Supporting Information

for

Understanding the anchoring and catalytic effect of Co@C2N monolayer in Lithium-selenium Batteries：A first-principles study

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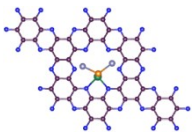
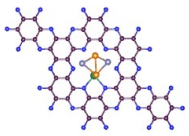
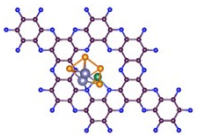
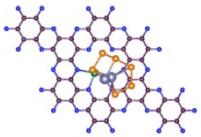
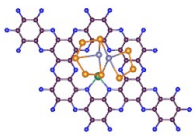
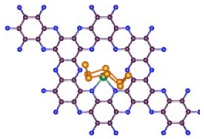
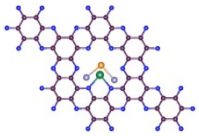
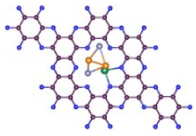
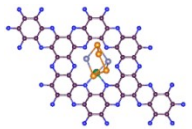
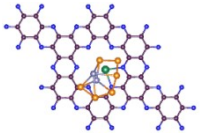
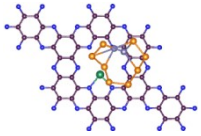
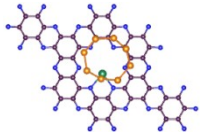
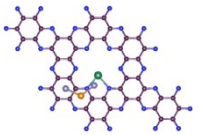
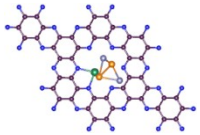
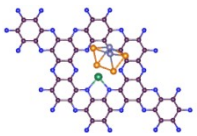
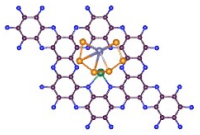
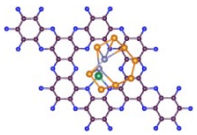
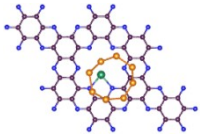
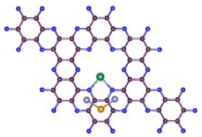
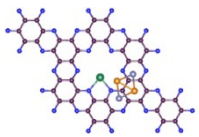
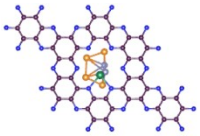
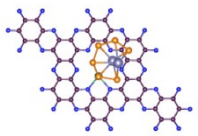
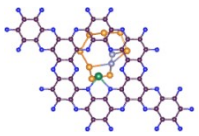
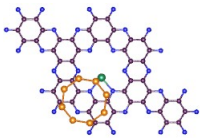
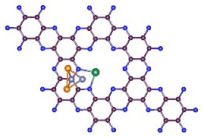
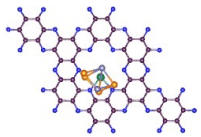
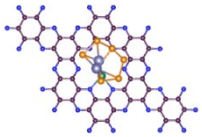
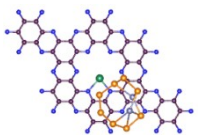
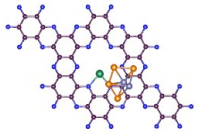
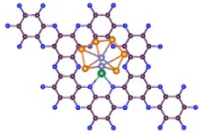
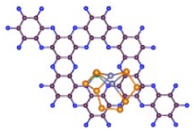
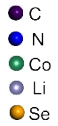
Table S1. Adsorbed structures and binding energies (E_b) of Se_8 and Li_2Se_n (n=1, 2, 4, 6, and 8) at different lithiation stages on the surface of Co@C_2N in different positions. Monkhorst-Pack grids are set to Gamma point, other methods and computational details are shown in the main article.

E_b / structures	Li_2Se-Co@C_2N	Li_2Se_2-Co@C_2N	Li_2Se_4-Co@C_2N	Li_2Se_6-Co@C_2N	Li_2Se_8-Co@C_2N	Se_8-Co@C_2N
						
	E_b = 3.7 eV	E_b =2.47 eV	E_b = 1.87 eV	E_b =1.79 eV	E_b =1.19 eV	E_b =1.04eV
						
	E_b = 2.28 eV	E_b =2.16 eV	E_b = 1.82 eV	E_b = 1.58 eV	E_b = 0.94eV	E_b = 0.93 eV
						
	E_b = 0.89 eV	E_b =1.97 eV	E_b = 1.29 eV	E_b =1.56 eV	E_b = 0.57eV	E_b = 0.89 eV
						
	E_b = 0.80 eV	E_b = 0.95 eV	E_b = 0.85 eV	E_b =1.53 eV	E_b = 0.52eV	E_b = 0.71 eV

					
	E_b =0.61 eV	E_b = 0.56 eV	E_b = 1.47eV	E_b = 0.37 eV	
					
		E_b = 0.51 eV	E_b = 1.14 eV	E_b = 0.04 eV	