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

Supporting information:

Graphene/C_2N lateral heterostructures as promising anode materials in lithium-ion batteries

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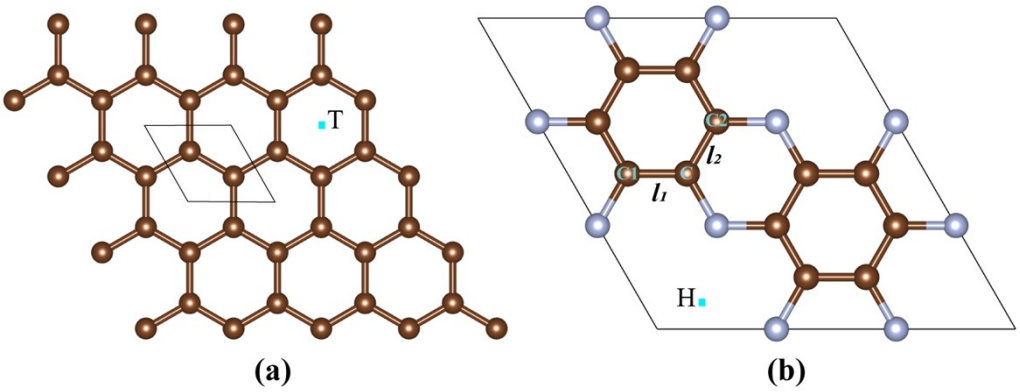

Fig. S1 Geometrical structures of (a) graphene and (b) C_2N monolayers. Brown and gray balls represent C and N atoms. T and H denote the stable sites for Li atom adsorption.

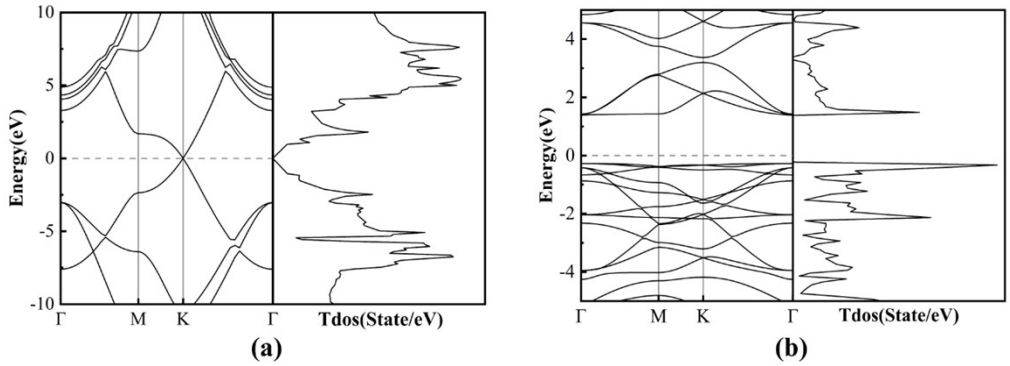

Fig. S2 Band structures and density of states (DOSs) of (a) graphene and (b) C_2N monolayers.

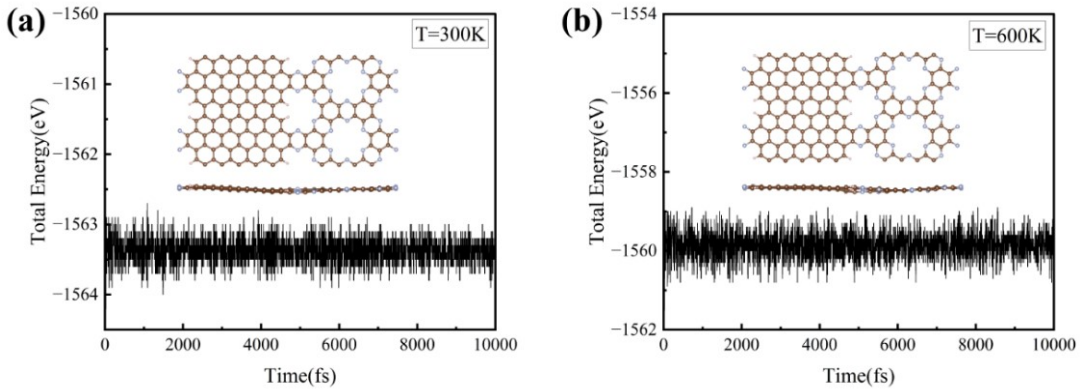

Fig. S3 Molecular dynamics simulation of model (11, 26) at (a) 300 K and (b) 600 K. The final snapshots of (11, 26) G/C_2N-LH viewed from different directions are displayed.

