Supporting Information for

Pentagonal B_2C monolayer with offering extremely high theoretical capacity for Li-/Na-ion batteries

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Contents of Supporting Information

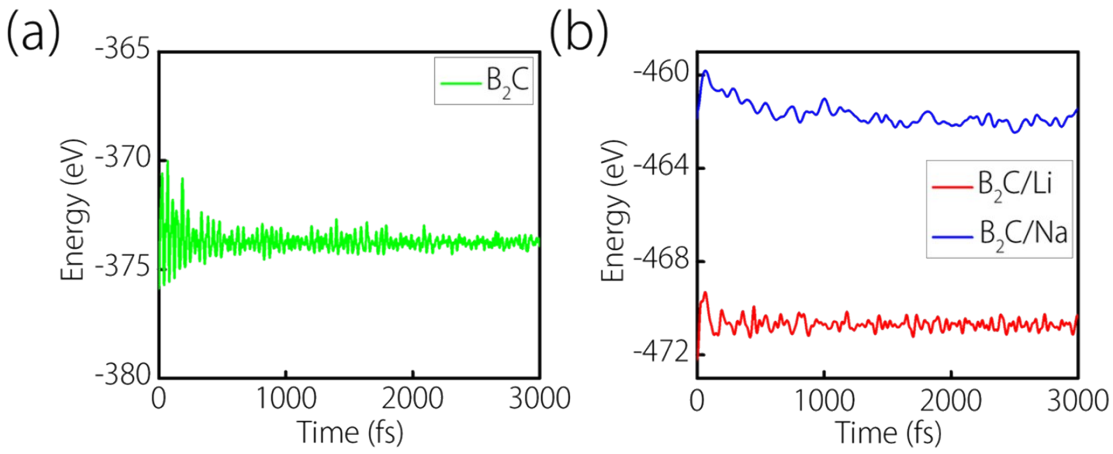

Figure S1 Evolution of the potential energy versus simulation time for Penta-B_2C (a) before and (b) after adsorption Li/Na during AIMD simulations at the temperature of 300 K.

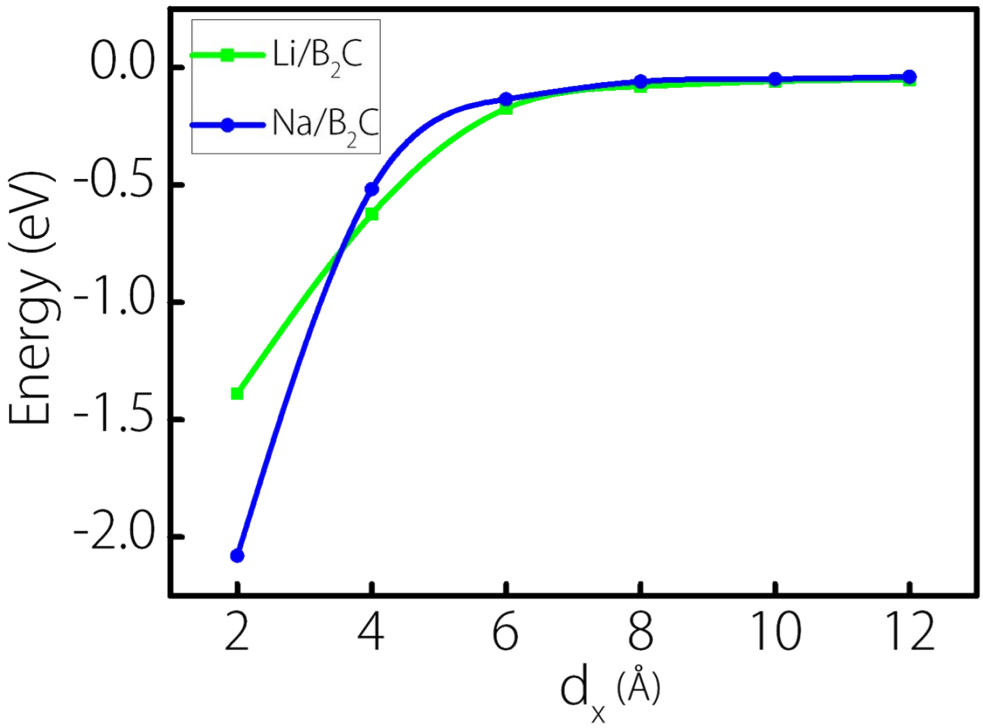

Figure S2 Changes of potential energy with the distance between a single Li/Na atom and Penta-B_2C.