Supporting Information

Electron-Rich Graphite-Like Electrode: Stability vs. Voltage for Al Battery

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Figure S1: Molecular dynamics simulation analysis of C_3N phases at 300 K temperature as a function of time step, and the top and side view of the obtained structures for (a) 3D C_3N bulk, (b) 2D C_3N bilayer, and (c) 1D C_3N-NT.

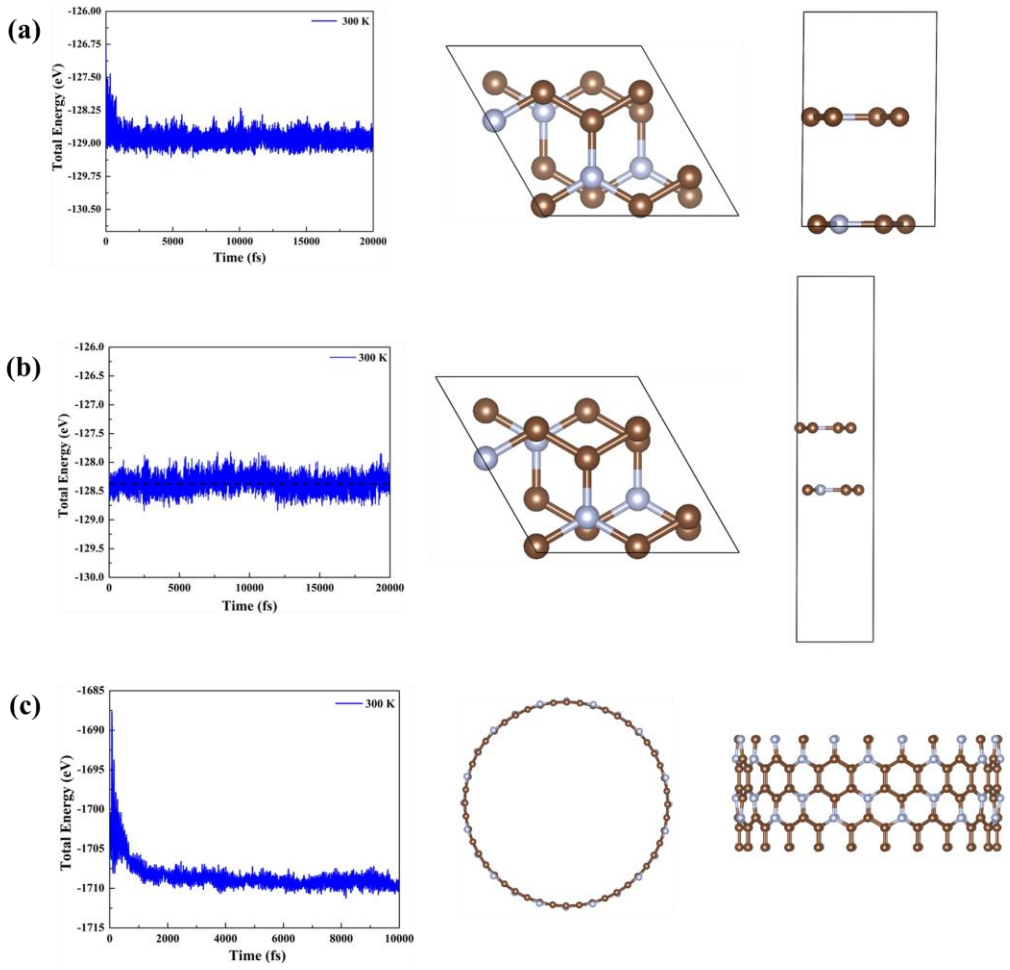

Table S1: Relative energy difference (ΔE) of stable binding sites in 3D C_3N bulk, 2D C_3N bilayer, and 1D C_3N-NT.

Sites	ΔE (eV)			
	3D C_3N bulk	**2D C_3N bilayer**	**1D C_3N-NT**	
			Inner surface adsorption	**Outer surface adsorption**
H-NC	-	0.003	0.000	0.035
H-CC	-	0.013	0.051	0.046
B-NC	0.140	0.016	0.008	0.032
B-CC	0.012	0.000	0.020	0.039
T-NC/T-NN	0.000	-	0.016	0.000
T-CC	0.004	-	0.013	0.038

Figure S2: Schematic picture of the structural change of C_3N bulk form AB to AA stacking on $AlCl_4$ intercalation.

