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C_3N/phosphorene heterostructure: a promising anode material in lithium-ion batteries

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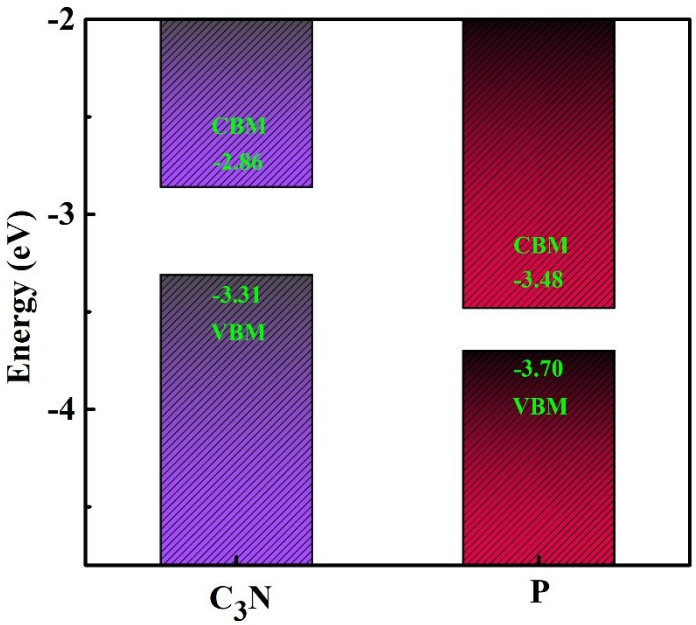

Fig. S1. Band alignment of stress-containing C_3N and phosphorene. CBM and VBM are calculated by PBE method.

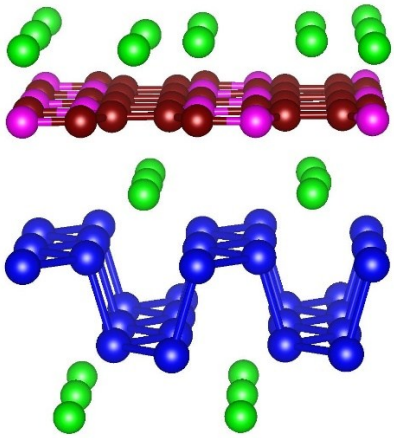

Fig. S2 Optimized structure of $Li_{2.5}C_3NP$.

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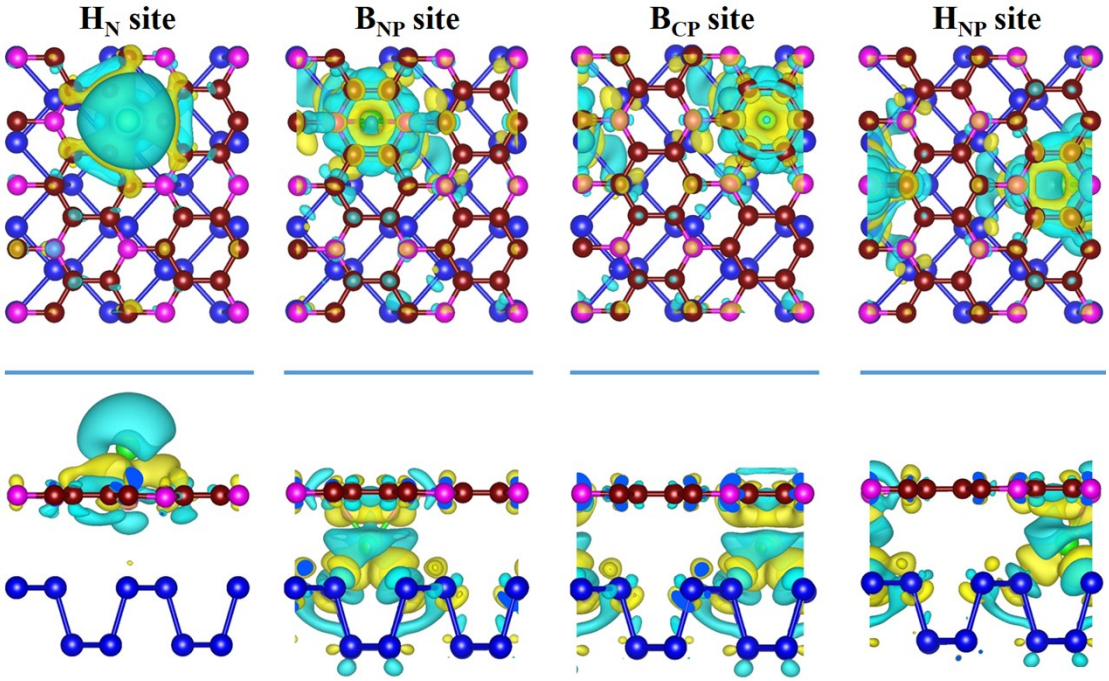

Fig. S3 Top and side views of the diff charge density of Li inserted into (a) H_N site, (b) B_{NP} site, (c) B_{CP} site and (d) H_{NP} site. The loss of electrons is indicated in blue and gain of electrons is indicated in yellow.