Supporting Information

B_2C_3N Monolayer with high theoretical capacity as Anode Materials for Lithium-Ion Batteries: A First-Principles Calculations

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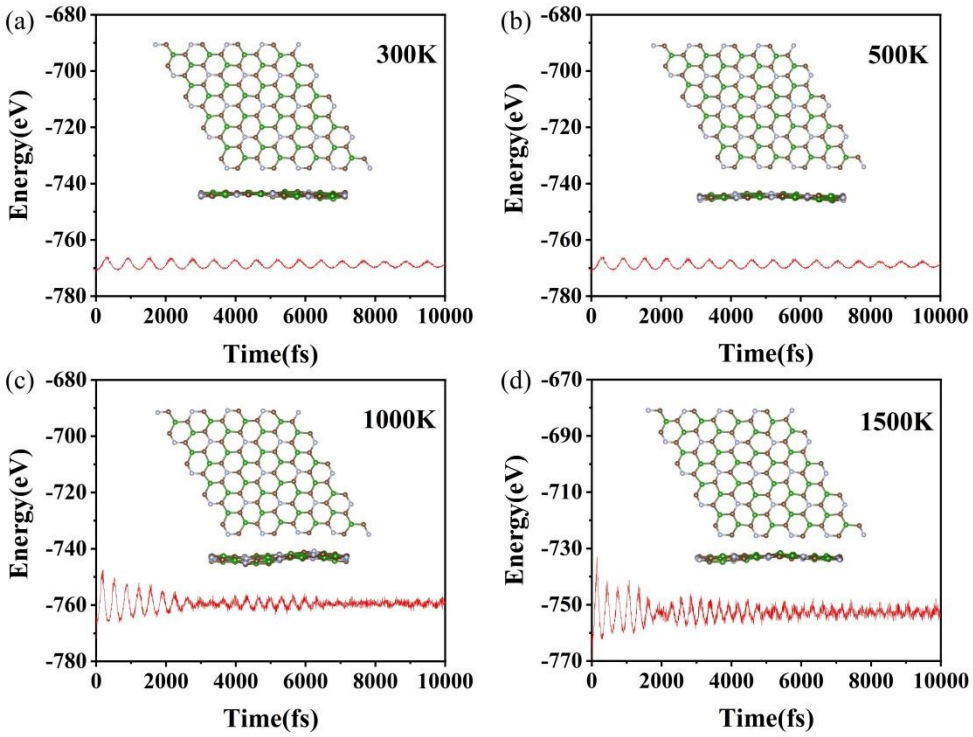

Fig. S1. Molecular dynamics simulations of B_2C_3N monolayer at (a) 300K, (b) 500K, (C) 1000K, and (b) 1500K, respectively.

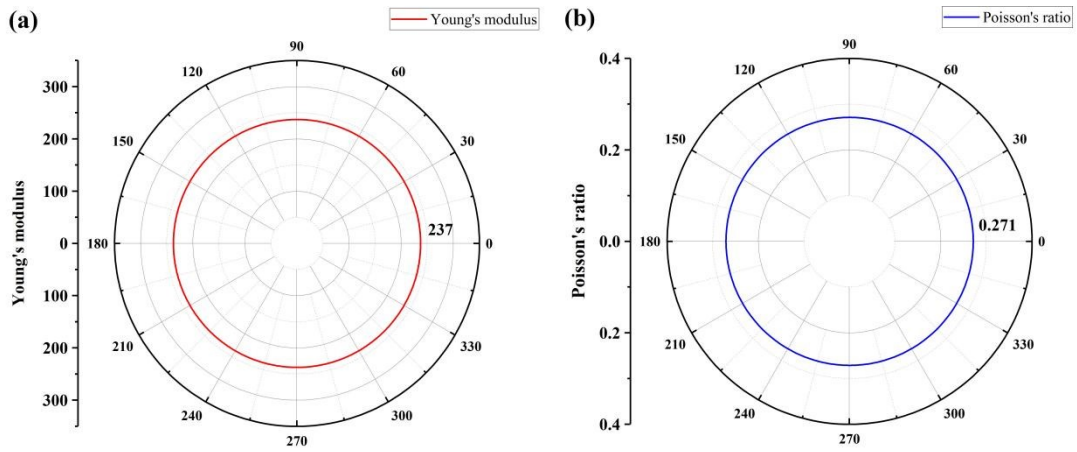

Fig. S2. Angle-dependent (a) Young's modulus and (b) Poisson's ratio of B_2C_3N monolayer.

