

Supporting Information

for

Unraveling the superior anchoring of lithium polyselenides to the confinement bilayer C₂N: an efficient host material for lithium-selenium batteries

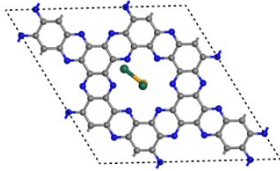
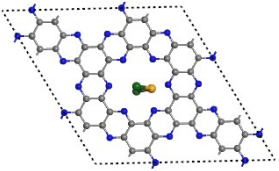
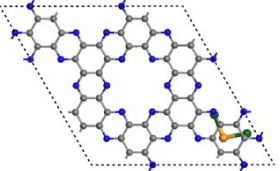
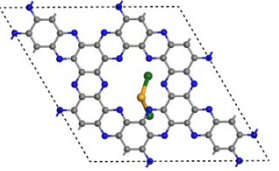
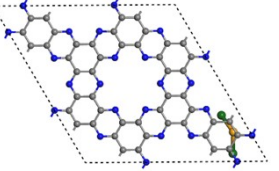
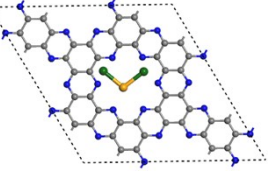
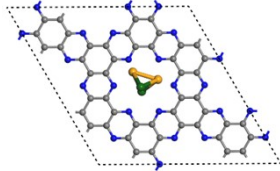
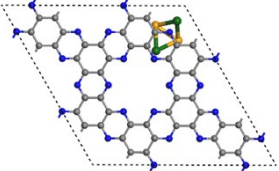
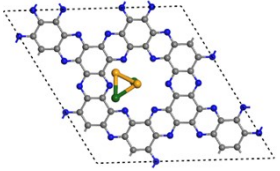
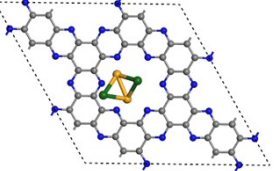
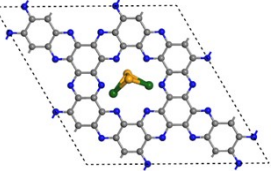
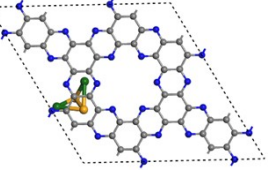
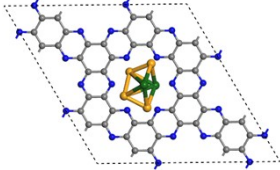
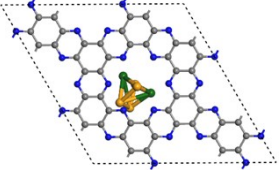
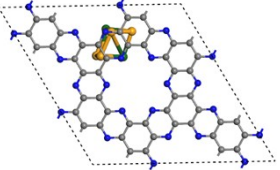
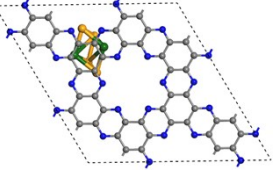
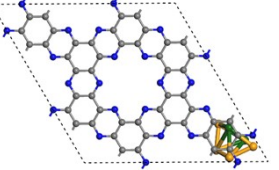
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Table S1. The adsorbed structures and binding energies (E_b) for Se_8 and LiPSes at different lithiation stages on the surface of AA-stacking C_2N at different sites.

structure						
E_b						
Li_2Se	 $E_b=3.62$ eV	 $E_b=2.74$ eV	 $E_b=2.45$ eV	 $E_b=2.16$ eV	 $E_b=2.04$ eV	 $E_b=1.56$ eV
Li_2Se_2	 $E_b=3.03$ eV	 $E_b=2.09$ eV	 $E_b=1.95$ eV	 $E_b=1.75$ eV	 $E_b=1.34$ eV	 $E_b=1.23$ eV
Li_2Se_4	 $E_b=3.01$ eV	 $E_b=1.58$ eV	 $E_b=1.56$ eV	 $E_b=1.39$ eV	 $E_b=1.31$ eV	

