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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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Table S1. 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

Li ₂ Se	Li ₂ Se ₂	Li ₂ Se ₄	Li ₂ Se ₆	Li ₂ Se ₈	Se ₈
$E_{\rm b} = 4.79 \; {\rm eV}$	$E_{\rm b}$ =4.53 eV	$E_{\rm b}$ = 2.74 eV	$E_{\rm b} = 2.34 \; {\rm eV}$	$E_{\rm b} = 2.31 \; {\rm eV}$	$E_{\rm b} = 1.10 \; {\rm eV}$
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	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	Torong to	proport	(marga)	
'aaaa	Agada,	, diddd	popolo/	4444/	/0,0,0,0,/
$E_{\rm b} = 4.74 \; \rm eV$	$E_{\rm b} = 4.16 \; {\rm eV}$	$E_{\rm b} = 2.62 \; {\rm eV}$	$E_{\rm b} = 2.30 \; {\rm eV}$	$E_{\rm b} = 2.21 \; {\rm eV}$	$E_{\rm b} = 1.06 \; {\rm eV}$
	Agagagay.	apploto			
\$\$\$\$\$		0000	papa/		
$E_{\rm b} = 4.64 \; {\rm eV}$	$E_{\rm b} = 4.01 \; {\rm eV}$	$E_{\rm b} = 2.59 \; {\rm eV}$	$E_{\rm b} = 2.04 \; {\rm eV}$	$E_{\rm b} = 1.94 \; {\rm eV}$	$E_{\rm b} = 1.00 \; {\rm eV}$
	Jorgan V		To a control	To cook	
Total Control	Johannay.	oranga/	/organa/	Joseph John John John John John John John Joh	(C)
$E_{\rm b} = 4.64 \; {\rm eV}$	$E_{\rm b} = 3.32 \; {\rm eV}$	$E_{\rm b} = 1.96 \; {\rm eV}$	$E_{\rm b} = 1.37 \; {\rm eV}$	$E_{\rm b} = 1.85 \rm eV$	$E_{\rm b} = 0.69 \; \rm eV$
\\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\	L _b 3.32 C V	0000	L_b 1.37 CV	0000	A COOL
Torono /		Total Total		papara/	44444
$E_{\rm b} = 4.06 \; {\rm eV}$		$E_{\rm b} = 1.14 \; {\rm eV}$		$E_{\rm b} = 1.03 \; {\rm eV}$	$E_{\rm b} = 0.08 \; {\rm eV}$

AA-stacking bilayer C₄N₃.

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 ₂ Se	Li ₂ Se ₂	Li ₂ Se ₄	Li ₂ Se ₆	Li ₂ Se ₈	Se ₈
	TOTAL .		TOTAL.	Total a	
$E_{\rm b} = 6.29 \; {\rm eV}$	$E_{\rm b}$ =5.59 eV	$E_{\rm b} = 3.67 \; {\rm eV}$	$E_{\rm b} = 2.62 \; {\rm eV}$	$E_{\rm b} = 3.50 \; {\rm eV}$	$E_{\rm b}$ =0.96 eV
$E_{\rm b} = 4.18~{\rm eV}$	$E_{\rm b} = 5.23 \text{ eV}$	$E_{\rm b}$ =2.83 eV	$E_{\rm b} = 2.37 \; {\rm eV}$	$E_{\rm b} = 1.62 \; {\rm eV}$	$E_{\rm b}$ =0.80 eV
$E_{\rm b} = 4.17 \; {\rm eV}$	$E_{\rm b}$ =4.77 eV	$E_{\rm b}$ =2.79 eV	$E_{\rm b}$ =2.36 eV	$E_{\rm b} = 1.59 \; {\rm eV}$	$E_{\rm b}$ =0.79 eV
$E_{\rm b}$ = 3.48 eV	$E_{\rm b} = 4.17 \; {\rm eV}$	$E_{\rm b}$ =2.71 eV	$E_{\rm b} = 1.96 \; \rm eV$	$E_{\rm b} = 1.35 \; {\rm eV}$	$E_{\rm b} = 0.68 \; \rm eV$
$E_{\rm b} = 1.79 \; {\rm eV}$	$E_{\rm b}$ = 4.05 eV	$E_{\rm b} = 1.97~{\rm eV}$			$E_{\rm b} = 0.59 \; {\rm eV}$

Table S3. The optimized configurations for Se₈ and Li₂Se_n (n = 1, 2, 4, 6, and 8) interacting with the different electrolytes (EC, DEC, and DOL).

	Li ₂ Se	Li ₂ Se ₂	Li ₂ Se ₄	Li ₂ Se ₆	Li ₂ Se ₈	Se ₈
EC						
DEC						
DOL						