Supporting Information

First principle investigation on the Na-ion storage in two-dimensional boron-rich B_2N, B_3N, and B_5N

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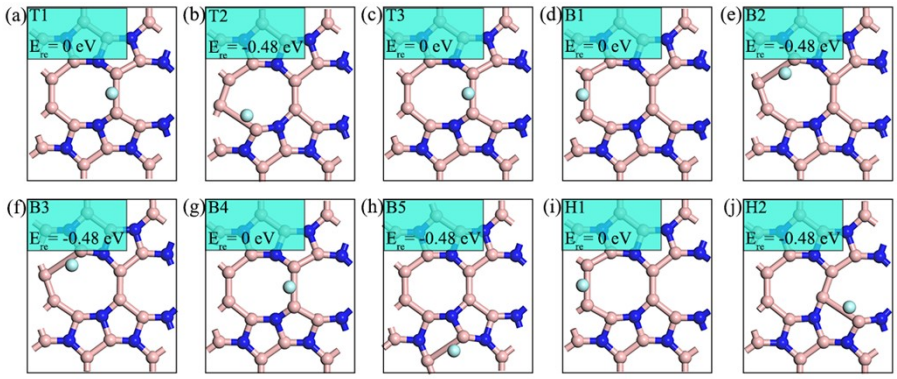

Figure S1. The relaxed configurations of B_2N with adsorbed fluorine atom. The energies are referenced by the configuration with the highest energy.

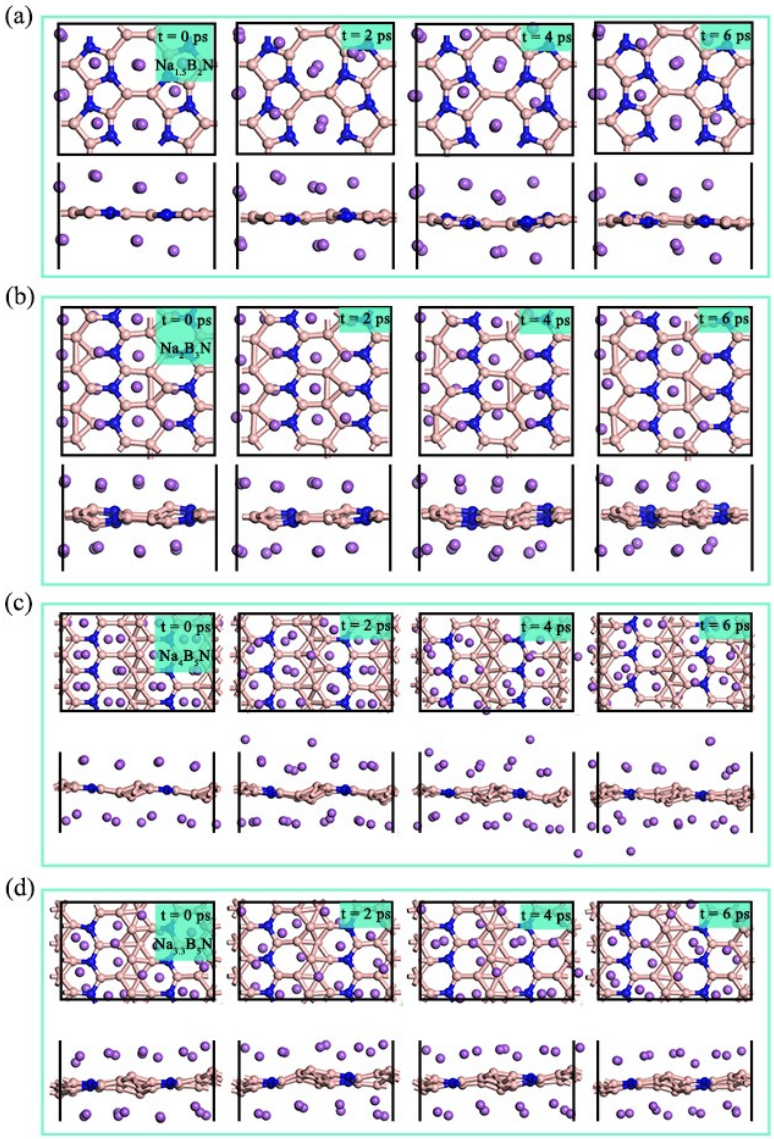

Figure S2. Snap shots of the AIMD simulations performed at 400 K for (a) $Na_{1.5}B_2N$, (b) Na_2B_3N, (c) Na_4B_5N, and (d) $Na_{3.3}B_5N$ electrode with a time interval of 2ps.

