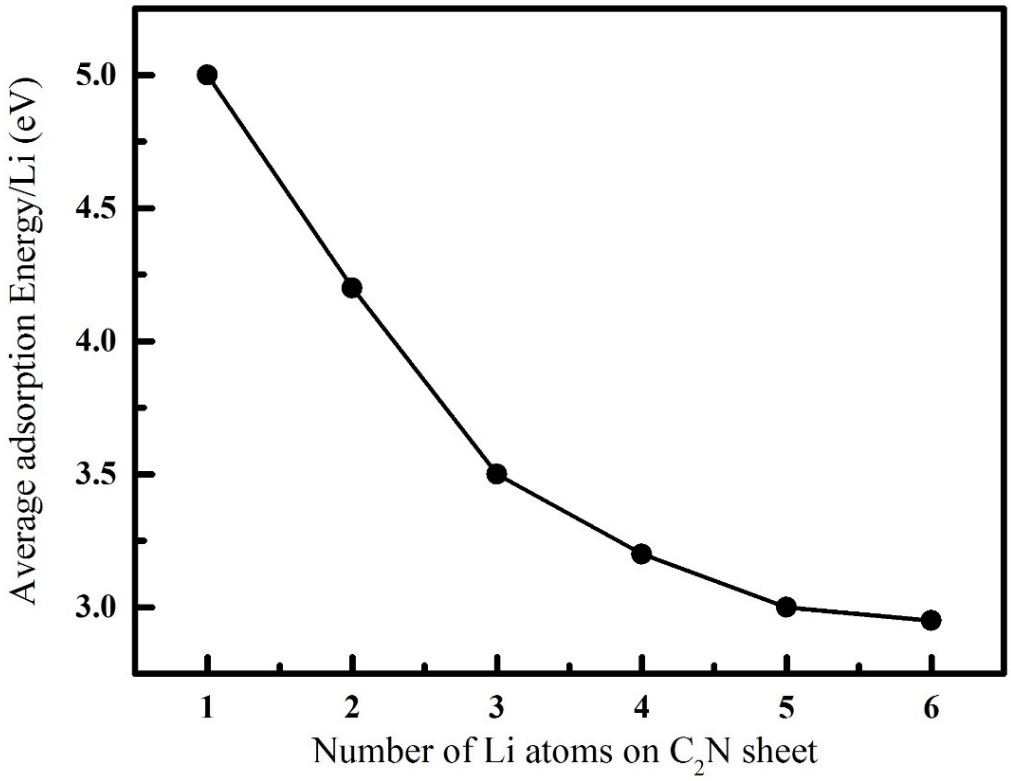

Fig. S2 Variation in binding energy with increasing Li content at holey C_2N layer.

