Supporting information

DFT study of N, S co-doped graphene anodes for Na-ion storage and diffusion

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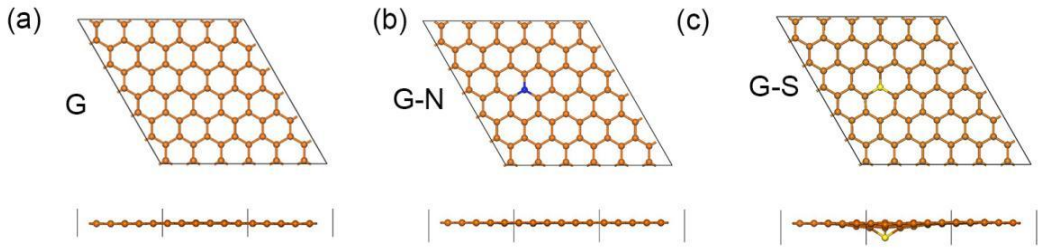

Fig. S1 Optimized configurations of graphene models: (a) bare, (b) N-doped and (c) S-doped. The upper part shows the top-view, lower part is the side-view; the golden, blue and yellow balls represent C, N and S elements, respectively.

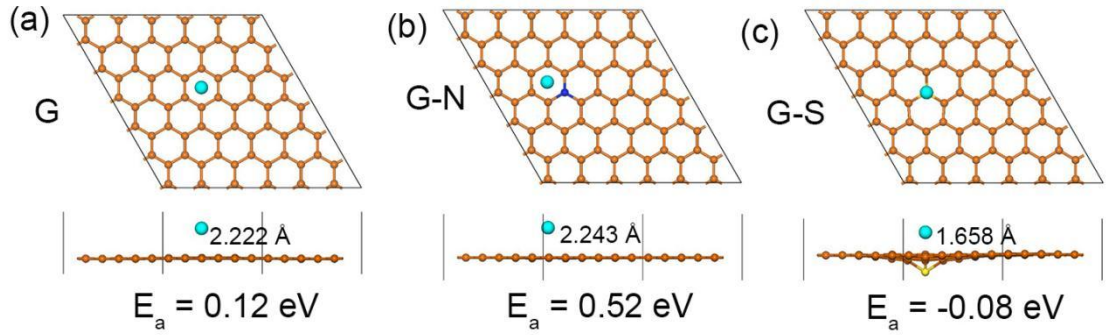

Fig. S2 Optimized configurations of Na adsorbed on graphene models: (a) bare, (b) N-doped and (c) S-doped. The upper part shows the top-view, lower part is the side-view; the corresponding adsorption energy (Ea) and the distance between Na and graphene models were also given in each figure; the golden, blue, yellow and cyan balls represent C, N, S, and Na elements, respectively.

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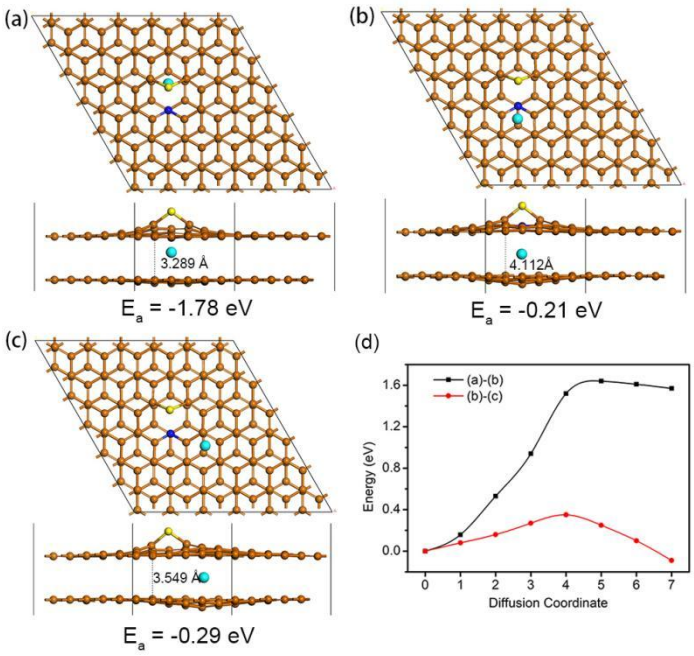

Fig. S3 The Schematic diagram of Na ion adsorption configuration sites and diffusion energy barriers of bi-layer N,S co-doped graphene models: (a) (b) (c) is the top and side view of the selected model, the corresponding adsorption energy (E_a) and the distance between bi-layer graphene models were also given in each figure; (d) the related Na ion diffusion energy barriers; the golden, blue, yellow and cyan balls represent C, N, S, and Na elements, respectively.

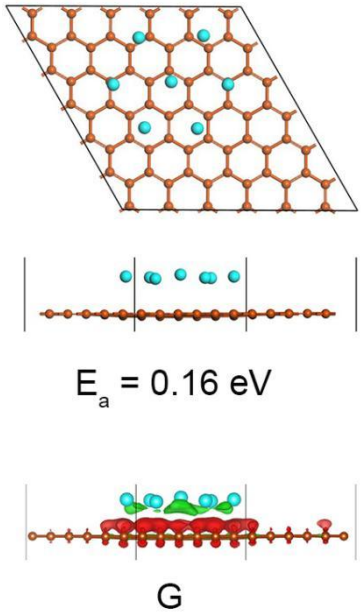

Fig. S4 Schematic diagram of 7 Na ions adsorption configurations, adsorption energies and the spatial distribution of charge densities difference of bare graphene (red and green isosurfaces indicate regions of charge accumulation and depletion (±0.01 eÅ^{-3}), respectively).