Supplemental Information

A Data-driven Framework to Accelerate the Discovery of Hybrid Cathode Materials for Metal-based Batteries

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Table S1: *Elements used to exclude compounds from the compositional spaces of the source materials datasets based on their scarcity, toxicity, and radioactivity.*

Scarce elements	Toxic elements	Radioactive elements
Au, Ag, Pt, Os, Te, Ru, Ir, Rh, Re, Ra, Po, Tc, Pm, and At	Pb, Hg, Tl, As, and Sb	Fr, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr

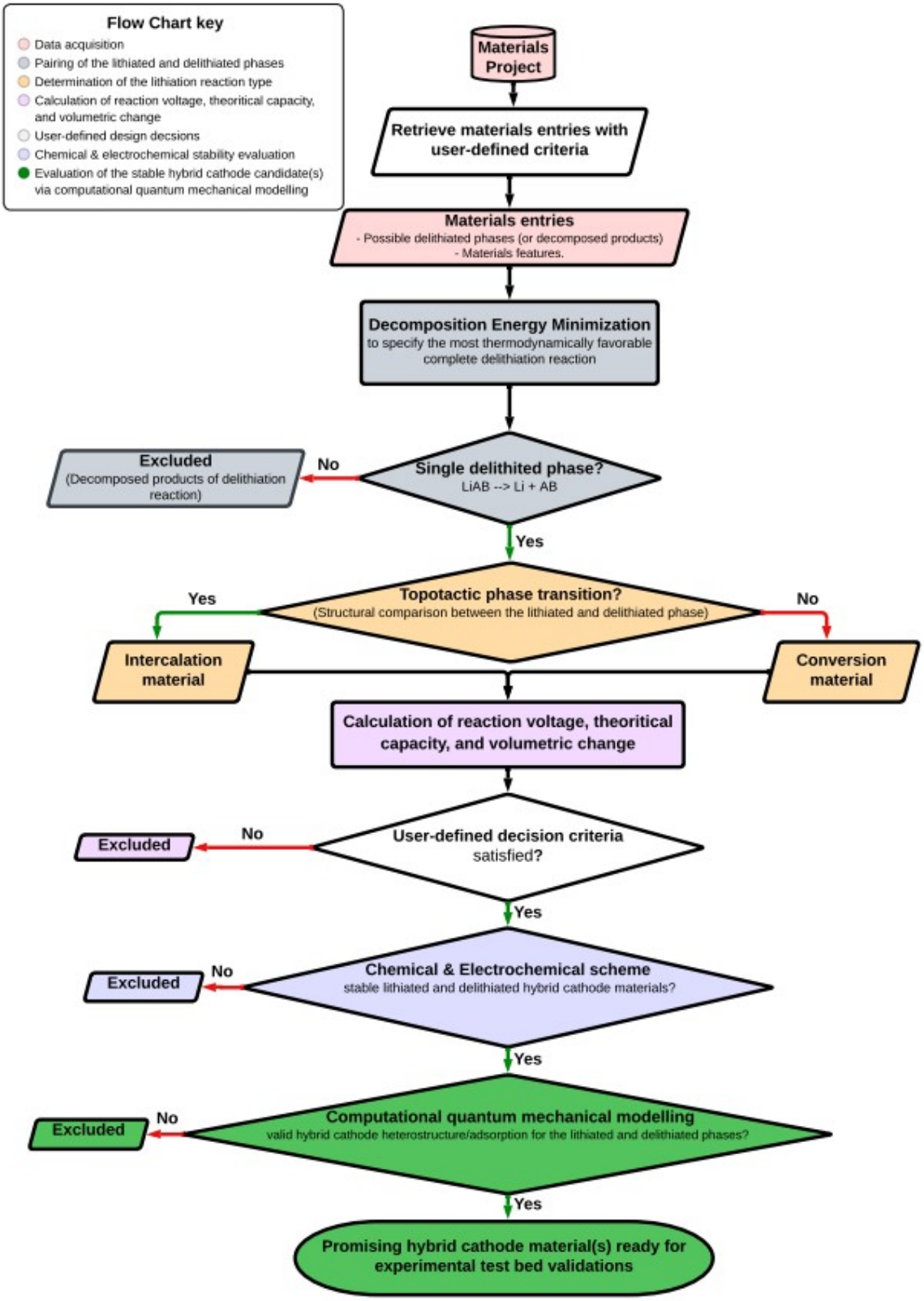

Figure S1*: The flowchart of the data-driven framework developed in this work for the discovery of hybrid cathode materials for metal-based batteries.*