Bandstructures of Li doped C_2N-h2D

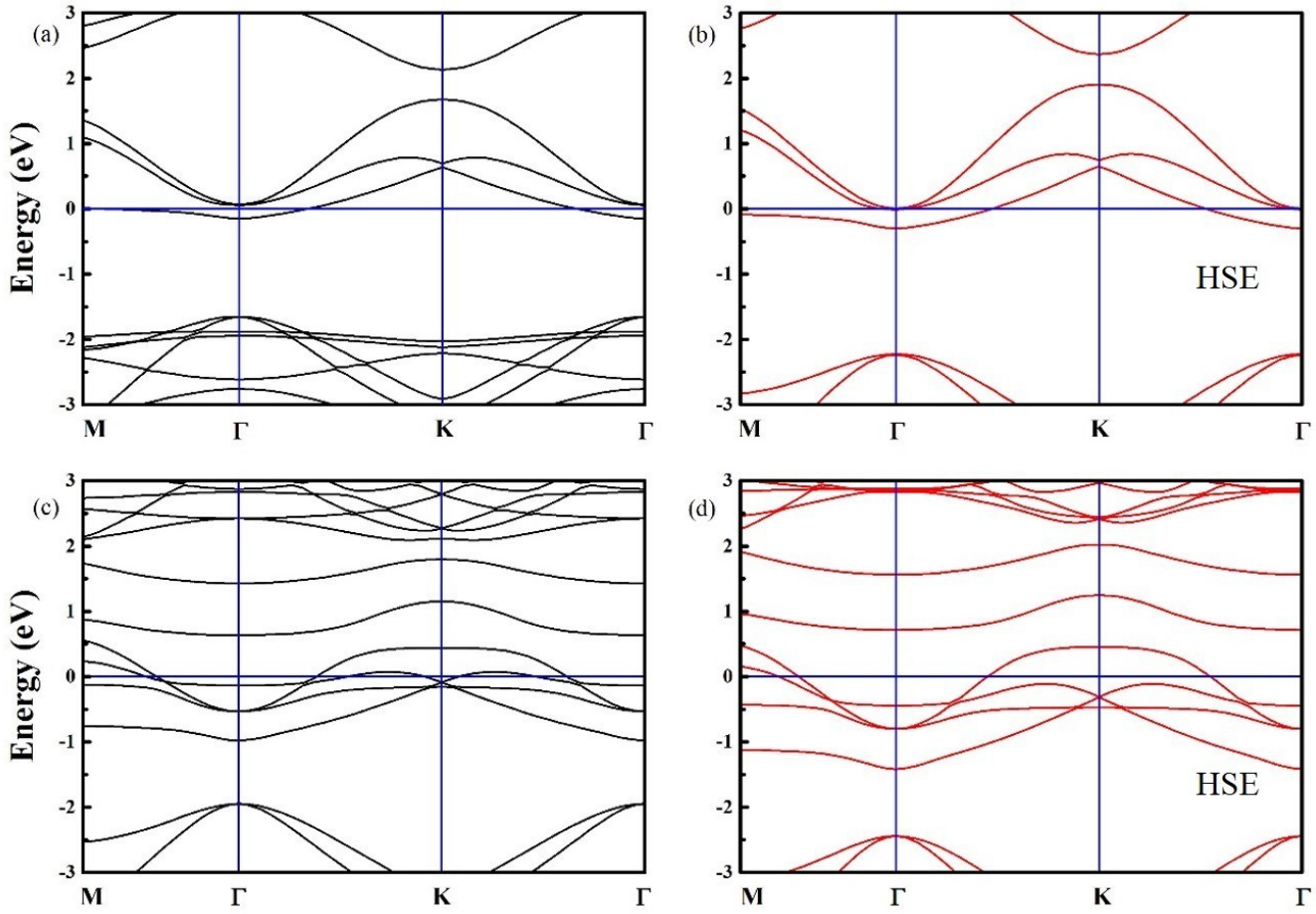

Fig. S3 Li doped calculated band structures. 1-Li doped C_2N layer bandstructures are shown (a) based on PBE+vdW (b) and HSE06 exchange correlation functional, respectively. 6-Li doped C_2N layer bandstructures (c) based on PBE+vdW (d) and HSE06. The blue solid line at zero indicates the Fermi level.

Adsorption Energies of H_2 at Li doped C_2N-h2D

Binding of Li at C_2N layer is calculated by

$$E_{ads} = \frac{E_{C_2N-Li} + nE_{H_2} - E_{tot}}{n}$$

Here E_{C_2N-Li} and E_{H_2} are the total energy of Li doped C_2N layer and energy of H_2 molecule in same slab, n is the number of H_2 molecules while E_{tot} is the energy of hydrogen adsorbed Li doped C_2N.