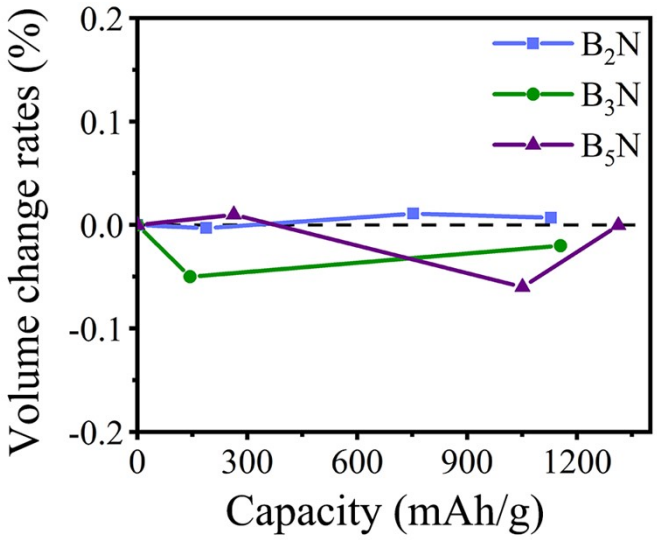

Figure S3. The volume change rate of the emerged stable intermediates.

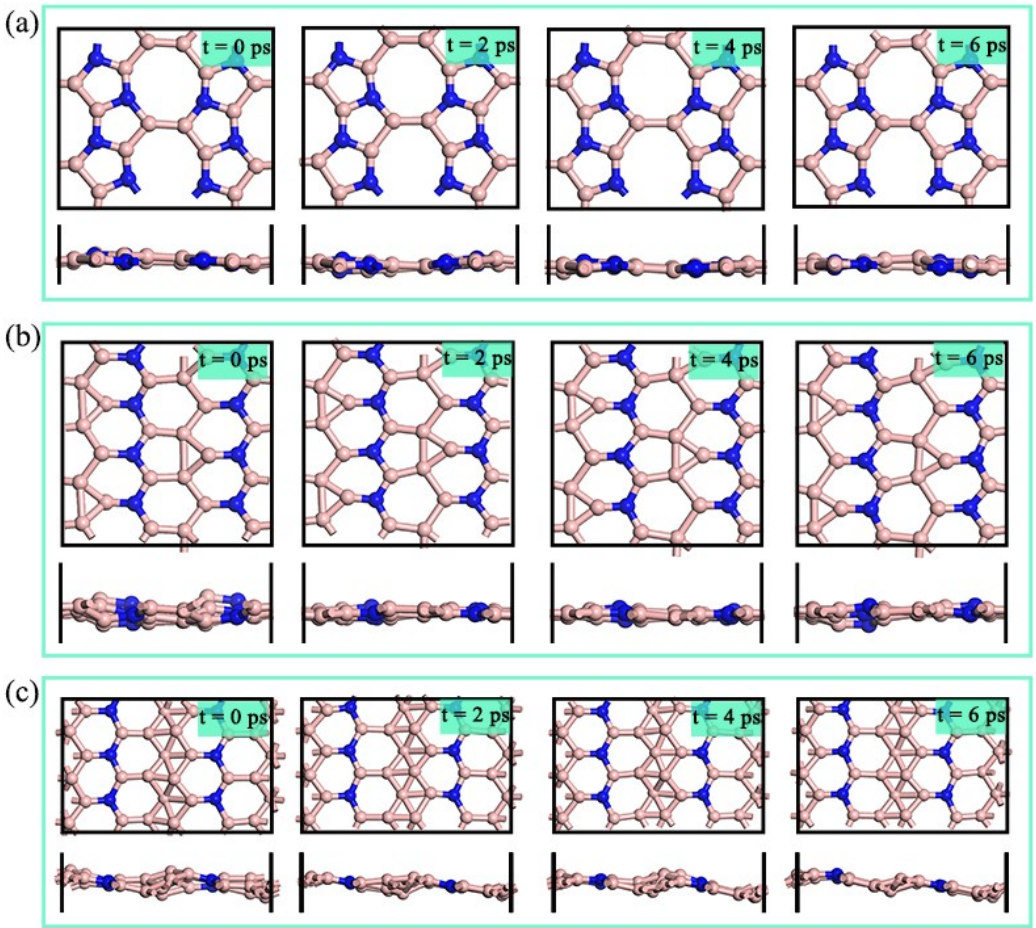

Figure S4. AIMD simulations of the recovery process of (a) B_2N, (b) B_3N, and (c) B_5N electrode with fully removed Na ions. The snap shots are taken with a time interval of 2ps.