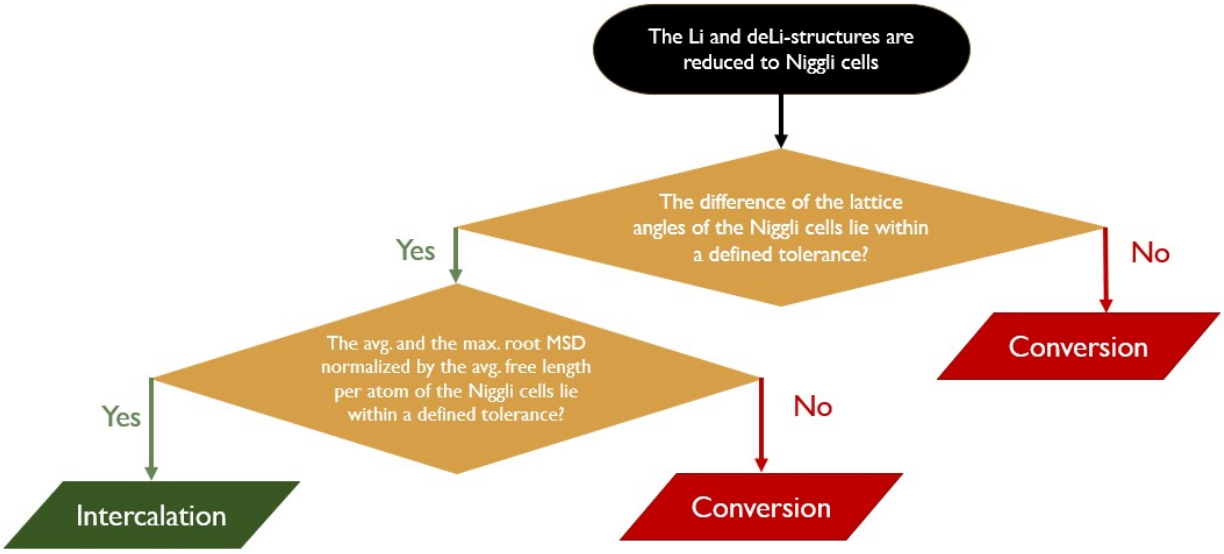

Figure S2: *The decision framework used in the StructureMatcher algorithm to identify whether a cathode material is an interaction or conversion material.*

Table S2: *List of intercalation phases that were excluded due to the instability of their delithiated phases.*

Lithiated phases	Delithiated phases	Reason for exclusion
mp-1206881 ($LiTaS_2$)	mp-1984 (TaS_2)	No μ_{Ta} overlap for TaS_2 and S_8
mp-1666120 ($LiCrPO_4$)	mp-25452 ($CrPO_4$)	No μ_O overlap for $CrPO_4$ and S_8
mp-26111 ($LiCr(PO_3)_3$)	mp-26112 ($Cr(PO_3)_3$)	No μ_O overlap for $Cr(PO_3)_3$ and S_8
mp-4226 ($LiCrS_2$)	mp-755263 (CrS_2)	CrS_2 has high energy above the hull
mp-752431 ($LiVPO_4$)	mp-767632 (VPO_4)	No μ_O overlap for VPO_4 and S_8
mp-755664 ($Li_2(TaS_2)_3$)	mp-1984 (TaS_2)	No μ_{Ta} overlap for TaS_2 and S_8
mp-757319 ($LiVPO_4$)	mp-18835 (VPO_4)	No μ_O overlap for VPO_4 and S_8
mp-765022 ($LiVPO_4$)	mp-18835 (VPO_4)	No μ_O overlap for VPO_4 and S_8
mp-767171 ($Li_5(NbS_2)_7$)	mp-10033 (NbS_2)	NbS_2 is not stable at all with S_8
mp-767218 ($Li_9(NbS_2)_{14}$)	mp-10033 (NbS_2)	NbS_2 is not stable at all with S_8
mp-7936 ($LiNbS_2$)	mp-10033 (NbS_2)	NbS_2 is not stable at all with S_8

