

## Thgraphene: a novel two-dimensional carbon allotrope as potential multifunctional material for electrochemical overall water splitting and potassium-ion batteries

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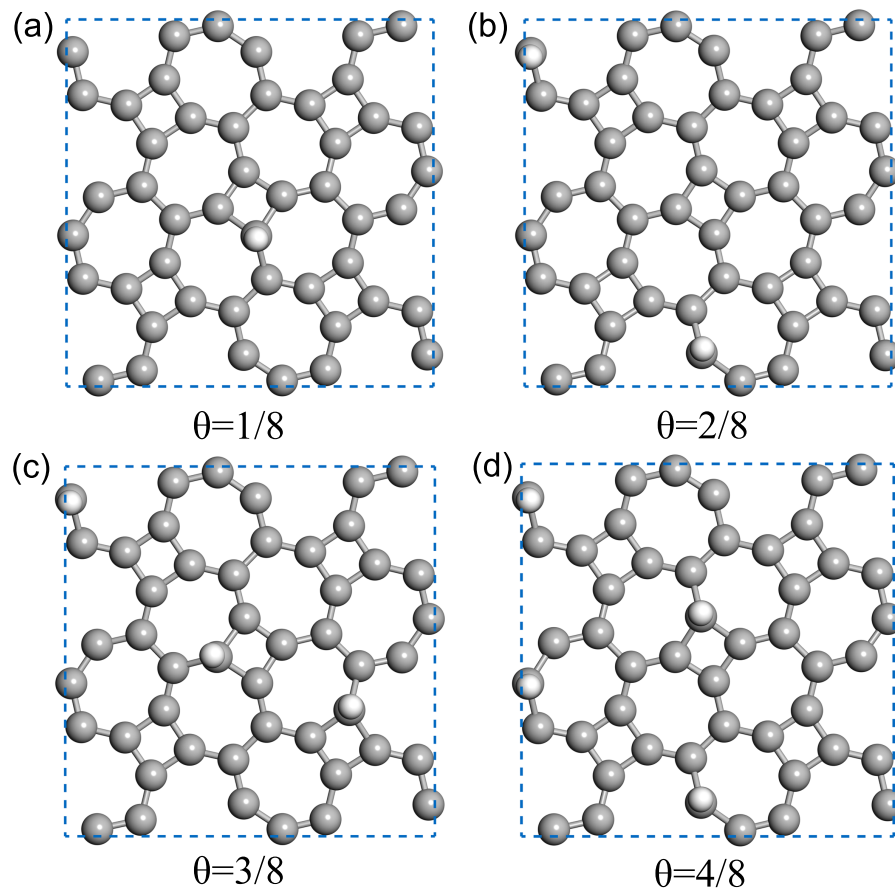


Fig. S1: (a-d) Optimized adsorption configurations of different hydrogen coverages  $\theta$  on thgraphene.

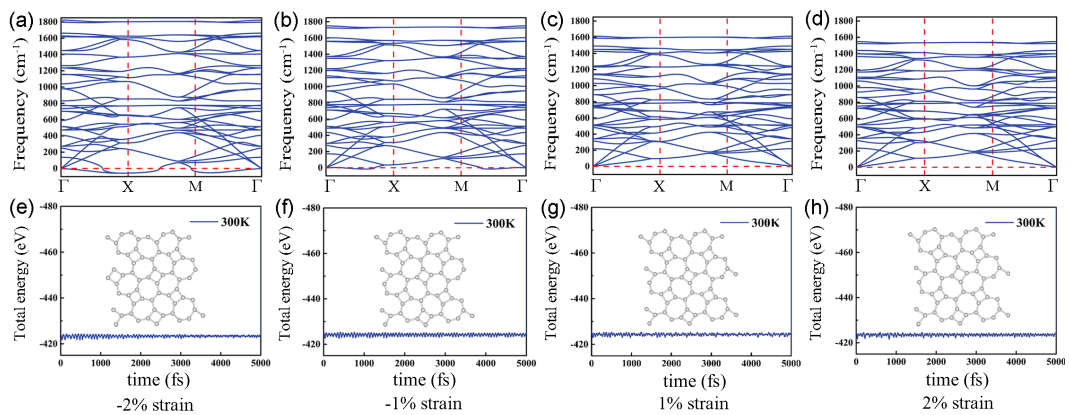


Fig. S2: Phonon dispersion (up panels) and energy fluctuation (down panels) curves of thgraphene at the strains of -2%, -1%, 1%, and 2%.

