Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

For

Anchoring and catalytic insights into bilayer C_4N_3 material for lithium-selenium batteries: a first-principles study

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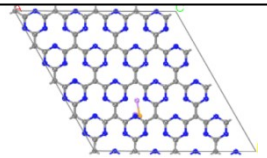
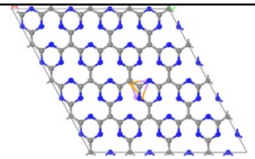
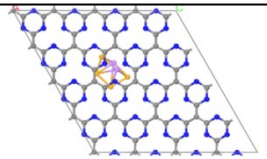
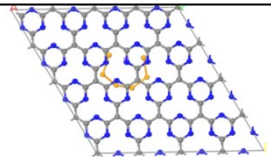
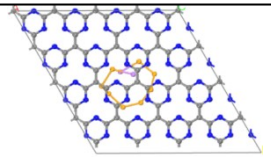
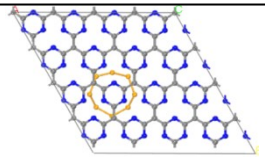
Li_2Se	Li_2Se_2	Li_2Se_4	Li_2Se_6	Li_2Se_8	Se_8
					
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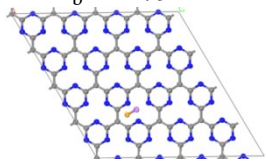
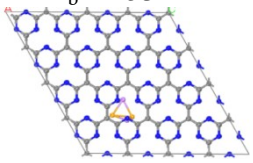
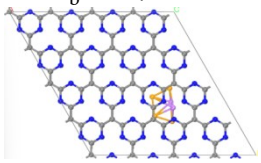
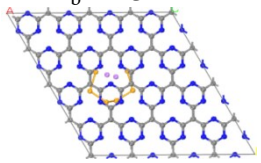
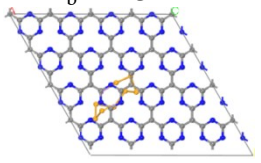
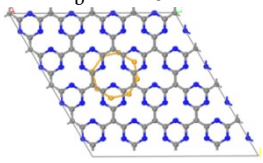
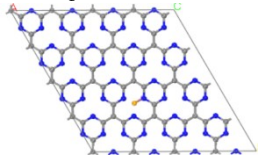
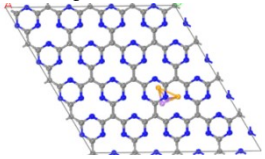
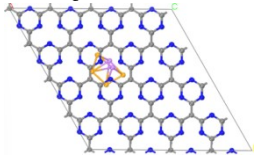
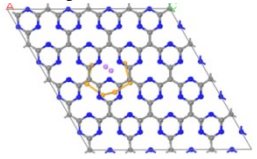
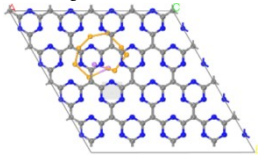
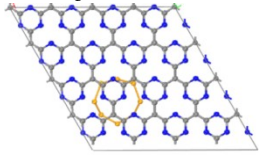
					
E_b = 4.74 eV	E_b =4.16 eV	E_b =2.62 eV	E_b = 2.30 eV	E_b = 2.21 eV	E_b =1.06 eV
					
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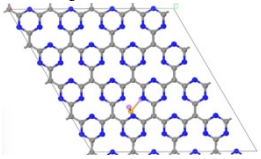
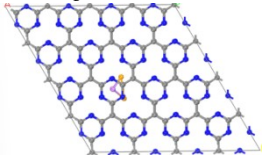
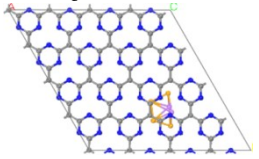
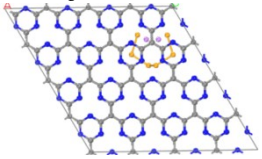
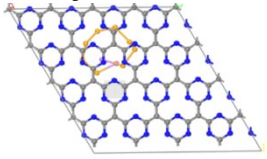
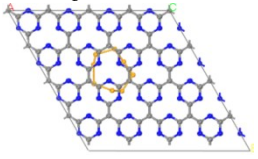
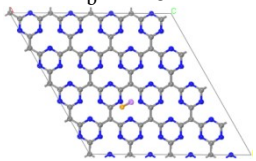
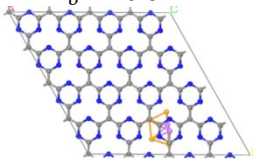
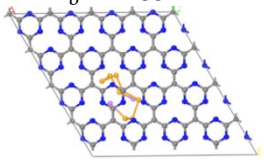
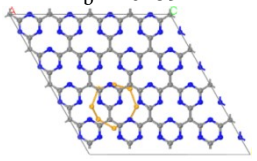
					
