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Supporting Information

Cr_2CO_2 Monolayer as Promising Cathode for Lithium and Non-lithium Ion Batteries: A Computational Exploration

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We considered four configurations of Cr_2CO_2 (see Figure S1): type I, in which all the O groups are attached on hollow sites of Cr atoms; type II, in which all the O groups are oriented above the C atoms on both sides of Cr_2C layer; type III, a combination of both types I and II, in which the O groups are placed above the hollow sites of Cr atoms on one side and above the top sites of C atoms on the other side, forming an asymmetric arrangement on the two sides of Cr_2C layer; type IV, the O groups are coordinated solely to the surface Cr atoms. Our computations revealed that type II is the lowest-energy structure.

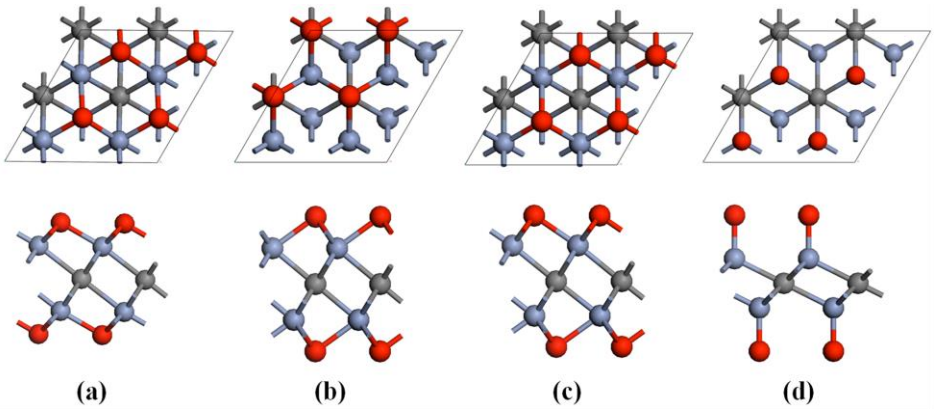

Figure S1. Top and side views of the optimized Cr_2CO_2 with type I (a), II (b), III (c) and IV (d) configurations. Color scheme: light purple, Cr; gray, C; red, O.

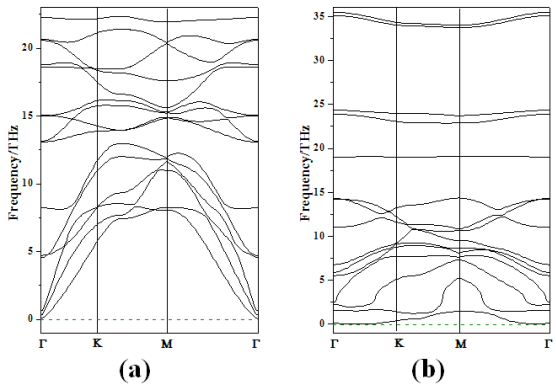

Figure S2. The phonon spectra of the optimized Cr_2CO_2 with type II configuration (a) and the most stable $Cr_2CO_2Li_2$ (b).

Table S1 The *k*-point (plane-wave cut off energy was chosen as 500 eV) and the plane-wave cut off energy testing (*k*-point mesh was chosen as 9×9×1) results based on type II Cr_2CO_2 monolayer.

k-point testing with E_{cut} of 500 eV				E_{cut} testing with k-point of 9×9×1			
	E/eV	*a*/Å	mag/μ_B		E/eV	*a*/Å	mag/μ_B
3×3×1	-42.156	2.699	0.000	300 eV	-44.505	2.617	0.000
5×5×1	-42.675	2.696	0.407	350 eV	-43.248	2.658	0.000
7×7×1	-42.714	2.693	0.000	400 eV	-42.836	2.681	0.000
9×9×1	-42.701	2.693	0.000	450 eV	-42.708	2.687	0.005
11×11×1	-42.706	2.693	0.000	500 eV	-42.701	2.693	0.000
13×13×1	-42.705	2.693	0.000	600 eV	-42.703	2.693	0.000

As shown in Table S1, the lattice parameter and magnetic moment become converged when the *k*-point and cut off energy are larger than 9×9×1 and 500 eV, and the energy difference between 9×9×1/500 eV and higher *k*-point/E_{cut} is less than 0.01 eV, so we chose 9×9×1 *k*-points mesh and 500 eV cut off energy in our computations.

Table S2 The total energy per unit cell (*E*), lattice parameter (*a*) and magnetic moment (mag) of the four possible Cr_2CO_2 structures with non-magnetic (NM), ferro-magnetic (FM) and antiferro-magnetic (AFM) configurations.

	type I				type II		
	E/eV	*a*/Å	mag/μ_B		*E*/eV	*a*/Å	mag/μ_B
NM	-42.094	2.805	--	NM	-42.700	2.692	--
FM	-42.520	2.888	3.980	FM	-42.700	2.692	0.000
AFM	-42.444	2.903	0.000	AFM	-42.700	2.692	0.000
	type III				type IV		
	E/eV	*a*/Å	mag/μ_B		*E*/eV	*a*/Å	mag/μ_B
NM	-42.379	2.732	--	NM	-41.001	3.146	--
FM	-42.594	2.797	2.070	FM	-40.999	3.146	0.263
AFM	-42.589	2.797	0.000	AFM	-40.998	3.146	0.000