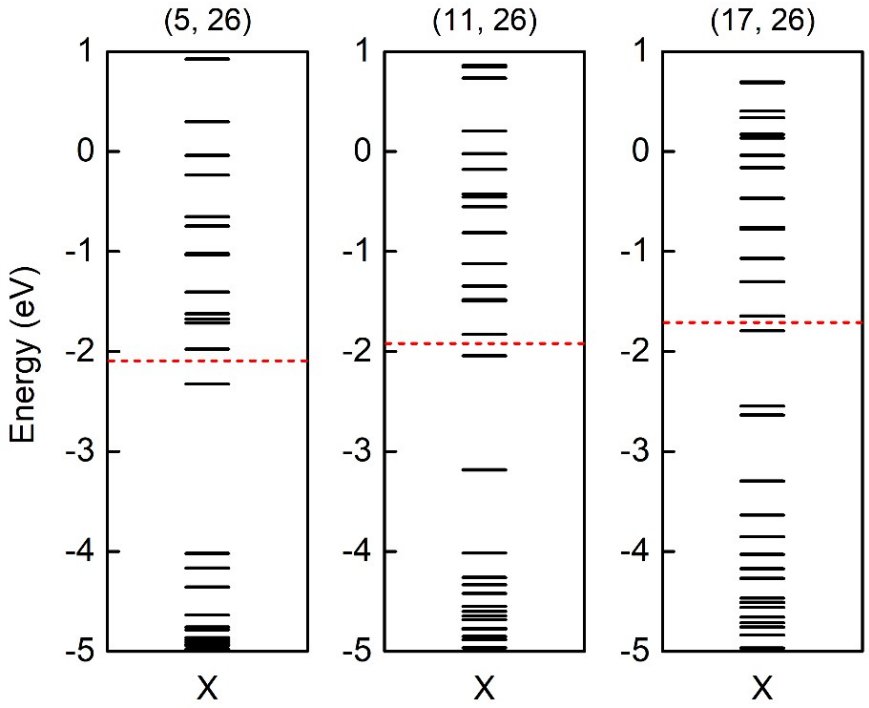

Fig. S4. Calculated energy eigenvalues for (5, 26), (11, 26), and (17, 26) G/C_2N-LHs at the X point using the HSE06 method. The Fermi level is denoted by the red dashed line.

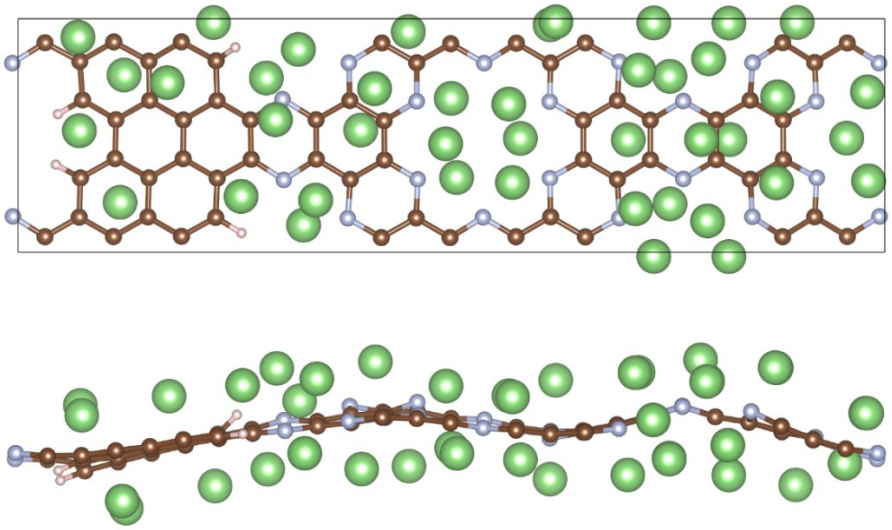

Fig. S5 Stable structure of model (5,26) after adsorption of 40 Li atoms. Brown, gray, green and pink balls represent C, N, Li and H atoms, respectively.