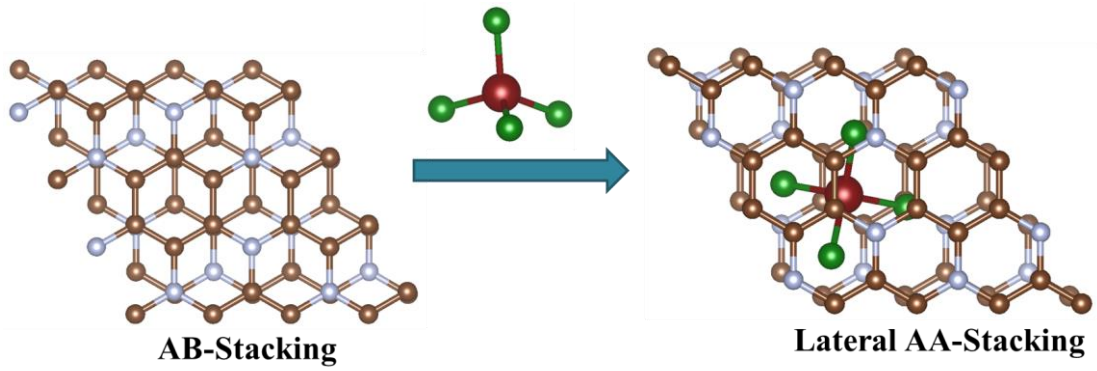

Figure S3: Schematic representation of $AlCl_4$ binding in C_3N bilayer, (a) inside the bilayer, and (b) on the top of bilayer surface. R.E. is the relative energy difference (eV) between the two binding possibilities.

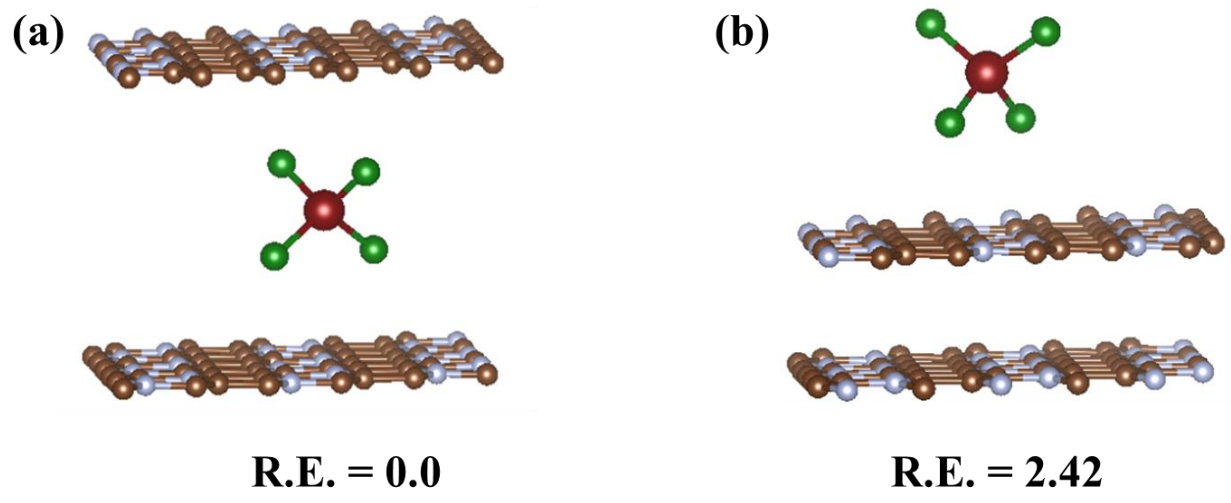

Figure S4: Total Charge density plots (Isosurface = 0.25 e/Å^3) and electron localization function plots of (001) section of one layer of (a) graphite, (b) BC_3, and (c) C_3N. The red and blue colours represent charge accumulation and depletion, respectively.