PDOS of the C2N decorated by Li before and after H2 adsorption

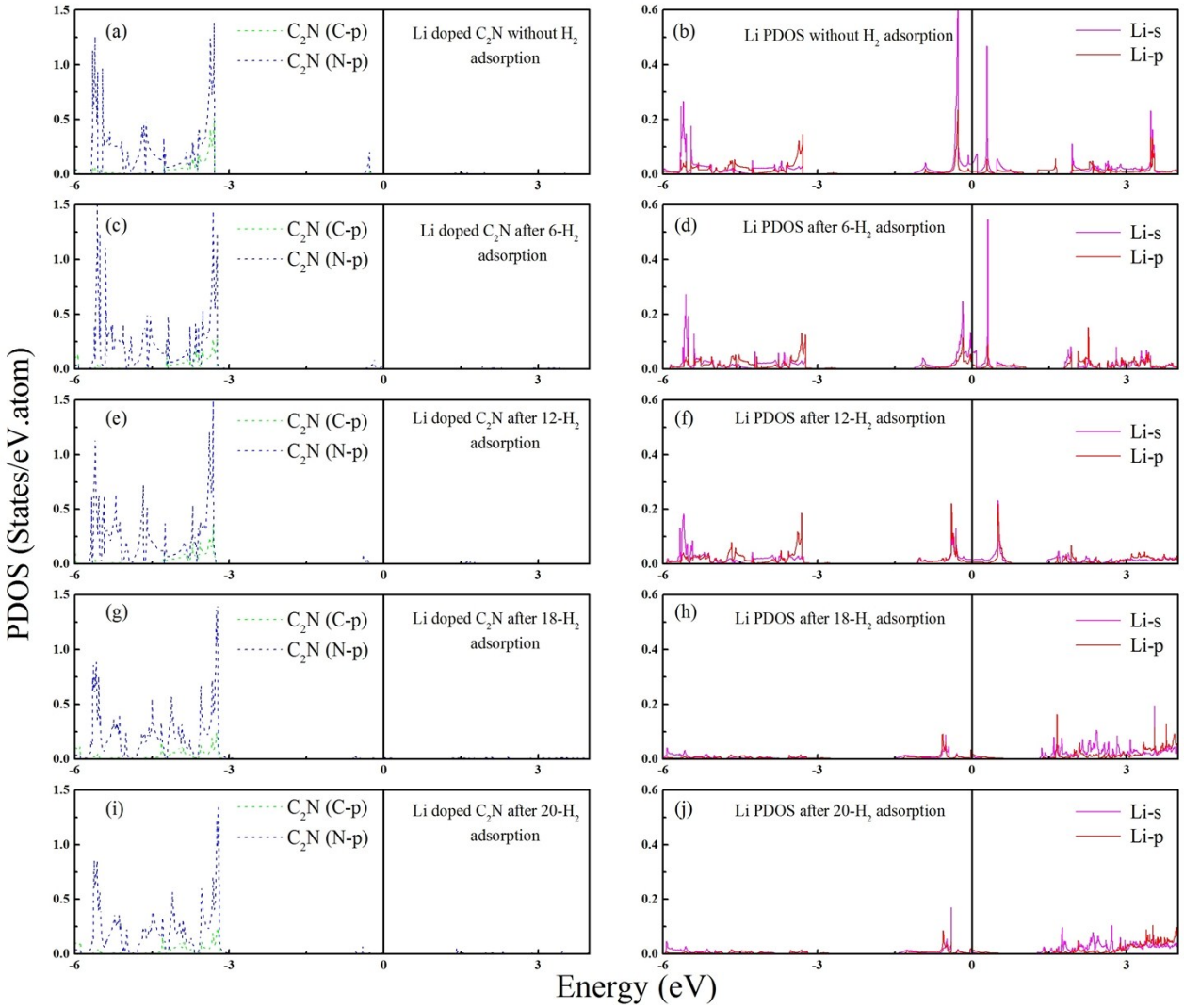

Fig. S4 The PDOS of the Li doped C_2N before and after H2 adsorption. Li doped C_2N before H_2 adsorption (a) Carbon & Nitrogen PDOS (b) Adsorbed Li PDOS. $6H_2$ adsorbed LiC_2N PDOS of (c) Carbon & Nitrogen (d) Li PDOS. (e-f) LiC_2N with $12H_2$ adsorbed PDOS of C2N and Li respectively. (g-h) PDOS of C2N & Li respectively with $18H_2$ molecules and (i-j) PDOS of C2N & Li respectively with $20H_2$ molecules.