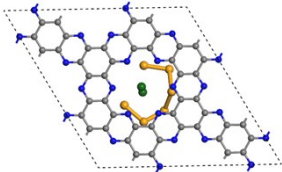
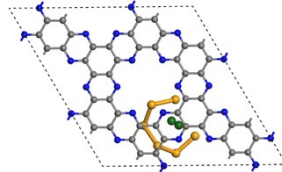
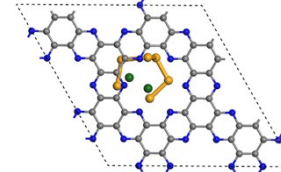
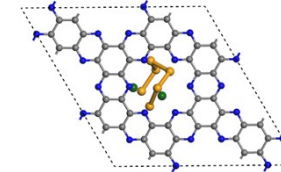
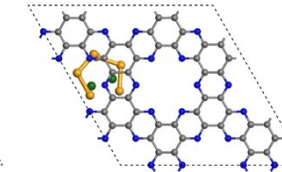
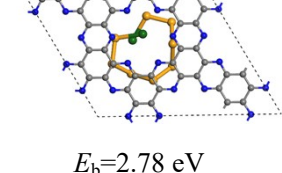
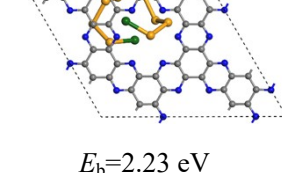
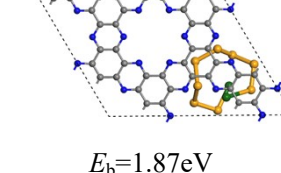
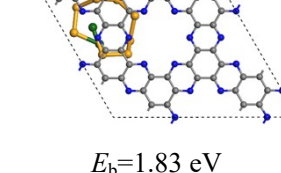
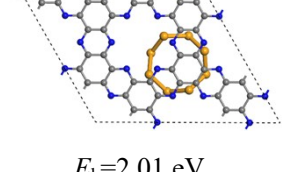
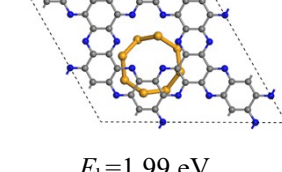
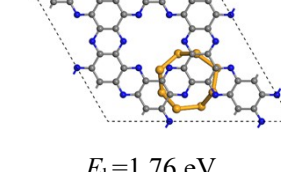
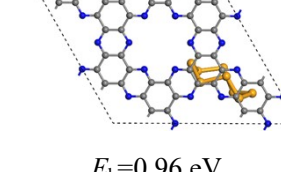
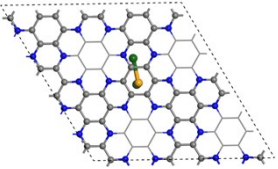
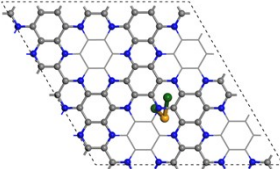
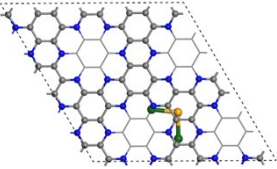
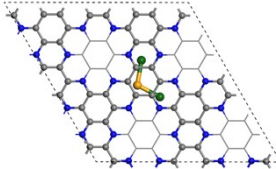
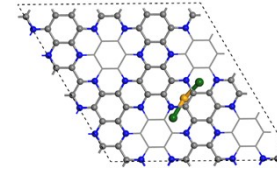
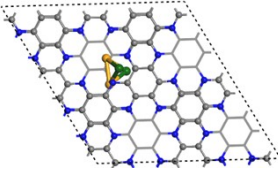
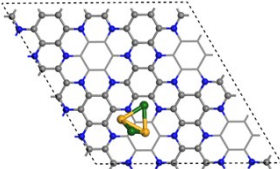
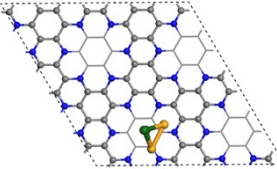
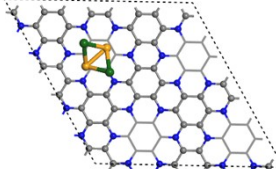
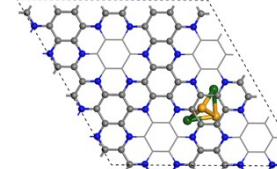
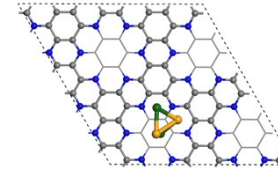
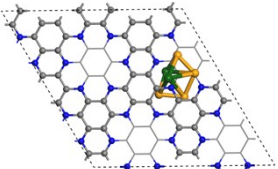
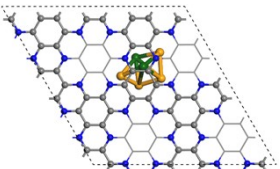
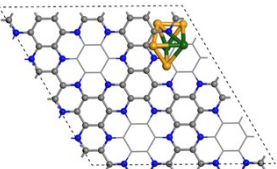
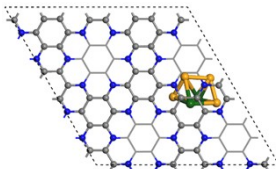
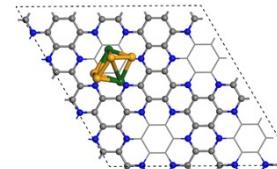
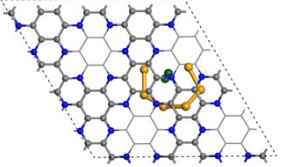
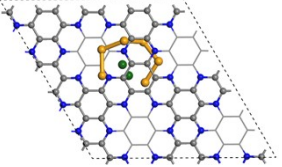
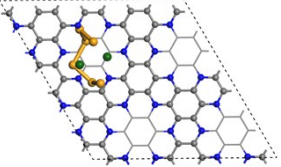
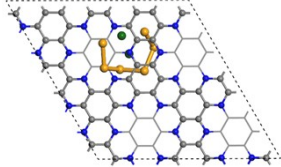
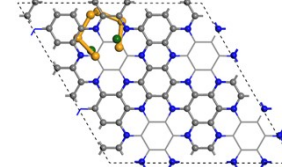
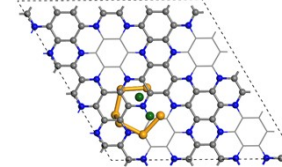
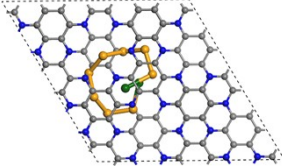
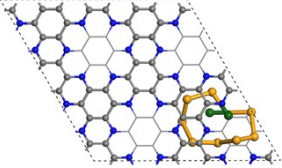
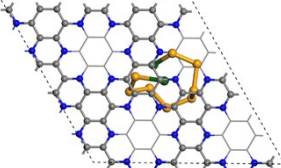
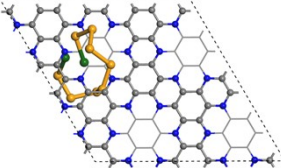
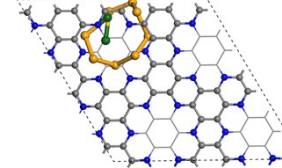
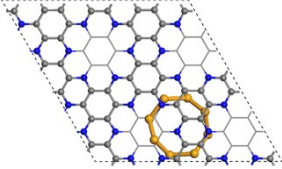
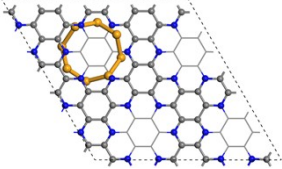
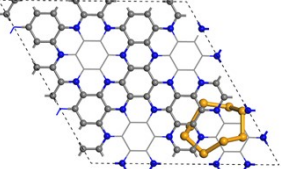
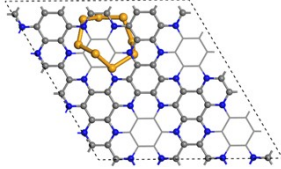
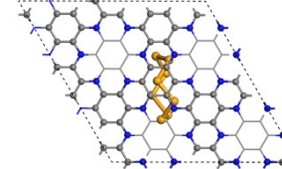
Li ₂ Se ₆					
	$E_b=2.98$ eV	$E_b=2.14$ eV	$E_b=1.80$ eV	$E_b=1.80$ eV	$E_b=1.73$ eV
Li ₂ Se ₈					
	$E_b=2.78$ eV	$E_b=2.23$ eV	$E_b=1.87$ eV	$E_b=1.83$ eV	
Se ₈					
	$E_b=2.01$ eV	$E_b=1.99$ eV	$E_b=1.76$ eV	$E_b=0.96$ eV	

