

39th Students' Symposium

Simulations **And** Informatics of
MATerials Group



High-throughput screening of intercalation electrodes for electrochemical ion capture and desalination

29th January 2026

Presenter: Sougat Purohit

PhD Scholar, sougatp@iisc.ac.in

Under the guidance of :

Dr. Sai Gautam Gopalakrishnan

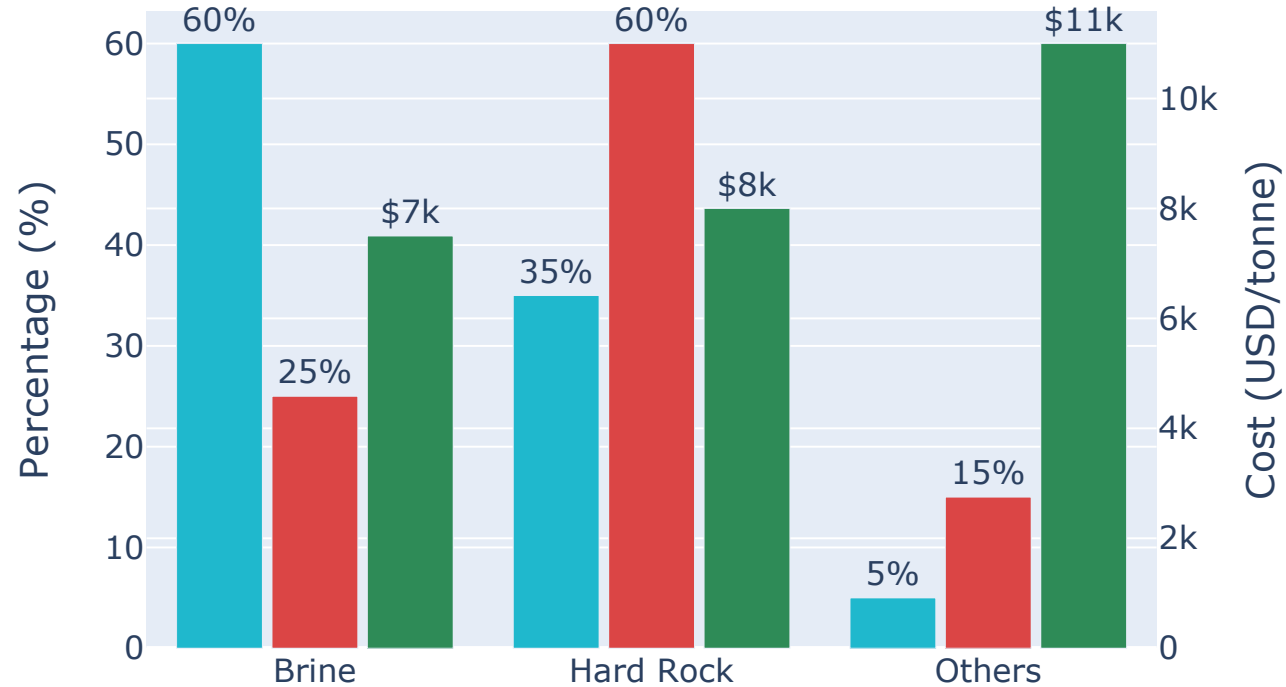


भारतीय विज्ञान संस्थान

Department of Materials Engineering
Indian Institute of Science, Bengaluru

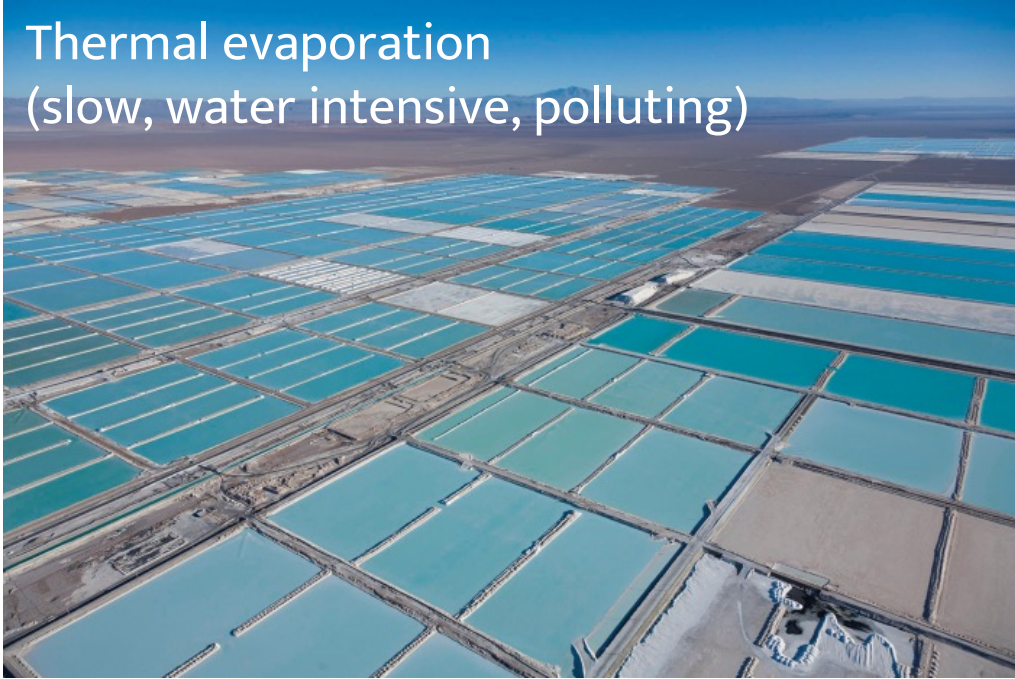
Problem with Li extraction from brines

■ Reserve % ■ Production % ■ Cost (USD/t)

