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The Potential Application of Phosphorene as Anode Materials in Li-ion Batteries

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Here are the supplementary figures:

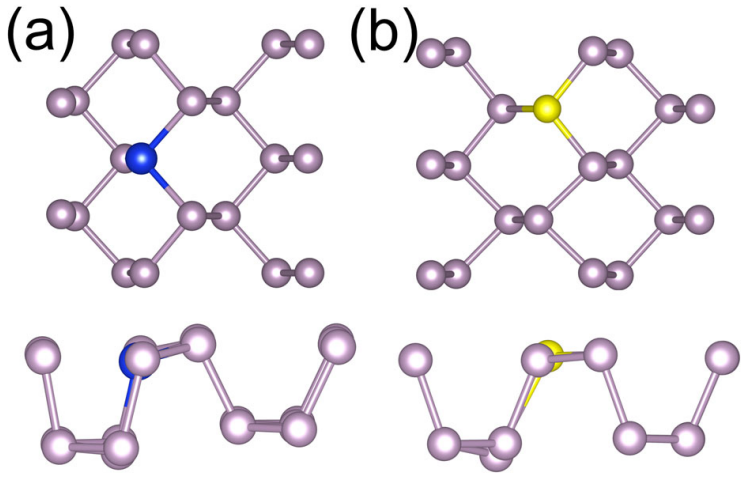

FIG. S1. Configurations of Si (a) and S (b) doped phosphorene monolayer.

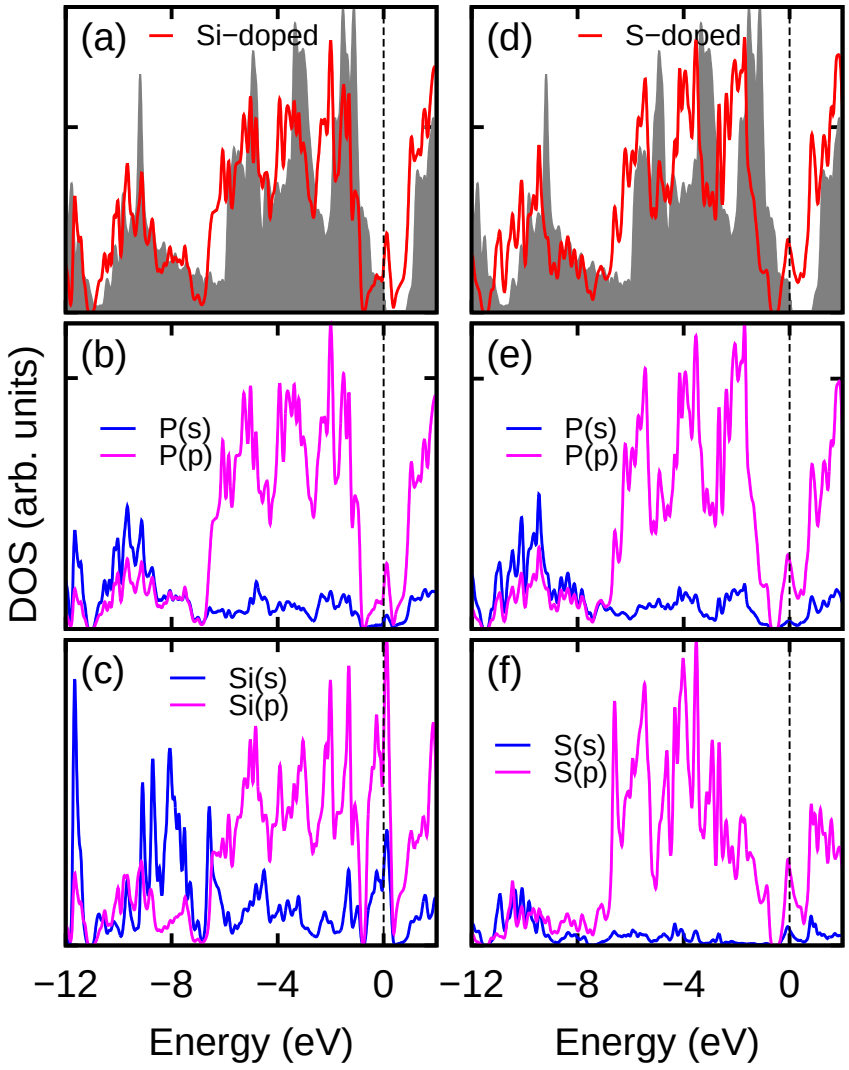

FIG. S2. Total and projected density of states (DOS) of Si-doped (panel a, b and c) and S-doped (panel d, e and f) phosphorene. The total DOS of pristine phosphorene is plotted as shaded area in (a) and (d).

