

Supporting Information for

**Anodic Potential and Conversion Chemistry of Anhydrous Iron (II) Oxalate in
Na-Ion Batteries**

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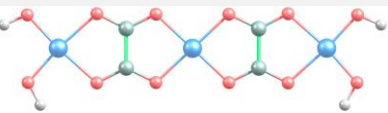
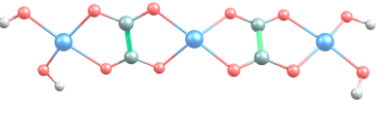
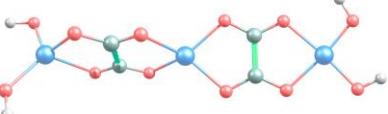
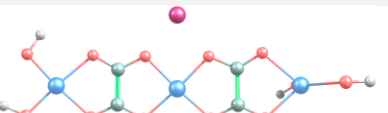
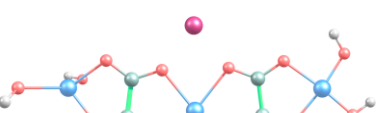
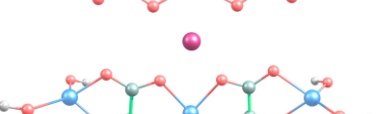


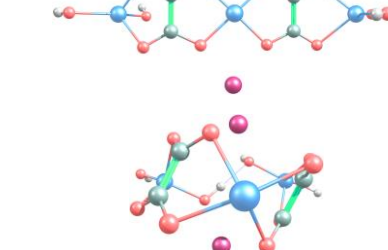
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Table S1. Properties of the non-periodic Na-free and Na-containing anhydrous ferrous oxalate (AFO) model at several spin states. ^{a, b}

Spin state	NUE	E (Hartree)	G (Hartree)	S^2	S^2A	IF	Structure
<div>  </div>							
Na-free AFO							
9tet	8	-4847.33889	-4847.39530	20.08	20.00	-	
11tet	10	-4847.35057	-4847.40958	30.06	30.00	-	
13tet	12	-4847.35780	-4847.41850	42.04	42.00	-	
AFO + 1 Na ⁰							
10tet	9	-5009.58392	-5009.64623	24.94	24.75	-	
12tet	11	-5009.60039	-5009.66378	35.92	35.75	-	
14tet	13	-5009.61206	-5009.67742	48.84	48.75	-	
AFO + 2 Na ⁰							
9tet	8	-5171.82100	-5171.88738	21.66	20.44	-	
11tet	10	-5171.83343	-5171.89850	30.62	30.04	-	
13tet	12	-5171.90942	-5171.97176	42.25	42.00	-	

^a Number of unpaired electrons in the system (NUE), zero-point energy-corrected electronic energy (E), Gibbs free energy at 298.15 K and 1 atm (G), total spin before (S^2) and after (S^2A) annihilation, and imaginary frequencies (IF).

^b The ground state is bolded.