E_b = 4.64 eV	E_b = 3.32 eV	E_b =1.96 eV	E_b =1.37 eV	E_b = 1.85 eV	E_b = 0.69 eV
					
E_b =4.06 eV		E_b = 1.14 eV		E_b = 1.03 eV	E_b = 0.08 eV

Table S2. The adsorbed structures and binding energies for Se_8 and Li_2Se_n (n =1, 2, 4, 6, 8) molecules at different lithiation stages within the AB-stacking bilayer C_4N_3.

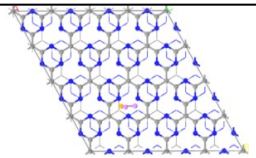
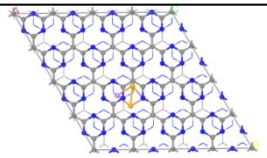
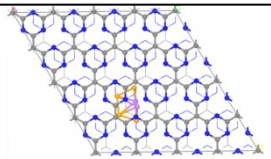
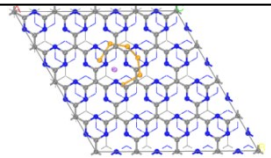
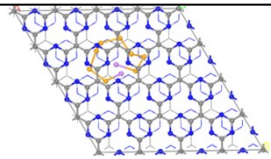
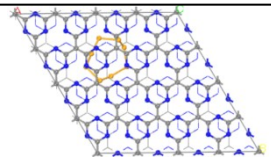
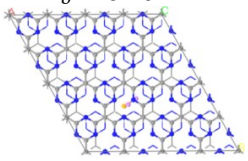
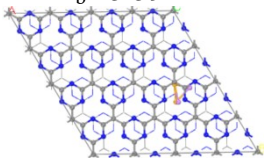
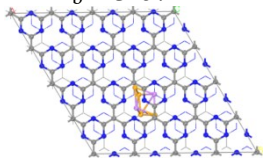
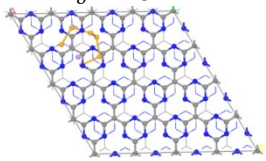
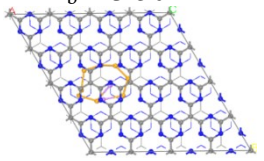
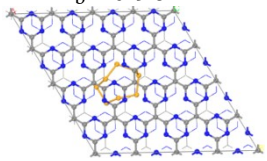
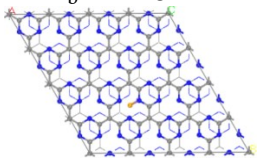
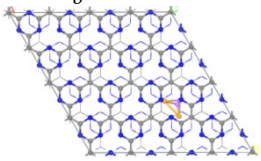
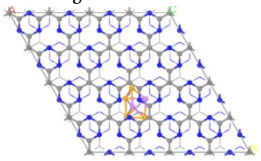
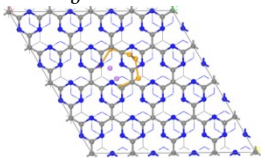
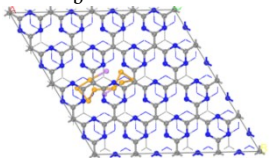
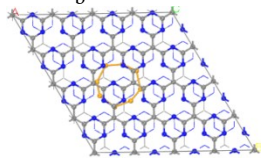
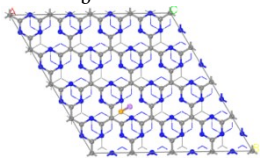
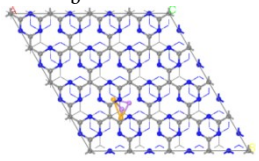
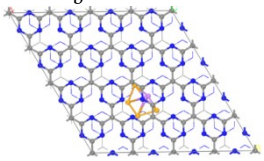
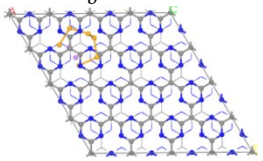
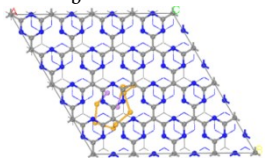
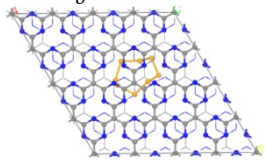
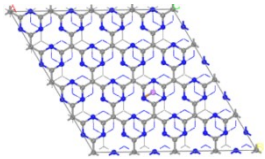