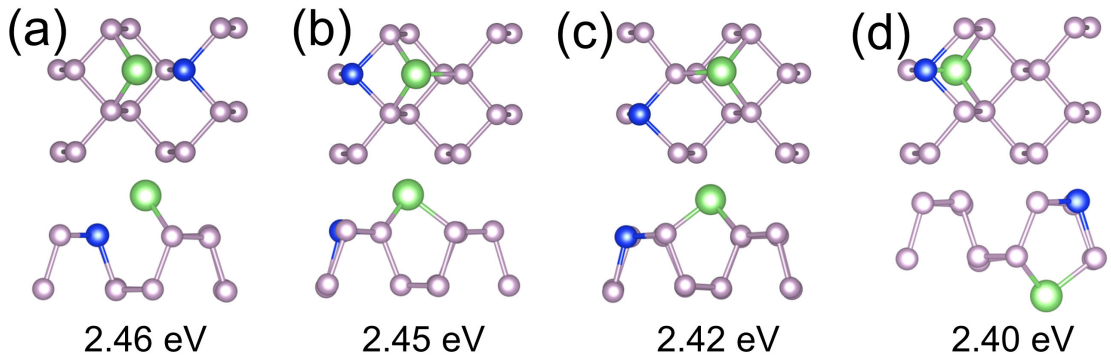

FIG. S3. Optimized configurations of Li adsorbed on Si-doped phosphorene.

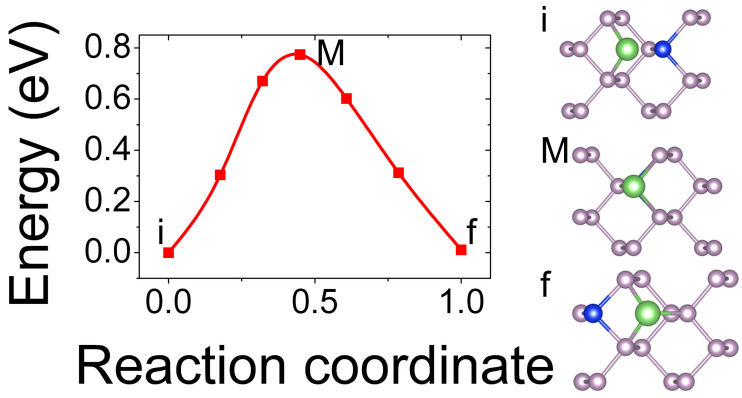

FIG. S4. Diffusion barrier and path of Li on Si-doped phosphorene.

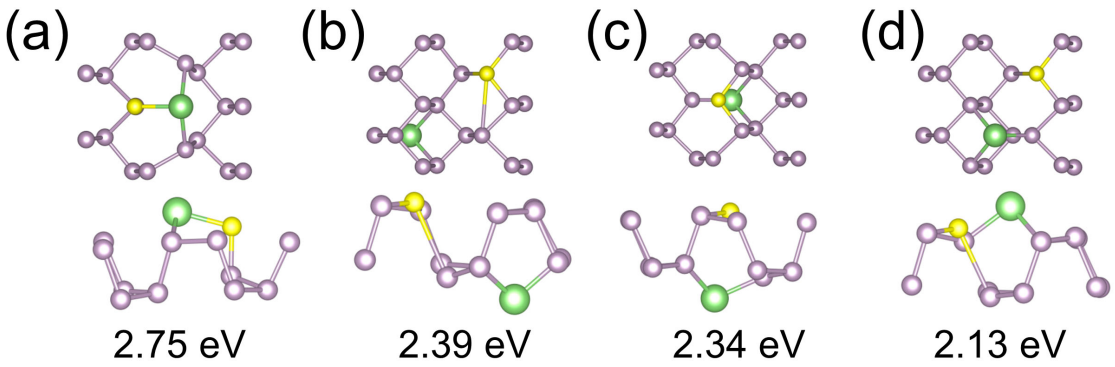

FIG. S5. Configurations of Li atoms adsorbed on S-doped phosphorene monolayer.