https://doi.org/10.1007/s11467-023-1385-0

RESEARCH ARTICLE

Modulation of charge in C_9N_4 monolayer for a high-capacity hydrogen storage as a switchable strategy

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Received December 14, 2023; accepted January 16, 2024

Supporting information

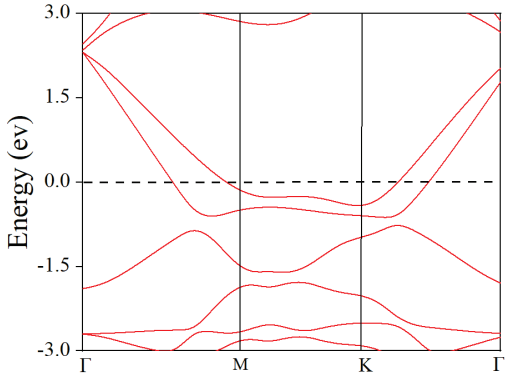

Fig. S1 The band structure of C_9N_4 monolayer at HSE06 level.

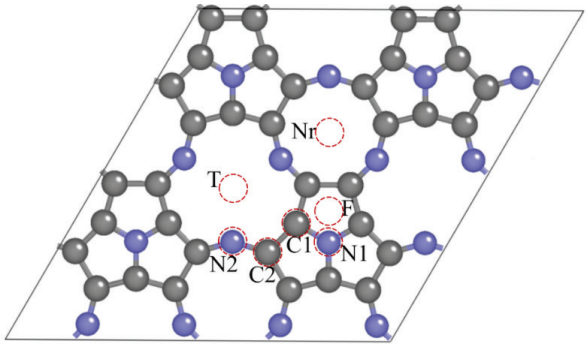

Fig. S2 we considered 7 kinds of sites for H_2 molecule adsorption. The red dotted line shows the specific location we have chosen for the adsorption, which are the top of (i) five-membered ring, marked with **F**, (ii) nine-membered ring, marked with **Nr**, (iii) twelve-membered ring, marked with **T**, (iv) N1 atom, marked with **N1**, (v) N2 atom, marked with **N2**, (vi) C1 atom, marked with **C1**, (vii) C2 atom, marked with **C2**.

Table S1 The energy of adsorption for individual hydrogen molecules at each site in the neutral state.

Adsorption sites	E_{ads} (eV)
T	0.23
Nr	0.32
F	0.29
C1	0.3
C2	0.32
N1	0.28
N2	0.28

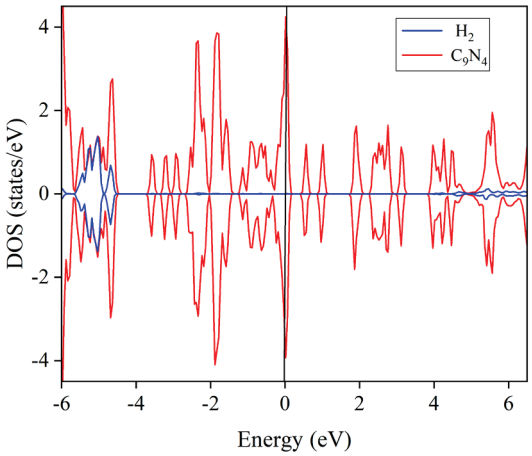

Fig. S3 The partial density of states of the adsorption system consisting of a C_9N_4 monolayer adsorbed by a hydrogen molecule.

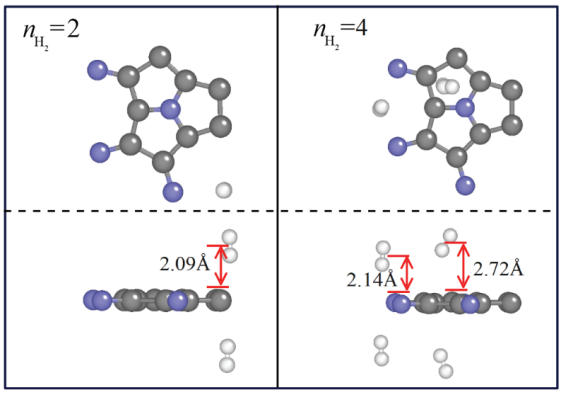

Fig. S4 Top and side views of the lowest-energy configuration of 3 e^- negatively charged C_9N_4 with the successive adsorption of 2 to 4 H_2 molecules. The perpendicular distance from the center of gravity of the H_2 molecule to the C_9N_4 is shown by the red bi-directional arrows.