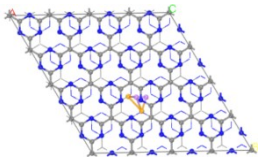
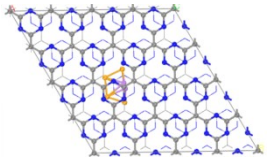
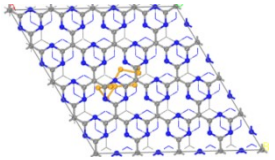
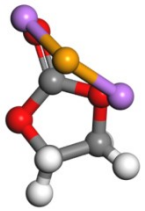
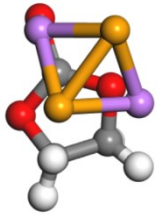
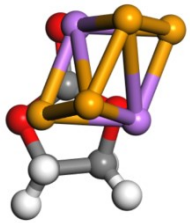
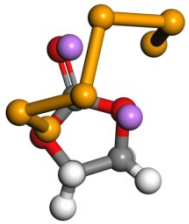
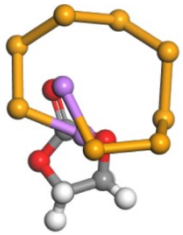
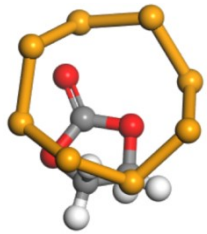
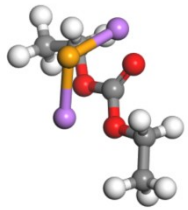
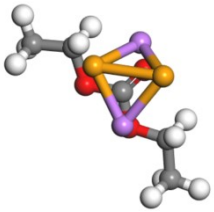
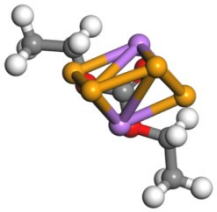
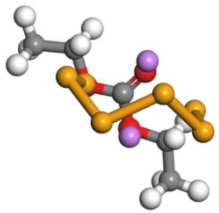
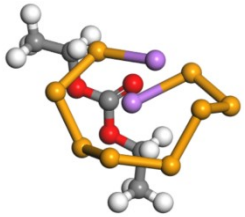
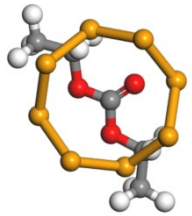
Li_2Se	Li_2Se_2	Li_2Se_4	Li_2Se_6	Li_2Se_8	Se_8
					
E_b = 6.29 eV	E_b =5.59 eV	E_b = 3.67 eV	E_b =2.62 eV	E_b = 3.50 eV	E_b =0.96 eV
					
E_b = 4.18 eV	E_b =5.23 eV	E_b =2.83 eV	E_b = 2.37 eV	E_b = 1.62 eV	E_b =0.80 eV
					
E_b = 4.17 eV	E_b =4.77 eV	E_b =2.79 eV	E_b =2.36 eV	E_b = 1.59 eV	E_b =0.79 eV
					
E_b = 3.48 eV	E_b = 4.17 eV	E_b =2.71 eV	E_b =1.96 eV	E_b = 1.35 eV	E_b = 0.68 eV
					
E_b = 1.79 eV	E_b = 4.05 eV	E_b = 1.97 eV			E_b = 0.59 eV

Table S3. The optimized configurations for Se_8 and Li_2Se_n (n = 1, 2, 4, 6, and 8) interacting with the different electrolytes (EC, DEC, and DOL).

	Li_2Se	**Li_2Se_2**	**Li_2Se_4**	**Li_2Se_6**	**Li_2Se_8**	**Se_8**
EC						
DEC						
DOL