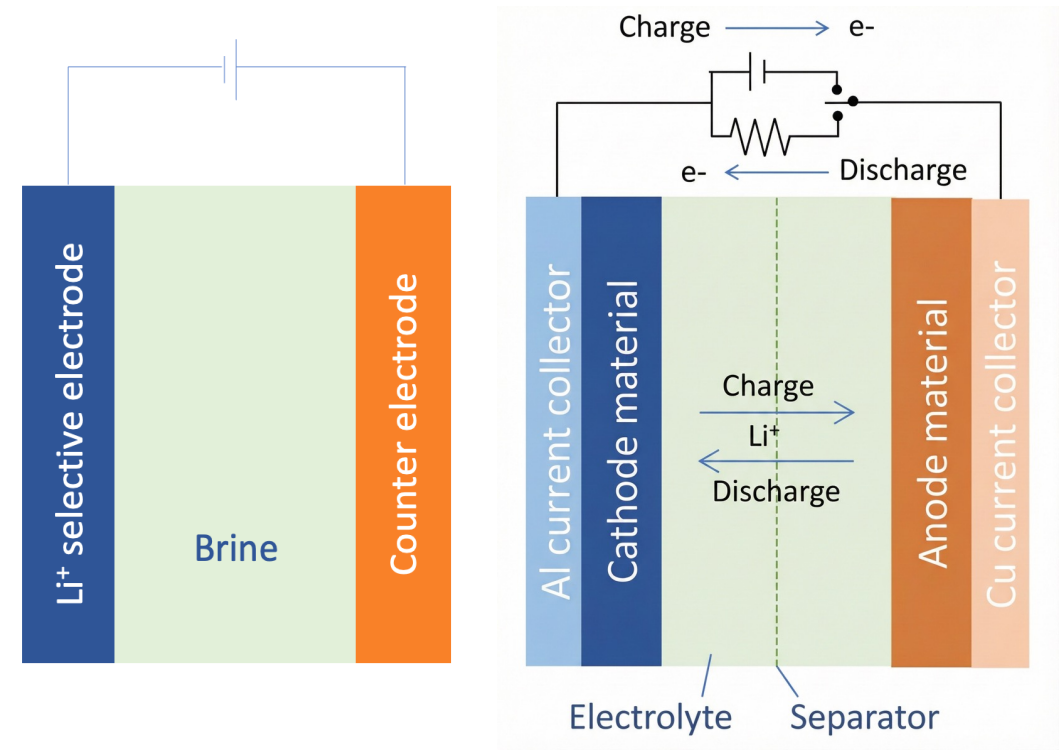
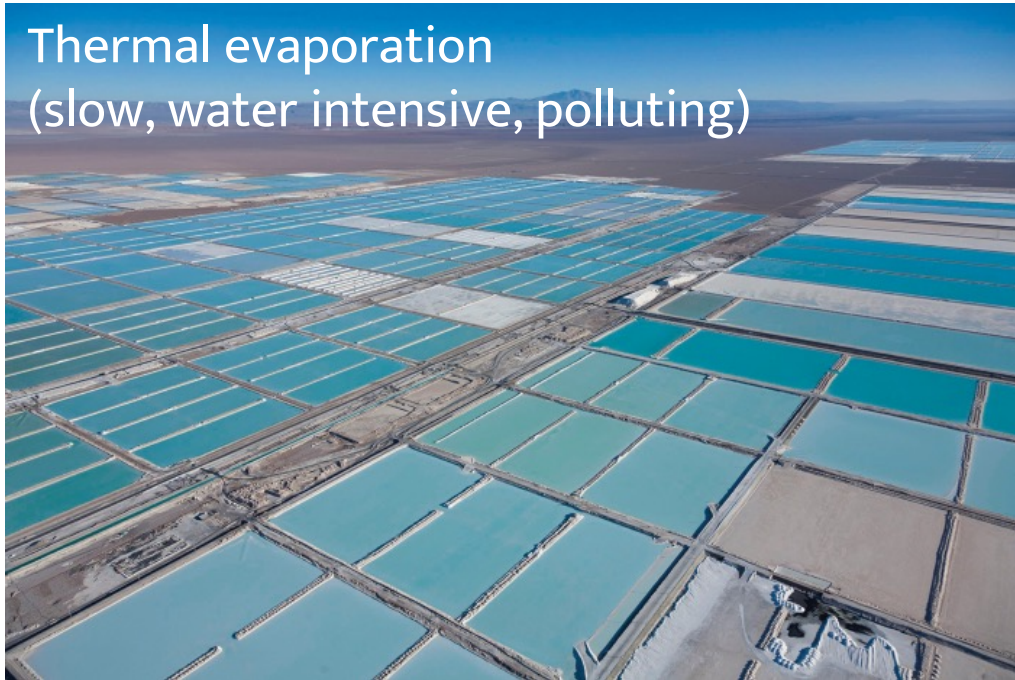


Problem with Li extraction from brines

Thermal evaporation
(slow, water intensive, polluting)



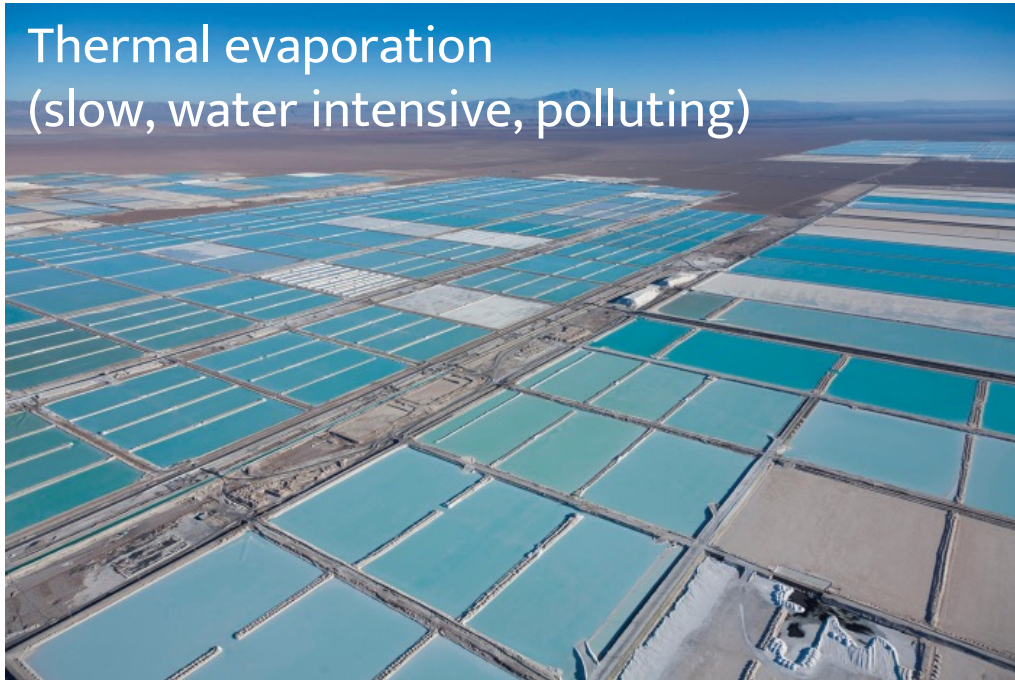
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Electrochemical ion-recovery:

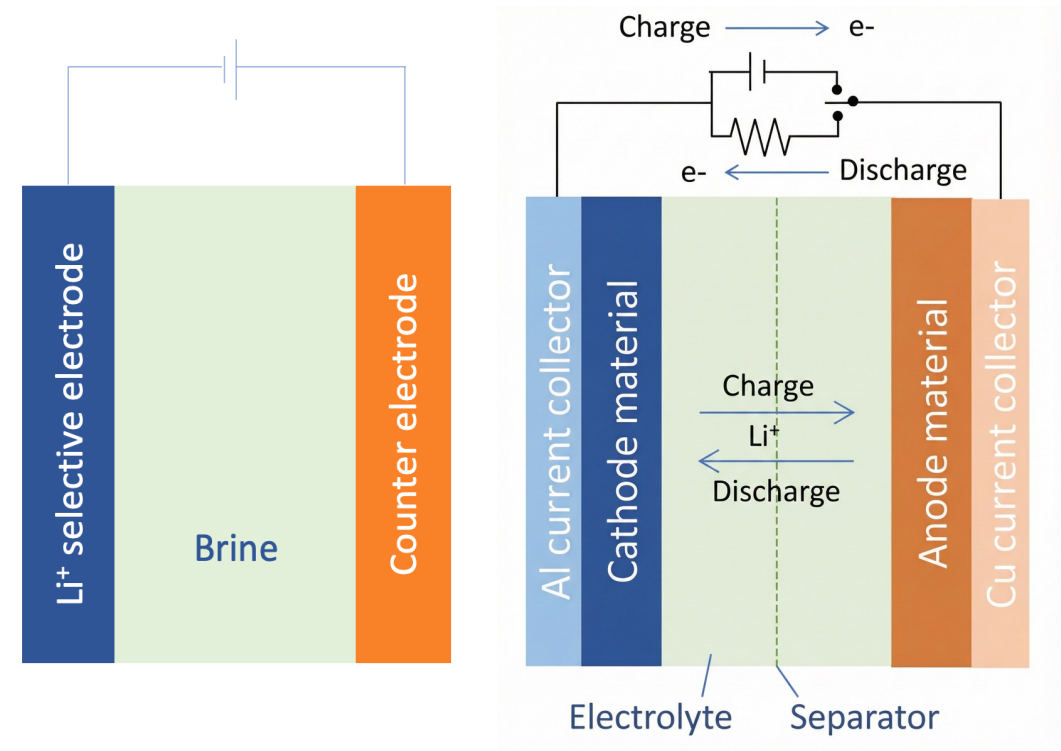
- Faster, low energy consumption
- Can handle various brine compositions including [seawater](#)
- Similar to Li-ion Battery (LIB)