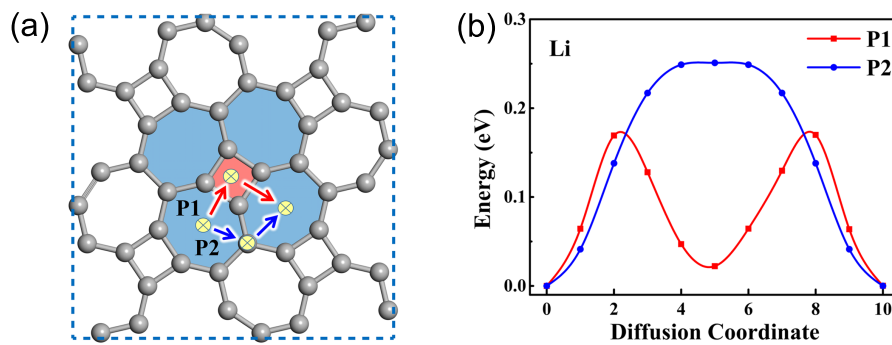


Fig. S3: (a) The illustration of possible ion diffusion paths for Li on thgraphene. (b) Corresponding ion diffusion profiles for Li.

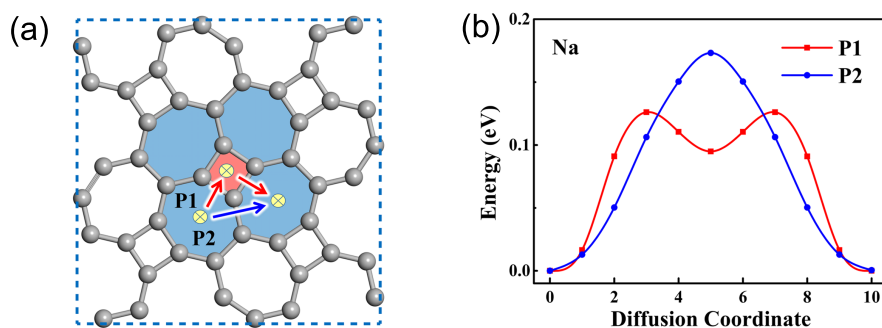


Fig. S4: (a) The illustration of possible ion diffusion paths for Na on thgraphene. (b) Corresponding ion diffusion profiles for Na.

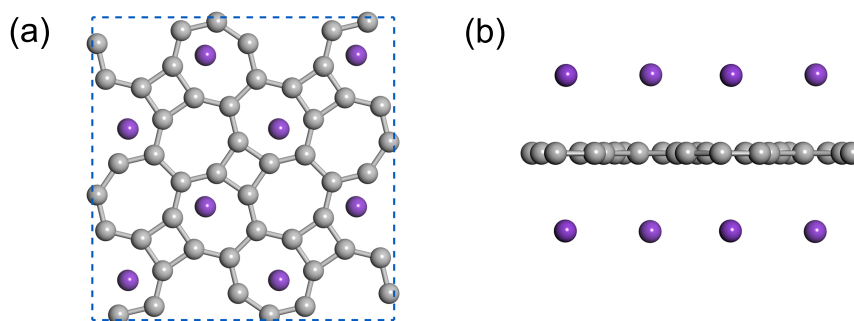


Fig. S5: (a-b) Top and side views of the optimized structure of K atoms adsorbed on thgraphene, gray and purple balls represent C and K atoms, respectively.