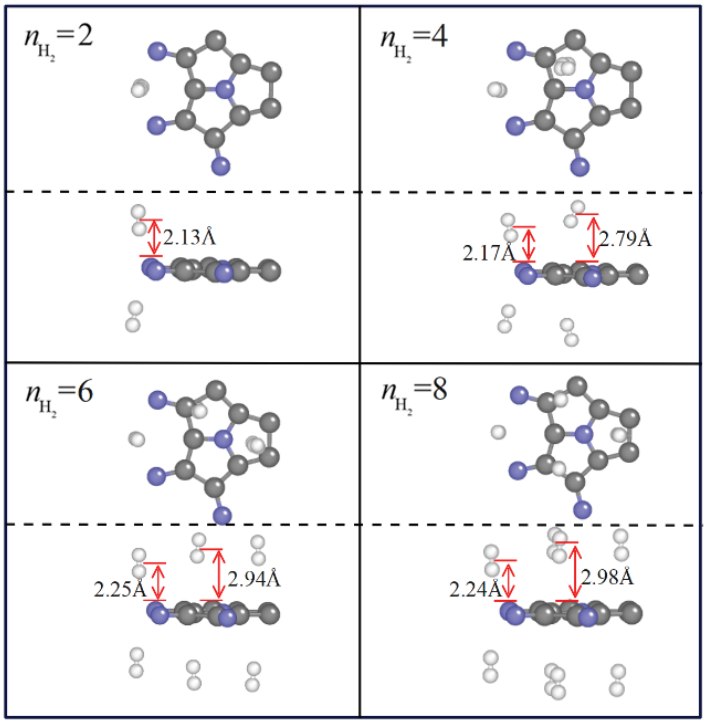

Fig. S5 Top and side views of the lowest-energy configuration of 4 e^- negatively charged C_9N_4 with the successive adsorption of 2 to 8 H_2 molecules. The red bi-directional arrows indicate the perpendicular distance from the center of gravity of the H_2 molecule to the C_9N_4.

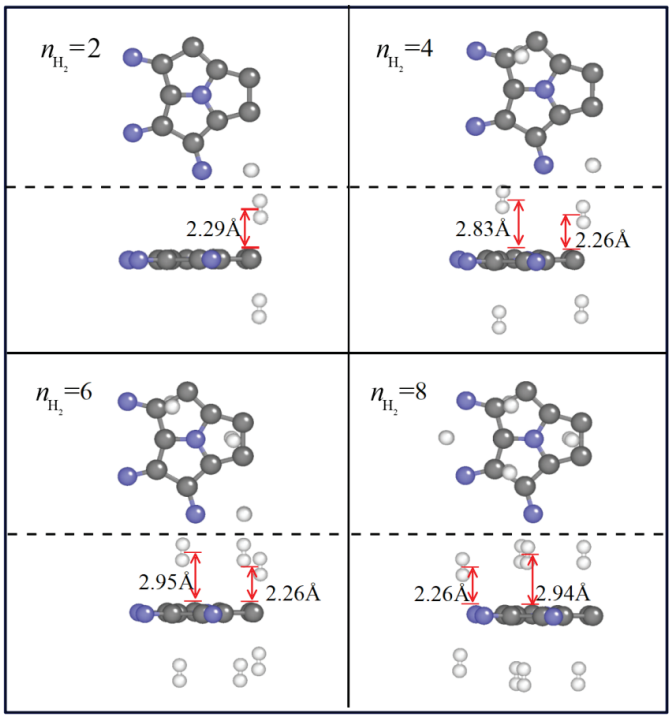

Fig. S6 Top and side views of the lowest-energy configuration of 5 e^- negatively charged C_9N_4 with the successive adsorption of 2 to 8 H_2 molecules. The red bi-directional arrows indicate the perpendicular distance from the center of gravity of the H_2 molecule to the C_9N_4.

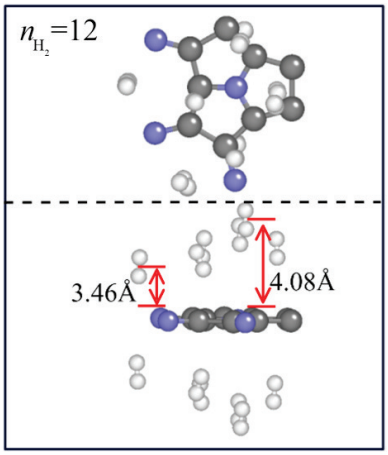

Fig. S7 Top and side views of the lowest-energy configuration of 4 e^- negatively charged C_9N_4 with the adsorption of 12 H_2 molecules. The red bi-directional arrows indicate the perpendicular distance from the center of gravity of the H_2 molecule to the C_9N_4.

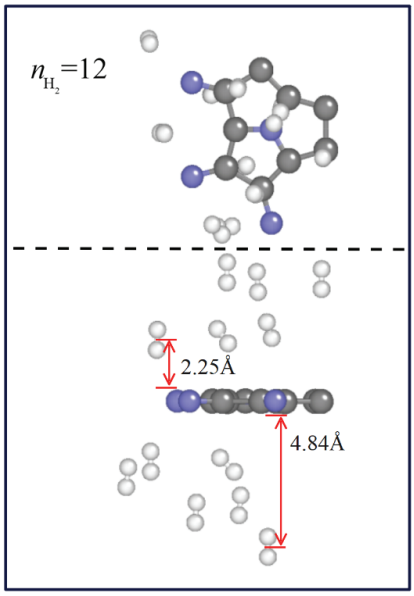

Fig. S8 Top and side views of the lowest-energy configuration of 5 e^- negatively charged C_9N_4 with the adsorption of 12 H_2 molecules. The red bi-directional arrows indicate the perpendicular distance from the centre of gravity of the H_2 molecule to the specified point.