Problem with Li extraction from brines



Necessary traits:

1. Must be **selective towards Li^+**
(doesn't intercalate Na^+ K^+ Ca^{+2} Mg^{+2})
2. Must be **stable in the brine**
3. Multi-ions intercalating electrodes: **desalination**

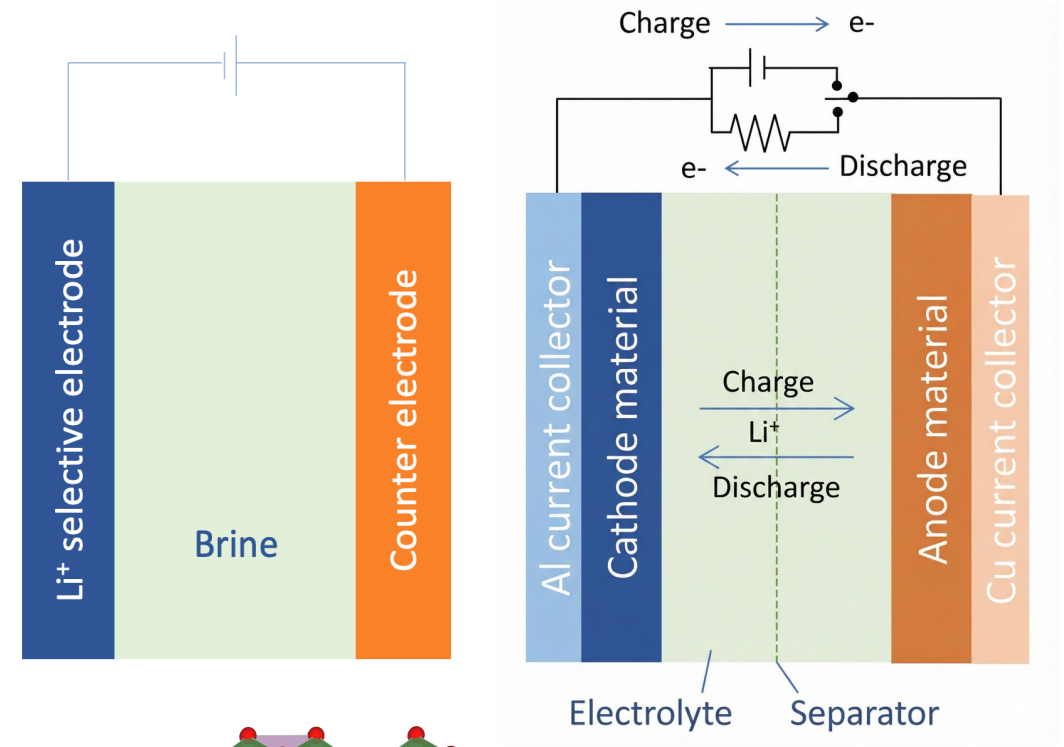
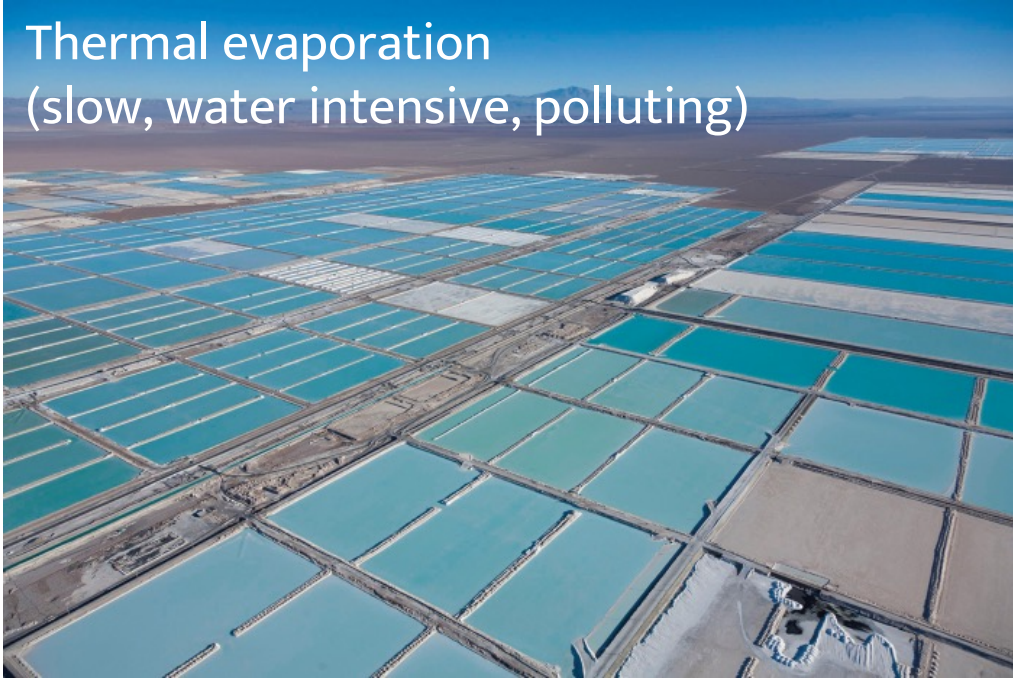


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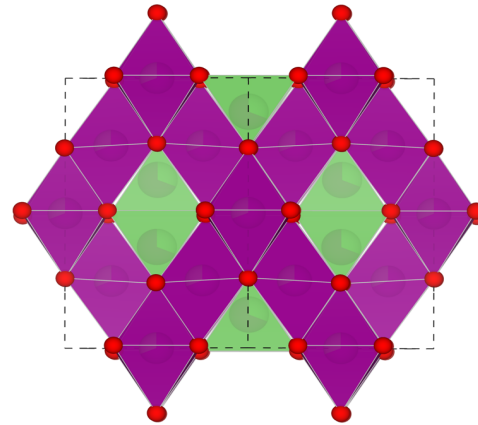
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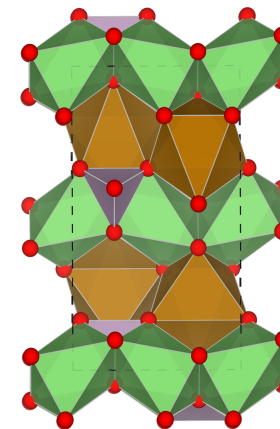
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State of the art
 Li^+ selective electrodes:



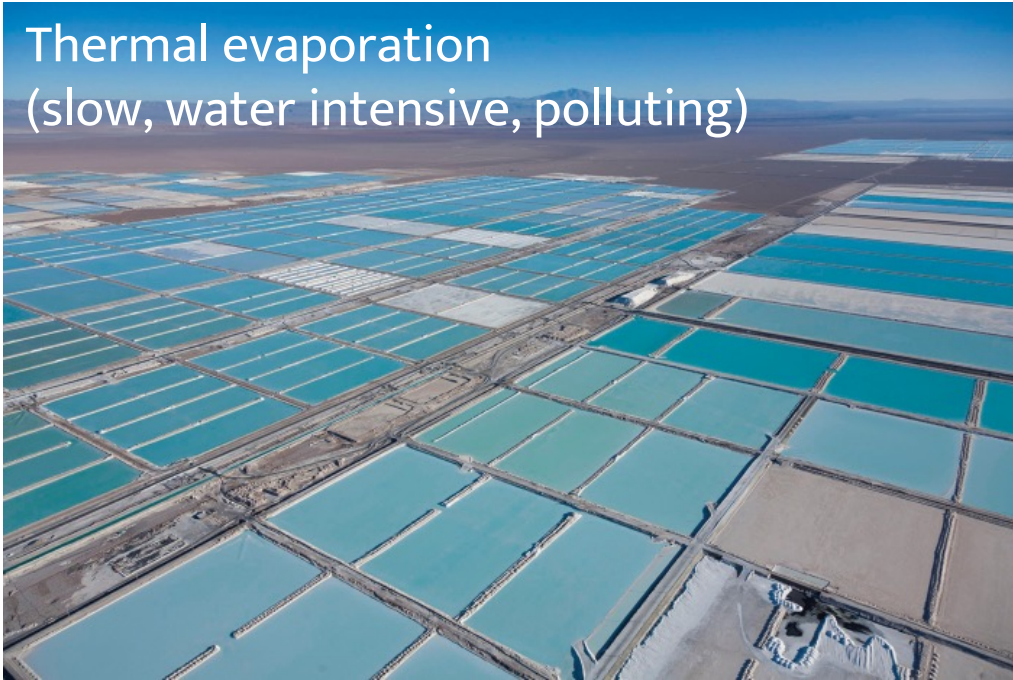
Spinel LiMn_2O_4



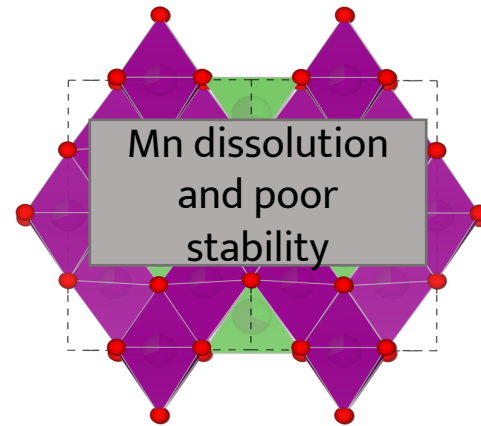
Olivine LiFePO_4

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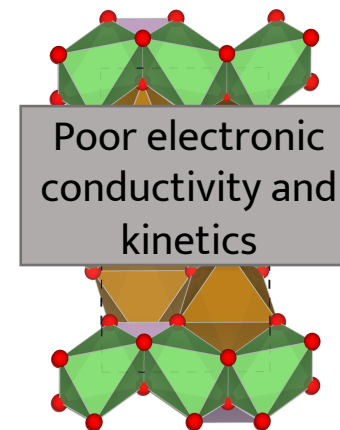
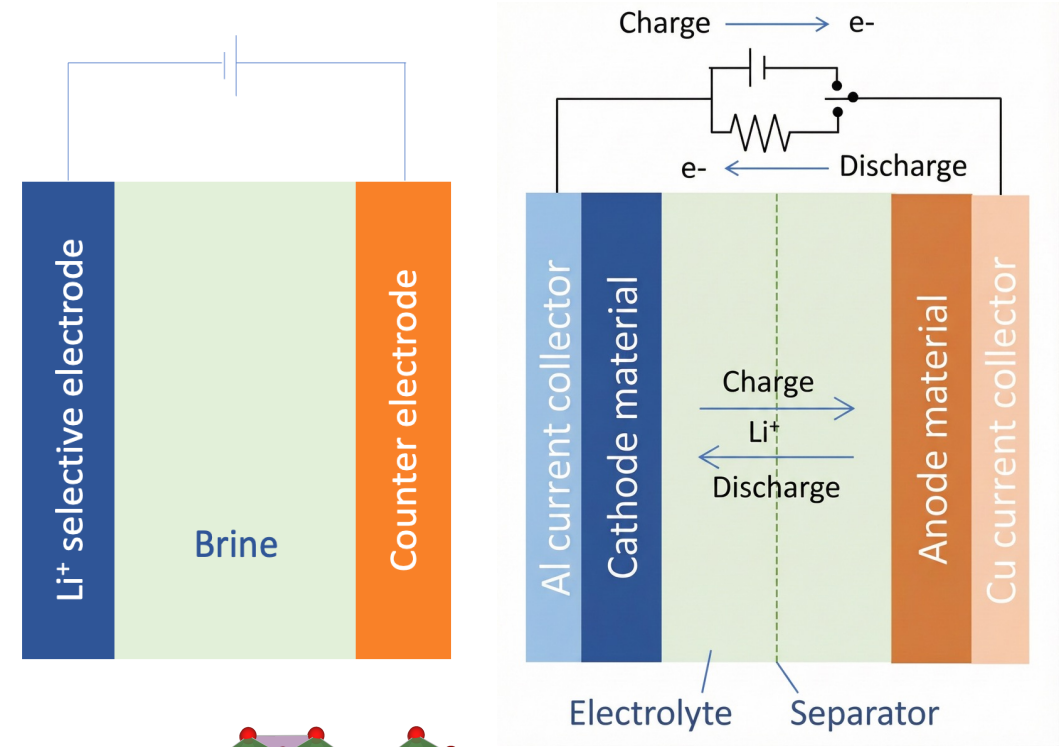
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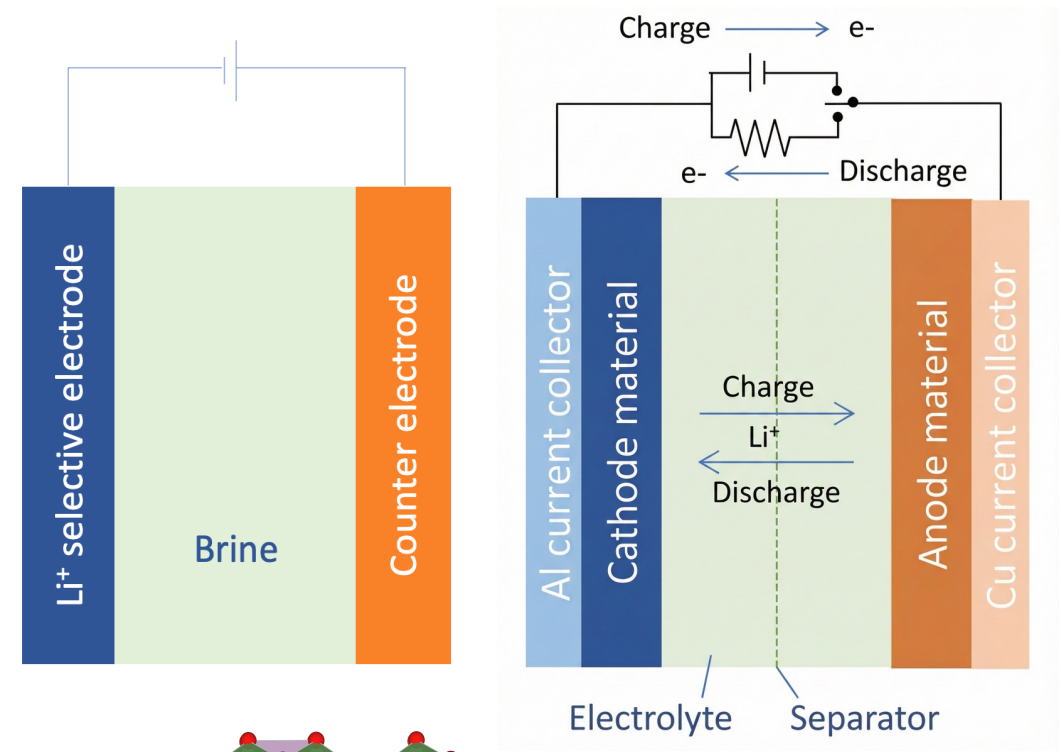
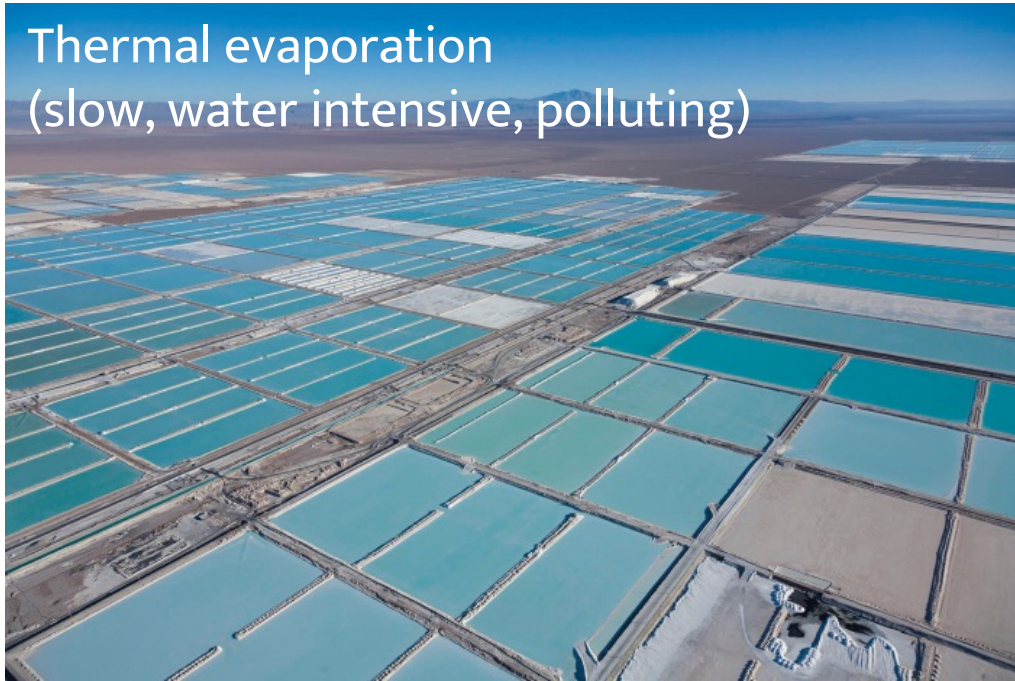
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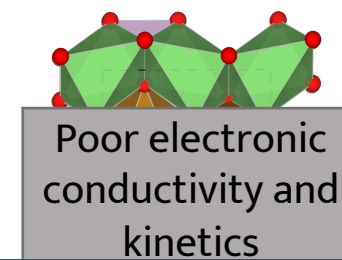
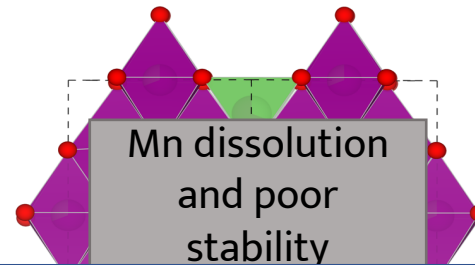
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State of the art
 Li^+ selective electrodes:



Objective: Find better alternatives to olivine LiFePO_4 and spinel LiMn_2O_4

Spinel LiMn_2O_4

Olivine LiFePO_4

High-throughput screening workflow

Step 1

Query first-principles cathodes' data across ions

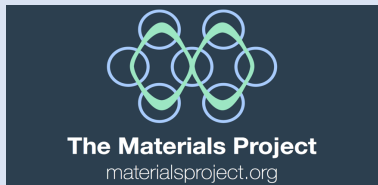


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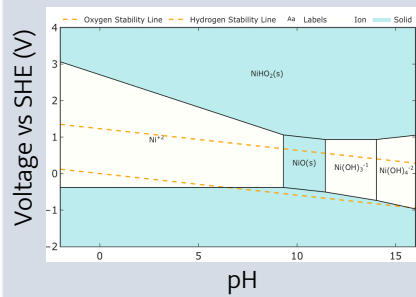
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Step 2

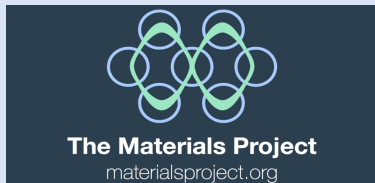
Determine aqueous stability of the cathodes



High-throughput screening workflow

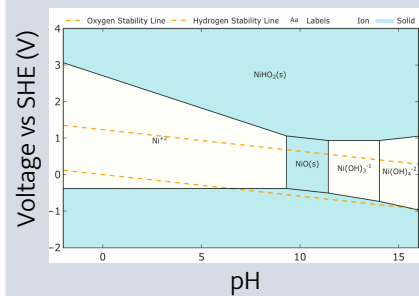
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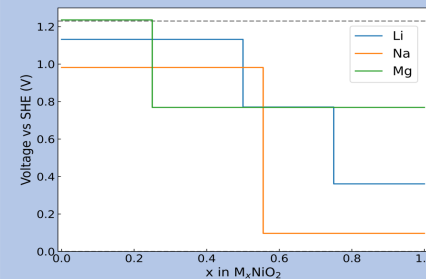
Step 2

Determine aqueous stability of the cathodes



Step 3

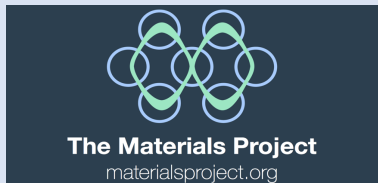
Calculate intercalation voltage



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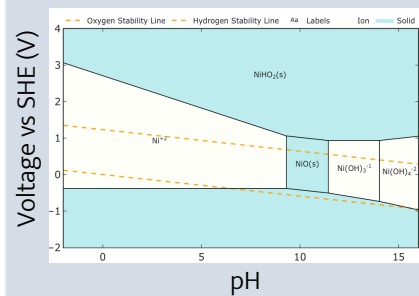
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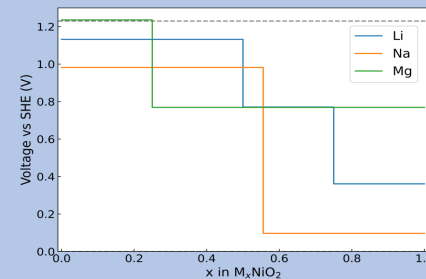
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Determine aqueous stability of the cathodes