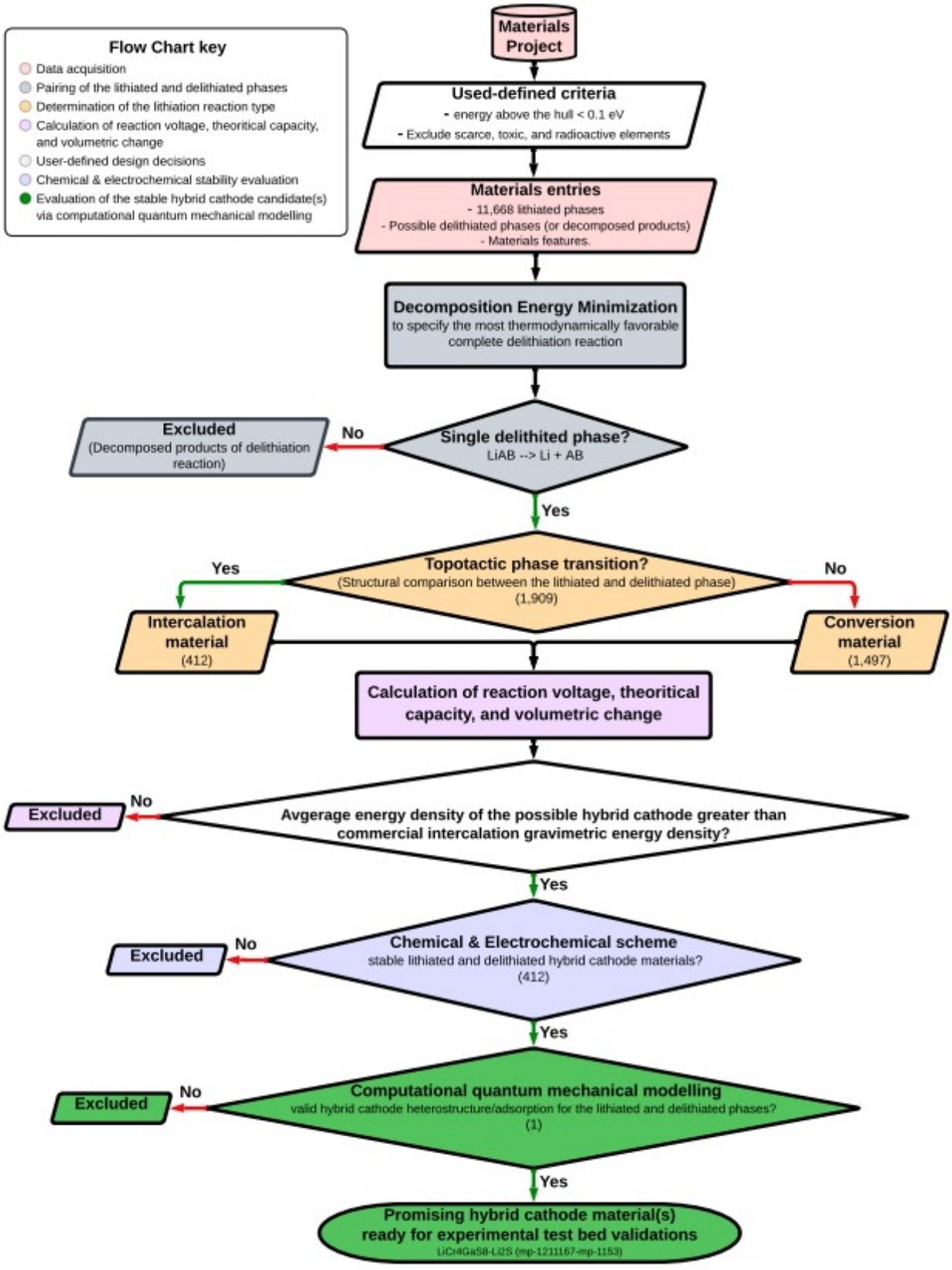

Figure S3: *The flowchart of the data-driven framework used in the case study to design a high-energy density Li hybrid cathode material.*

