Supporting Information

Flexible C_6BN Monolayers As Promising Anode Materials for High-Performance K-Ion Batteries

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Table S1. Structural details of the optimized C_6BN nanotubes.

	(N, M)	Diameter (Å)	Number of formula units	Total energy (Ha)	*c* lattice parameter (Å)
C6BN-I	(3, 0)	4.98	6	-1849.36	8.598
	(6, 0)	9.69	12	-3699.49	8.617
	(9, 0)	14.31	18	-5549.44	8.622
	(12, 0)	19.13	24	-7399.34	8.624
	(15, 0)	23.82	30	-9249.22	8.626
	(18, 0)	28.62	36	-11099.10	8.627
C6BN-II	(3, 0)	5.07	6	-1849.34	8.607
	(6, 0)	9.74	12	-3699.44	8.630
	(9, 0)	14.46	18	-5549.36	8.635
	(12, 0)	19.13	24	-7399.24	8.637
	(15, 0)	23.89	30	-9249.10	8.639
	(18, 0)	28.64	36	-11098.96	8.639
C6BN-III	(3, 0)	4.92	6	-1849.56	8.611
	(6, 0)	9.60	12	-3699.94	8.624
	(9, 0)	14.27	18	-5550.14	8.624
	(12, 0)	19.05	24	-7400.29	8.625
	(15, 0)	23.76	30	-9250.42	8.625
	(18, 0)	28.50	36	-11100.54	8.623

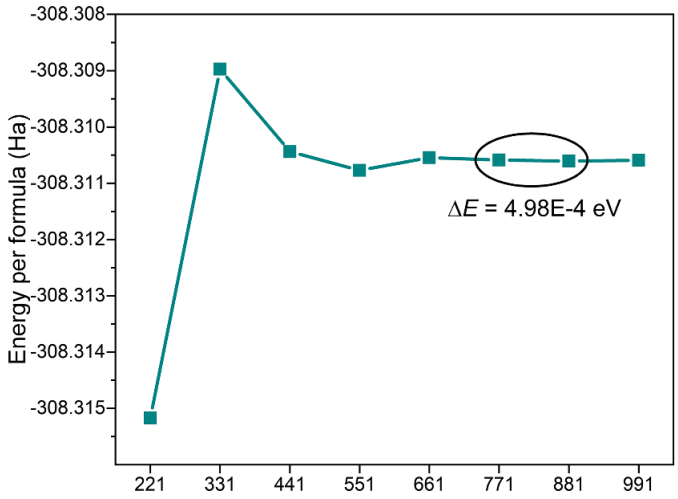

Figure S1. Total energy of C_6BN-I for different k-meshes.

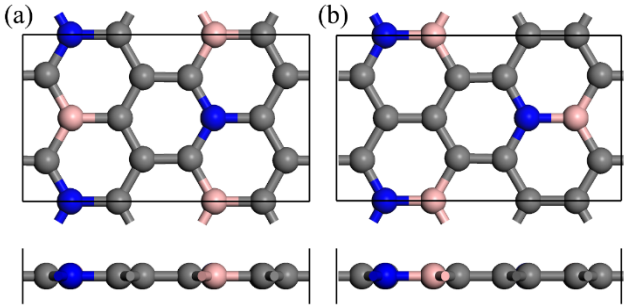

Figure S2. Top and side views of the unit cells of (a) C_6BN-II and (b) C_6BN-III.

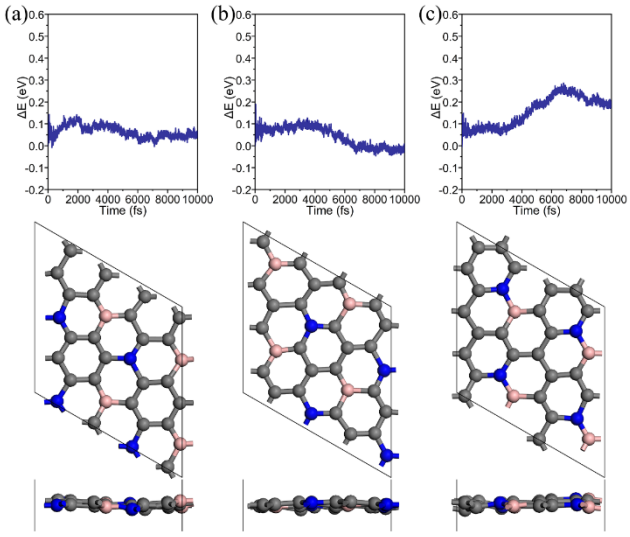

Figure S3. Total potential energy in 2 × 2 (a) C_6BN-I, (b) C_6BN-II, and (c) C_6BN-III at 1200 K and corresponding structure after the ab initio molecular dynamics simulation.

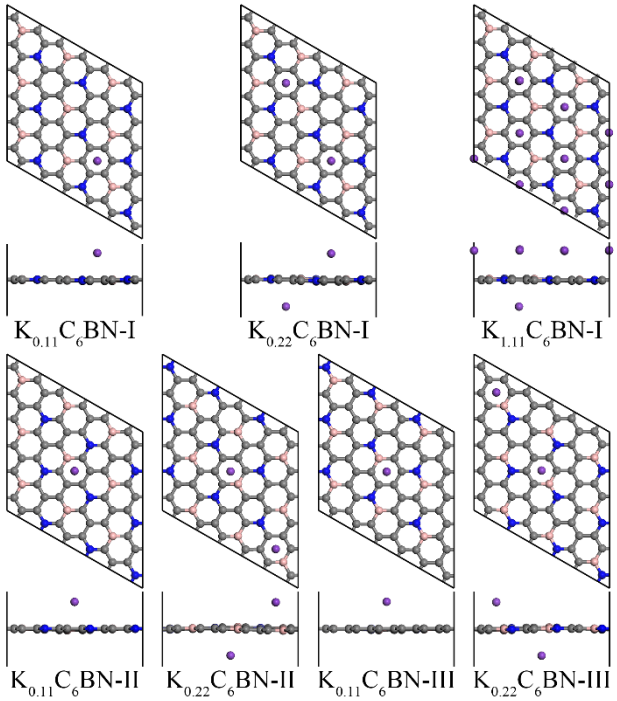

Figure S4. Intermediate structures during potassiation.

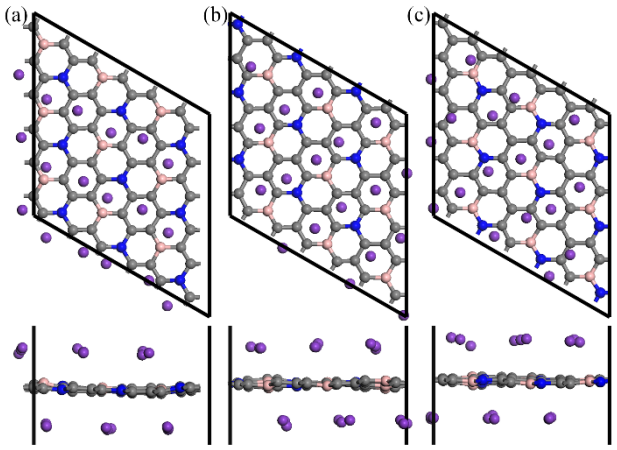

Figure S5. Maximally potassiated (a) C_6BN-I, (b) C_6BN-II, and (c) C_6BN-III after ab-initio molecular dynamics simulations at 300 K.