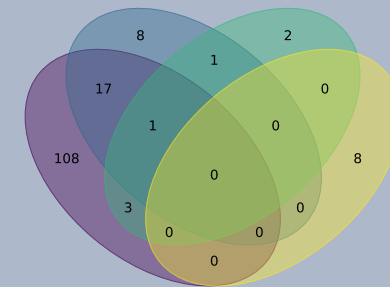
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Step 4

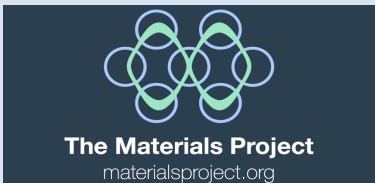
Compare structures across ions



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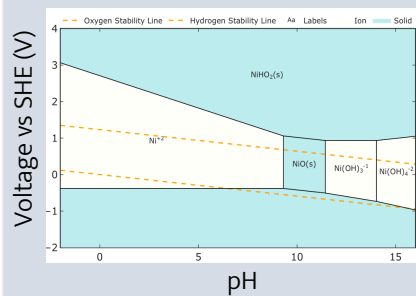
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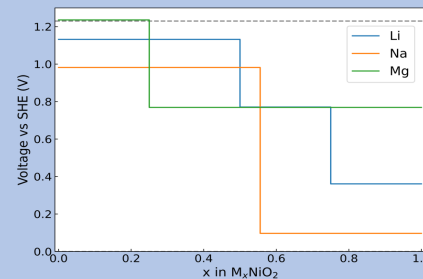
Step 2

Determine aqueous stability of the cathodes



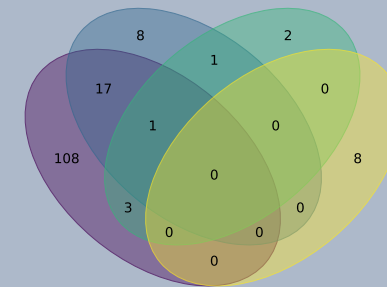
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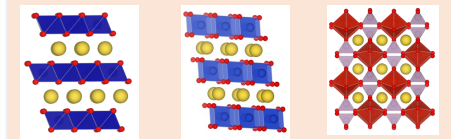
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Results

Li-capturing electrodes
(Selective-ion extraction)

All-ions-capturing electrodes
(Desalination)



Step 1: Querying Cathodes' data

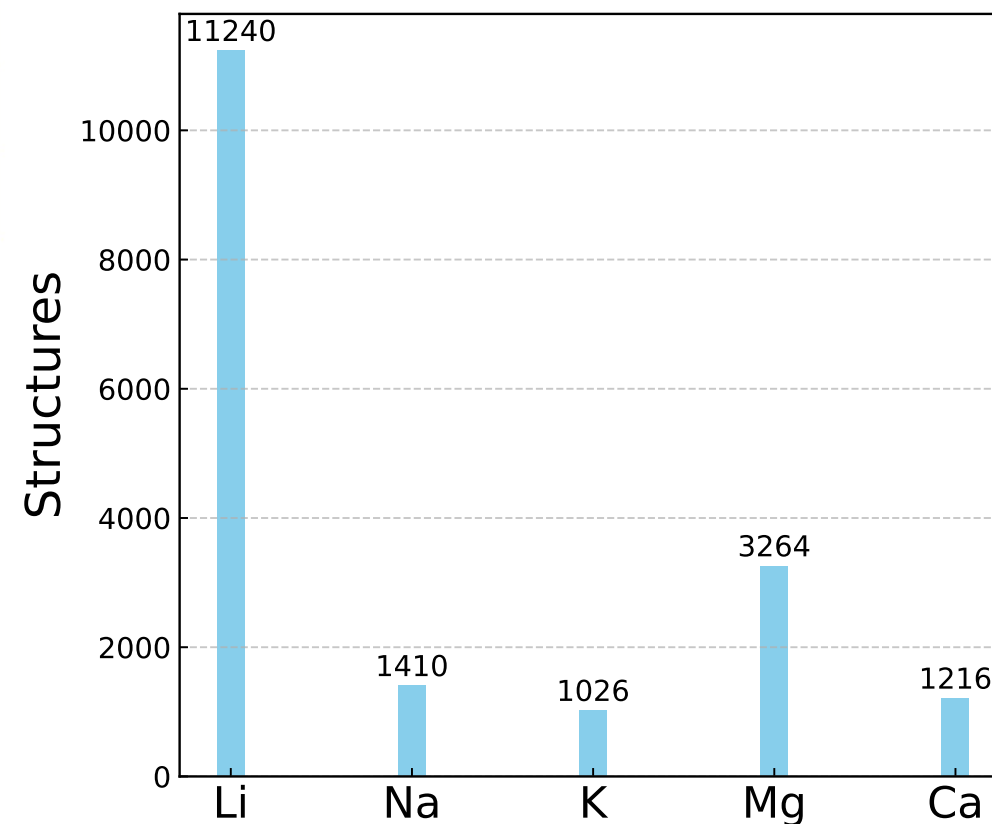
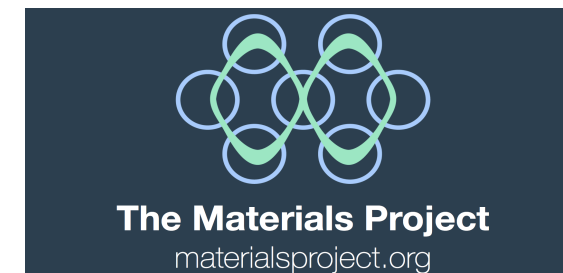
1 H Hydrogen 1.008																	2 He Helium 4.00260	
3 Li Lithium 7.0	4 Be Beryllium 9.012183																	10 Ne Neon 20.180
11 Na Sodium 22.9897693	12 Mg Magnesium 24.305																	18 Ar Argon 39.9
19 K Potassium 39.098	20 Ca Calcium 40.08	21 Sc Scandium 44.95591	22 Ti Titanium 47.87	23 V Vanadium 50.941	24 Cr Chromium 51.996	25 Mn Manganese 54.93804	26 Fe Iron 55.84	27 Co Cobalt 58.93319	28 Ni Nickel 58.693	29 Cu Copper 63.55	30 Zn Zinc 65.4	31 Ga Gallium 69.72	32 Ge Germanium 72.63	33 As Arsenic 74.63	34 Se Selenium 78.97	35 Br Bromine 79.904	36 Kr Krypton 83.80	
37 Rb Rubidium 85.468	38 Sr Strontium 87.6	39 Y Yttrium 88.9058	40 Zr Zirconium 91.22	41 Nb Niobium 92.906	42 Mo Molybdenum 95.9	43 Tc Technetium 97.9072	44 Ru Ruthenium 101.1	45 Rh Rhodium 101.1	46 Pd Palladium 106.4	47 Ag Silver 107.868	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.6	53 I Iodine 126.90	54 Xe Xenon 131.29	
55 Cs Caesium 132.905450	56 Ba Barium 137.33	57-71 Lanthanoids	72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.8	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.96657	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207	83 Bi Bismuth 208.9804	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222.01758	
87 Fr Francium 223.01871	88 Ra Radium 226.02541	89-103 Actinoids	104 Rf Rutherfordium 261.102	105 Db Dubnium 262.103	106 Sg Seaborgium 266.107	107 Bh Bohrium 264.104	108 Hs Hassium 277.102	109 Mt Meitnerium 276.106	110 Ds Darmstadtium 281.105	111 Rg Roentgenium 282.109	112 Cn Copernicium 285.107	113 Nh Nihonium 284.103	114 Fl Flerovium 289.101	115 Mc Moscovium 290.106	116 Lv Livermorium 293.105	117 Ts Tennessine 294.101	118 Og Oganesson 294.101	