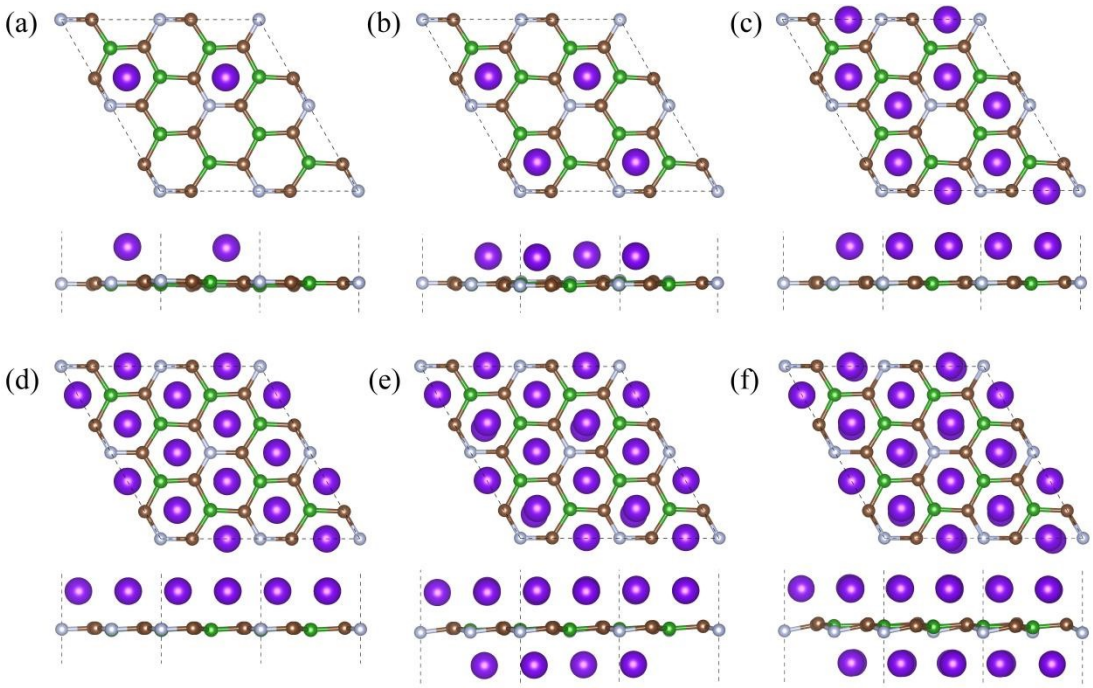

Fig. S3. Top and side view structural diagrams of B_2C_3N at different Li-ion concentrations: (a) $B_2C_3NLi_{0.5}$, (b) $B_2C_3NLi_1$, (c) $B_2C_3NLi_2$, (d) $B_2C_3NLi_3$, (e) $B_2C_3NLi_4$, (f) $B_2C_3NLi_5$.

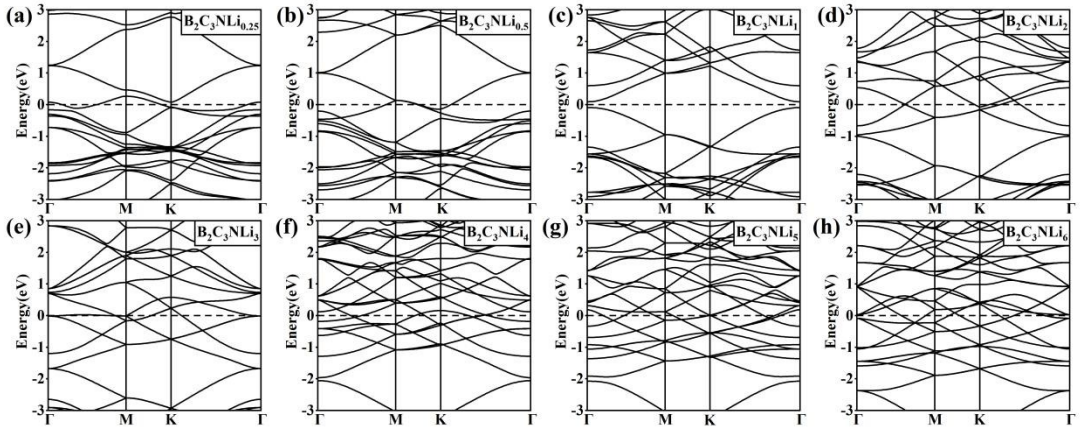

Fig. S4. Band structure diagrams of B_2C_3N with varying Li-ion concentrations: (a) $B_2C_3NLi_{0.25}$, (b) $B_2C_3NLi_{0.5}$, (c) $B_2C_3NLi_1$, (d) $B_2C_3NLi_2$, (e) $B_2C_3NLi_3$, (f) $B_2C_3NLi_4$, (g) $B_2C_3NLi_5$, (h) $B_2C_3NLi_6$.

Table SI. Average adsorption energy, average Bader charge transfer, lattice constant *a*, percentage change in lattice constant *a*, and volume expansion rate of B_2C_3N at various Li-ion concentrations.

Name	Average adsorption energy (eV)	Average Bader charge (e)	Lattice constant *a* (Å)	% change in lattice constant *a*	Volume expansion rate
$B_2C_3NLi_{0.25}$	-1.640	-0.92	8.919	0.15%	0.29%
$B_2C_3NLi_{0.5}$	-1.634	-0.89	8.934	0.31%	0.62%
$B_2C_3NLi_1$	-1.382	-0.88	8.976	0.79%	1.58%
$B_2C_3NLi_2$	-0.581	-0.70	8.994	0.98%	1.98%
$B_2C_3NLi_3$	-0.347	-0.73	9.092	2.08%	4.21%
$B_2C_3NLi_4$	-0.258	-0.75	9.167	2.93%	5.94%
$B_2C_3NLi_5$	-0.173	-0.73	9.212	3.43%	6.98%
$B_2C_3NLi_6$	-0.134	-0.73	9.296	4.38%	8.94%

Table SII. Structural information for B_2C_3N monolayer.

Name	Space group	Lattice parameters (Å)	Atomic positions		
B_2C_3N	*P*-62*m*	$a = b$ =4.454	C	3g	(0.31369, 0.00000, 0.50000)
			B	2d	(0.66667, 0.33333, 0.50000)
			N	1b	(0.00000, 0.00000, 0.50000)