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

First Principles study of 2 Dimensional C-silicyne monolayer for promising anode in Na/K ion secondary battery

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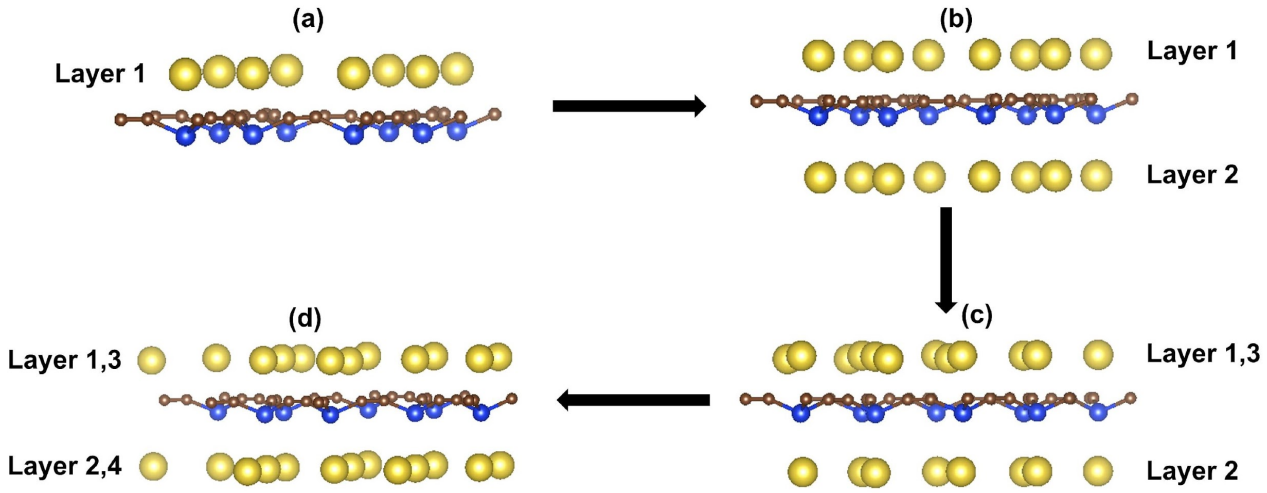

Figure S1 (A): (a) For storage capacity calculation, Na ions are introduced on the most favourable adsorption site (Si-T) to form layer 1 above the C-silicyne monolayer. (b) Next layer of Na ions is formed below the monolayer as layer 2. (c) After all the most favourable sites are occupied, next Na ions are introduced to the next favourable site; in the Ring. After relaxation, layer 3 is formed in between the layer 1 above the monolayer. (d) Layer 4 is formed below the monolayer in between layer 2.

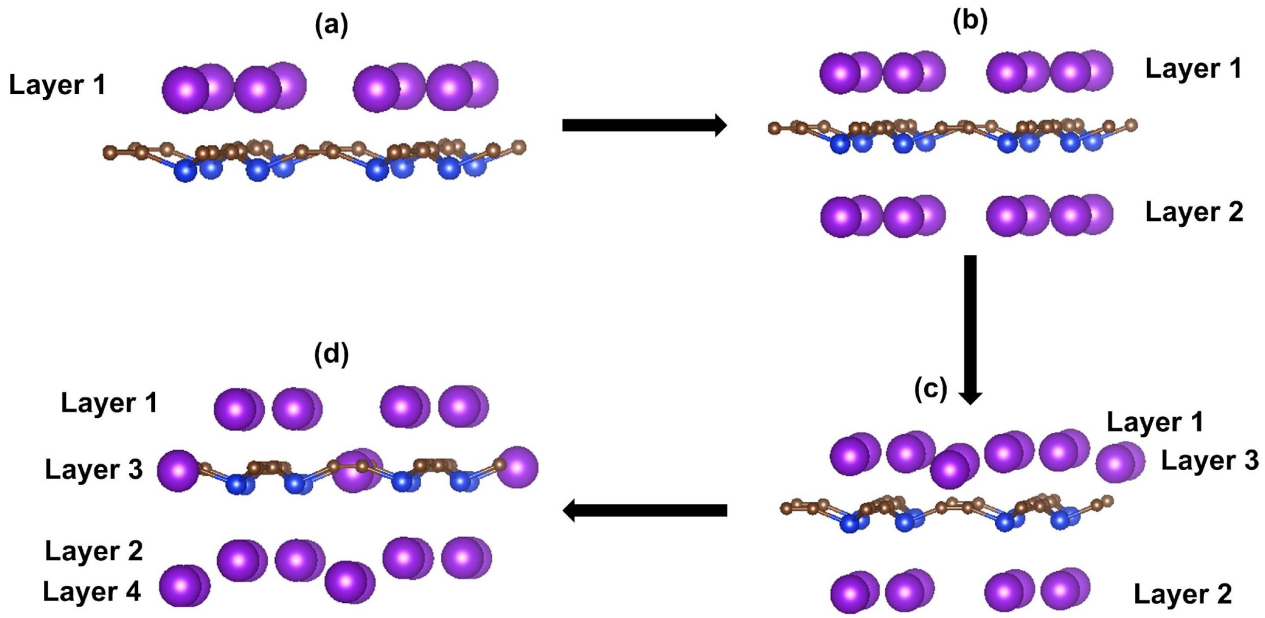

Figure S1 (B): (a) K ions are introduced on the most favourable adsorption site (Si-T) to form layer 1 above the C-silicyne monolayer. (b) Next layer of K ions is formed below the monolayer as layer 2. (c) After all the most favourable sites are occupied, next K ions are introduced to the next favourable site; in the Ring. After relaxation, layer 3 is formed slightly below the layer 1 above the C-silicyne monolayer. (d) As next K ions are introduced below the monolayer, the already adsorbed K ions rearrange themselves to accommodate next layer and thus the layer 3 shifts and layer 4 is formed below the monolayer slightly below layer 2.