15 Transition Metals (TMs)

9 Anions

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- Atmost 3 TMs or anions at a time

$^{15}C_1 + ^{15}C_2 + ^{15}C_3$ TM combinations

{‘Ti’ ‘V’, ‘Cr’, ... ‘Ti-V’ ‘Ti-Cr’ ... ‘Re-Os-Ir’}

$^9C_1 + ^9C_2 + ^9C_3$ anion combinations

{‘N’ ‘P’ ‘O’ ... ‘N-P’ ‘N-O’ ... ‘Cl-Br-I’}

M-Ti-N

M-V-N

•

M-Cr-N-O

M-Cr-N-S

•

M-Re-O-Ir-Cl-Br-I

M = Li/Na/K/Mg/Ca

Step 1

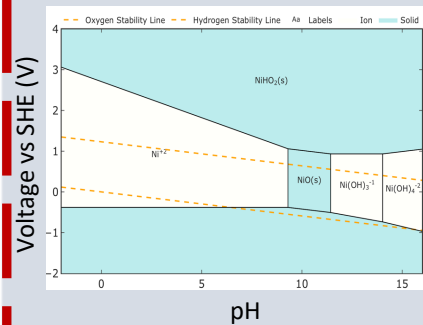
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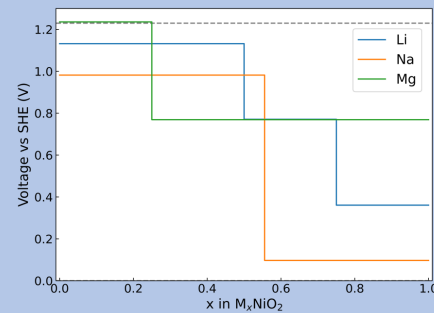
Step 2

Determine aqueous stability of the cathodes



Step 3

Calculate intercalation voltage



Step 4

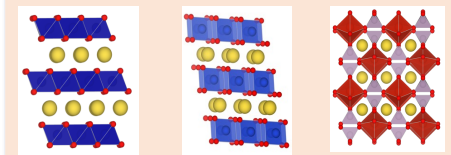
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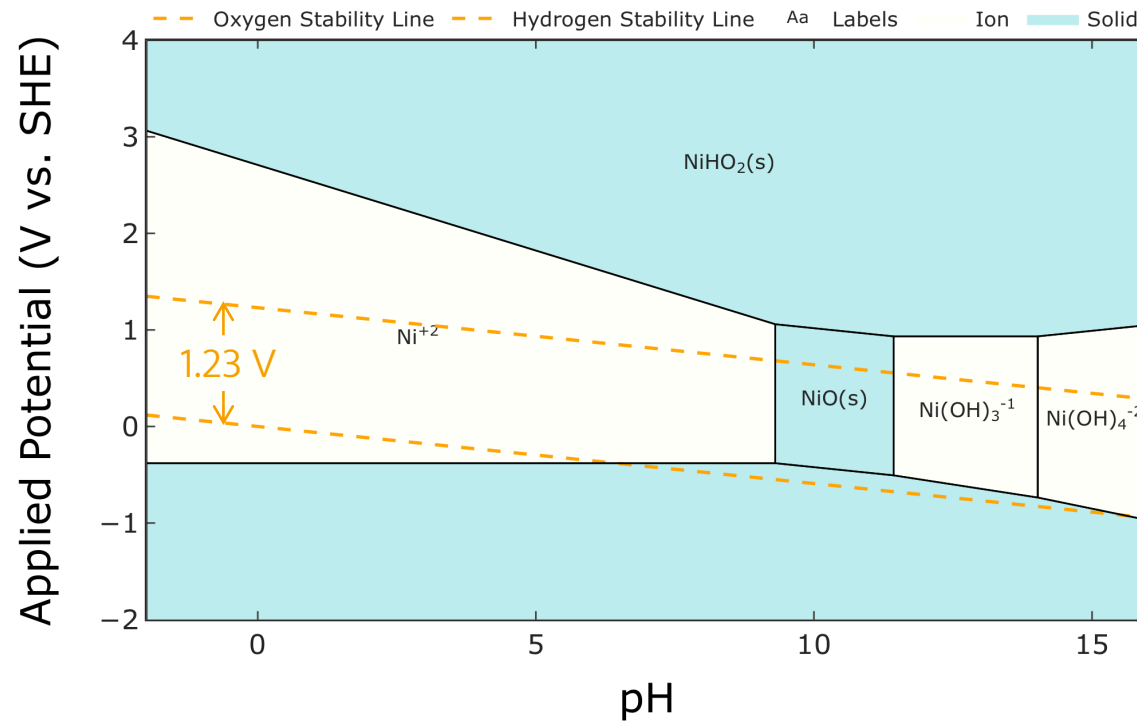
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Li-capturing electrodes
(Selective-ion extraction)

All-ions-capturing electrodes
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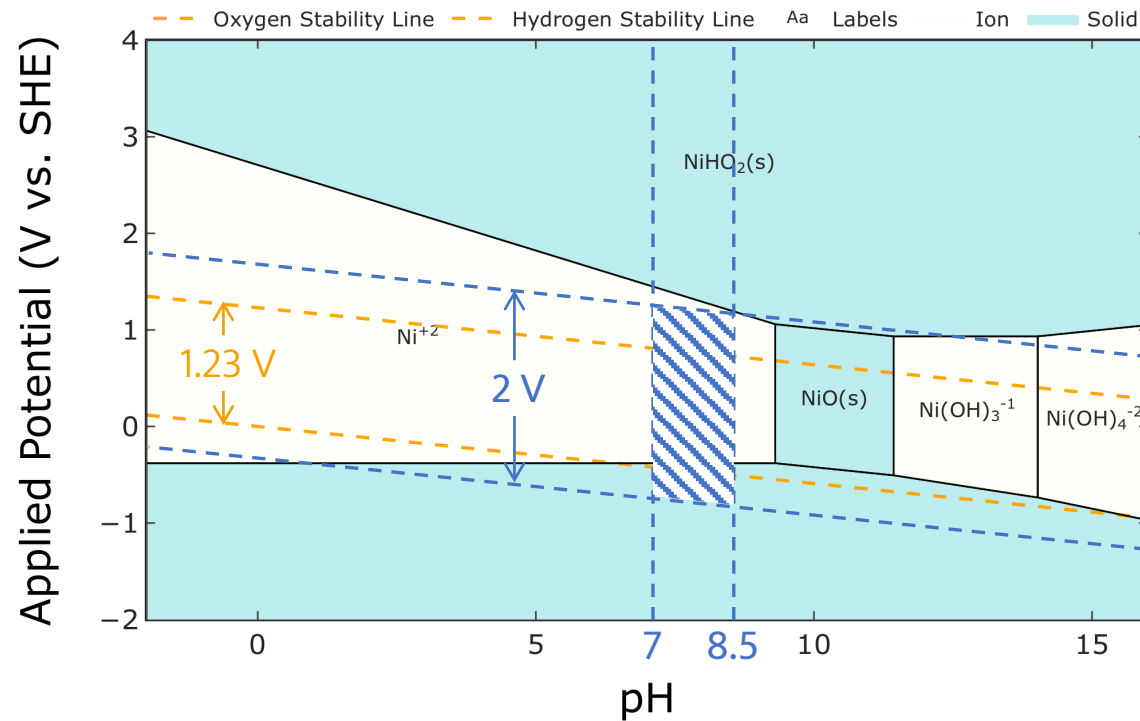