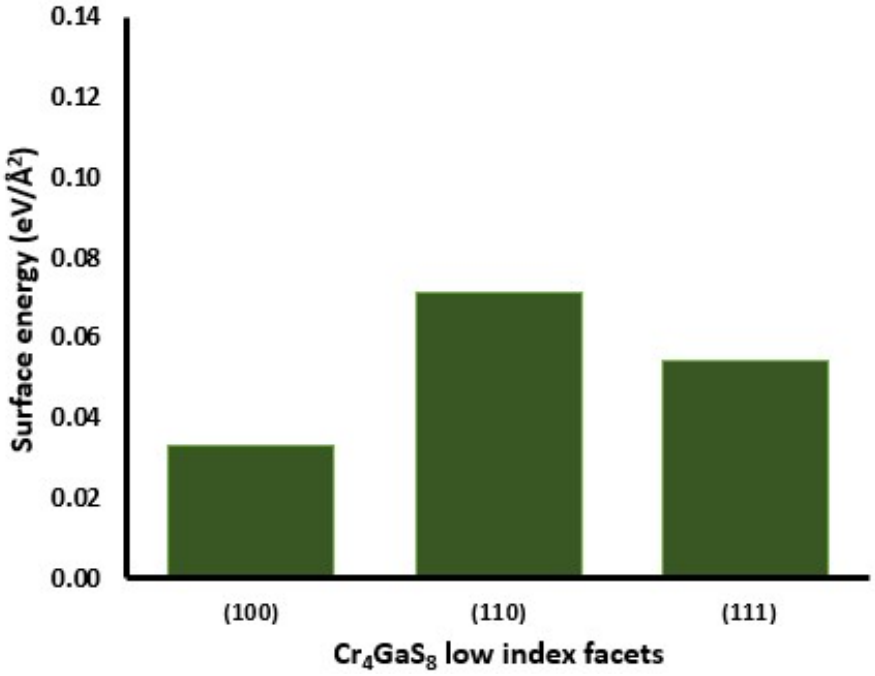

Figure S4: *Surface energies for the (100), (110), and (111) facets of Cr_4GaS_8 were compared at neutral charge. The (100) facet possesses the lowest surface energy and was adopted for the adsorption study.*

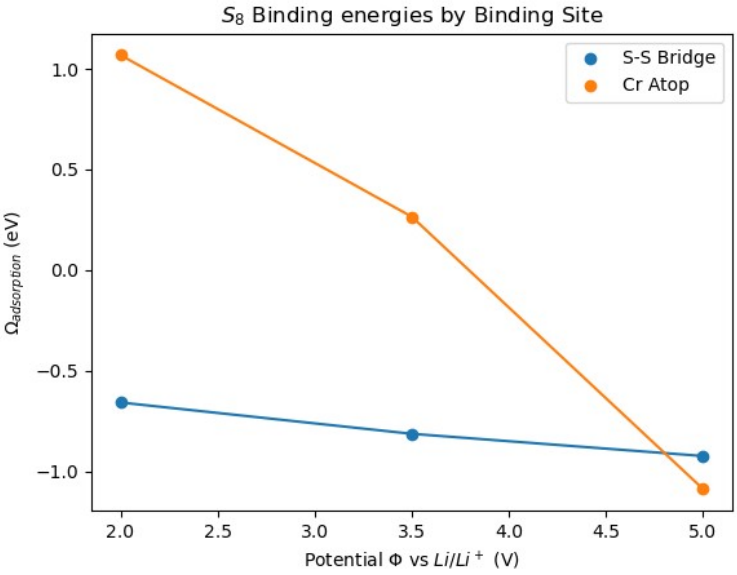

Figure S5: *S_8 binding energies at the S-S bridge and Cr-atop sites of Cr_4GaS_8, where the electron reservoir potential was sampled over the charging (delithiation) operating window*

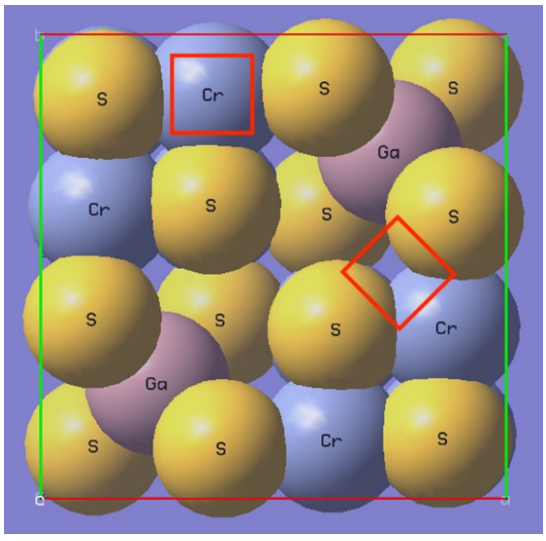

Figure S6: *The binding sites of S-S bridge and Cr-atop in Cr_4GaS_8 (100) facet. Cr-atop are indicated by red boxes.*