Table S2. The adsorbed structures and binding energies (E_b) for Se_8 and LiPSes at different lithiation stages on the surface of AB-stacking C_2N at different sites.

structure						
E_b						
Li_2Se	 $E_b=2.63$ eV	 $E_b=1.47$ eV	 $E_b=1.36$ eV	 $E_b=1.25$ eV	 $E_b=1.19$ eV	
Li_2Se_2	 $E_b=2.36$ eV	 $E_b=1.78$ eV	 $E_b=1.49$ eV	 $E_b=1.34$ eV	 $E_b=0.64$ eV	 $E_b=0.47$ eV
Li_2Se_4	 $E_b=1.79$ eV	 $E_b=1.52$ eV	 $E_b=1.26$ eV	 $E_b=1.18$ eV	 $E_b=1.16$ eV	

Li_2Se_6	 $E_b=1.69 \text{ eV}$	 $E_b=1.30 \text{ eV}$	 $E_b=1.02 \text{ eV}$	 $E_b=0.98 \text{ eV}$	 $E_b=0.91 \text{ eV}$	 $E_b=0.83 \text{ eV}$
Li_2Se_8	 $E_b=1.86 \text{ eV}$	 $E_b=1.51 \text{ eV}$	 $E_b=1.45 \text{ eV}$	 $E_b=1.30 \text{ eV}$	 $E_b=1.18 \text{ eV}$	
Se_8	 $E_b=1.19 \text{ eV}$	 $E_b=1.13 \text{ eV}$	 $E_b=0.99 \text{ eV}$	 $E_b=0.89 \text{ eV}$	 $E_b=0.77 \text{ eV}$	