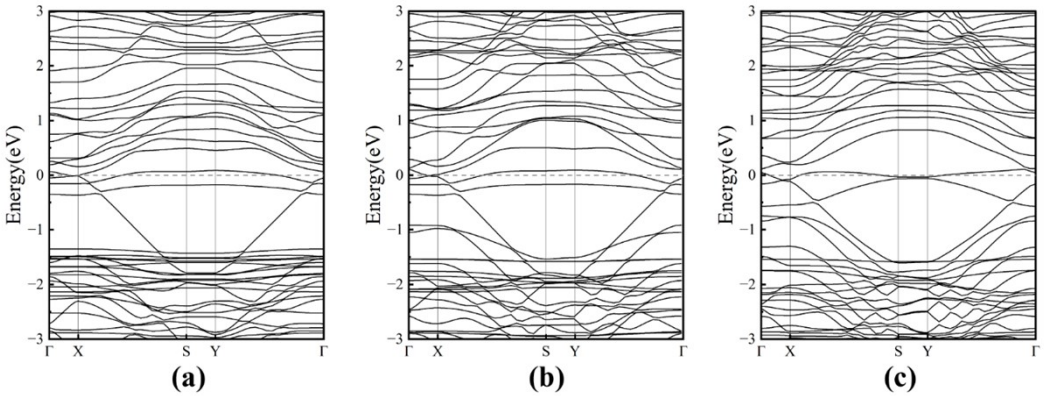

Fig. S6 Band structures of G/C_2N-LHs after adsorbing a lithium atom at a stable site: (a) (5,26), (b) (11, 26) and (c) (17, 26).

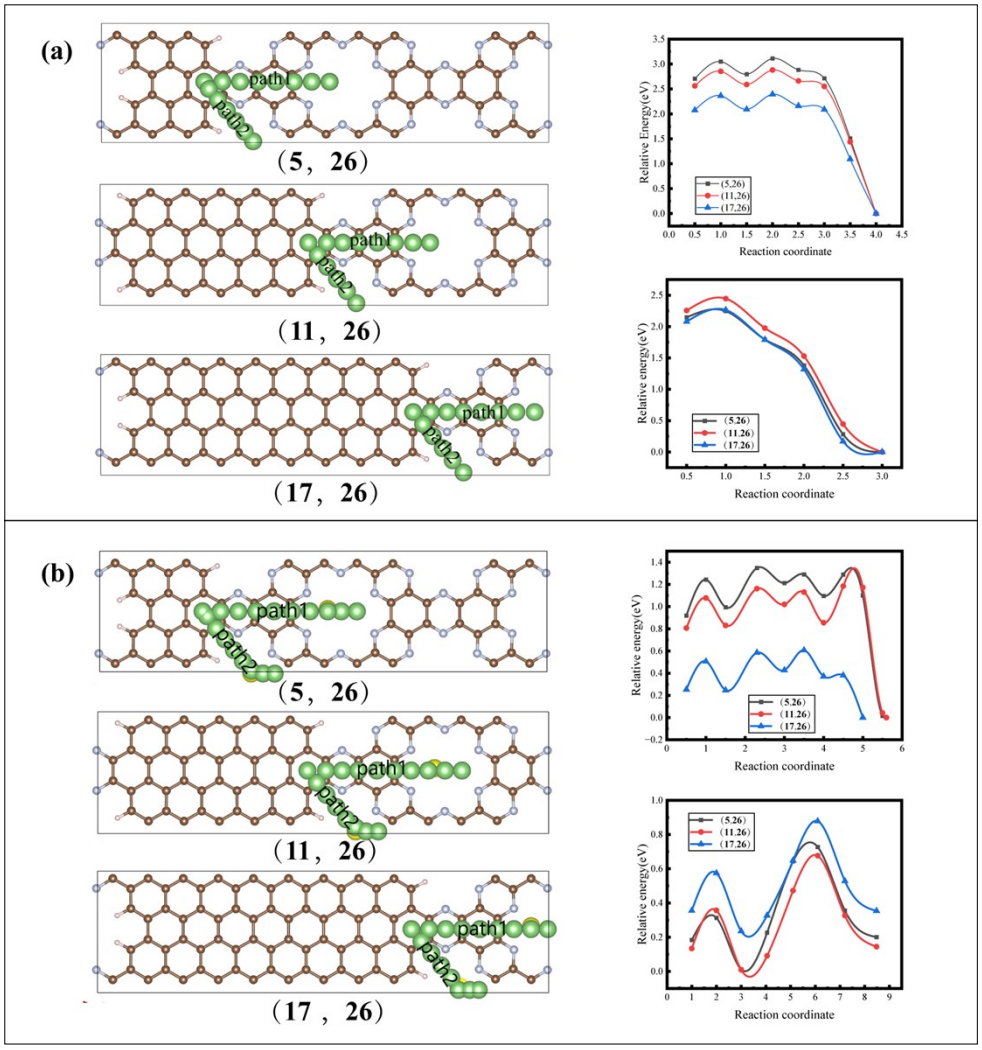

Fig. S7 Diffusion pathways and energy barrier for Li atom migrating on (a) bare G/C_2N-LHs and (b) one Li atom-adsorbed G/C_2N-LHs. Brown, gray, and pink balls represent C, N, and H atoms, respectively. Green balls represent lithium atoms in the diffusion process, and yellow balls represent a lithium atom attached to G/C_2N-LHs.