Step 2: Determining aqueous stability of cathodes



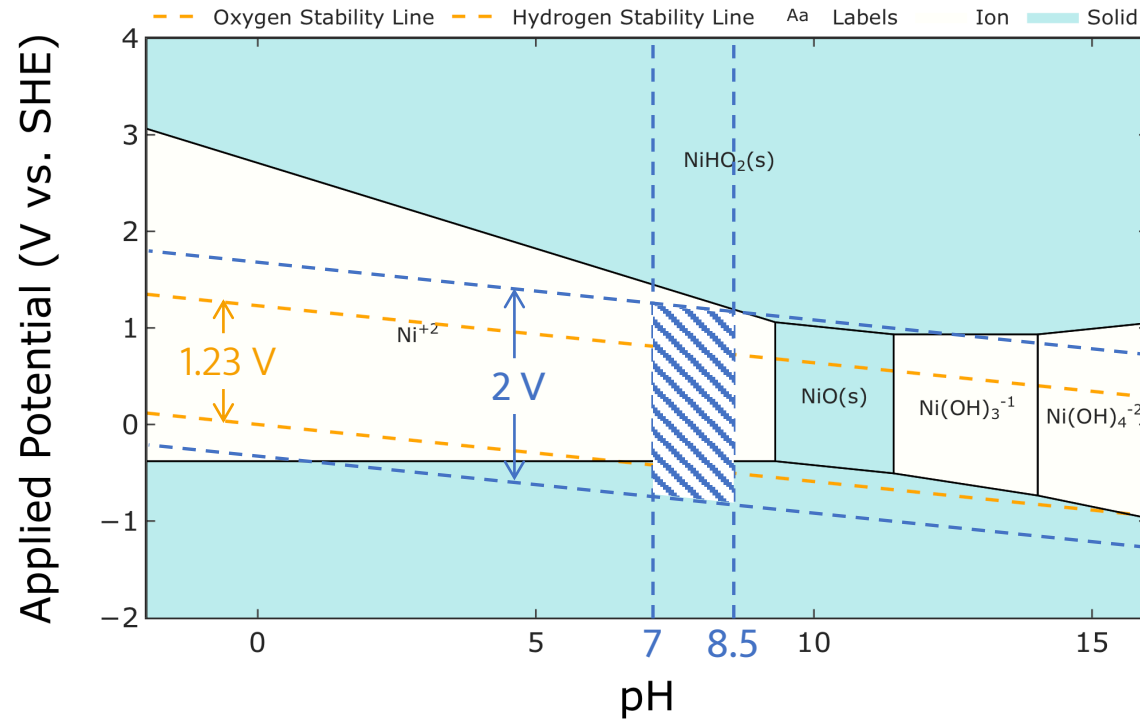
$$\Psi = G - \frac{\partial G}{\partial N_H} N_H - \frac{\partial G}{\partial Q} Q - \frac{\partial G}{\partial N_O} N_O$$

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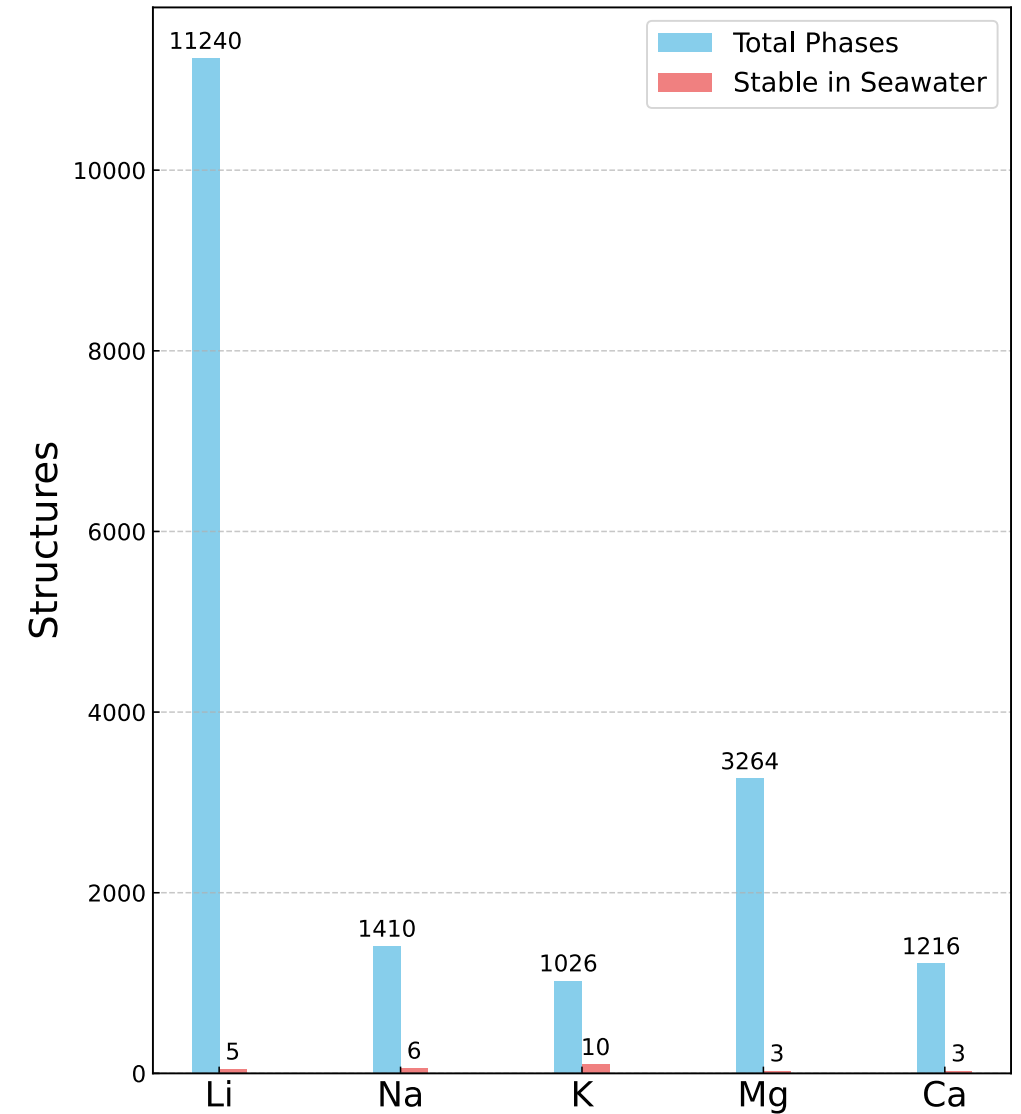


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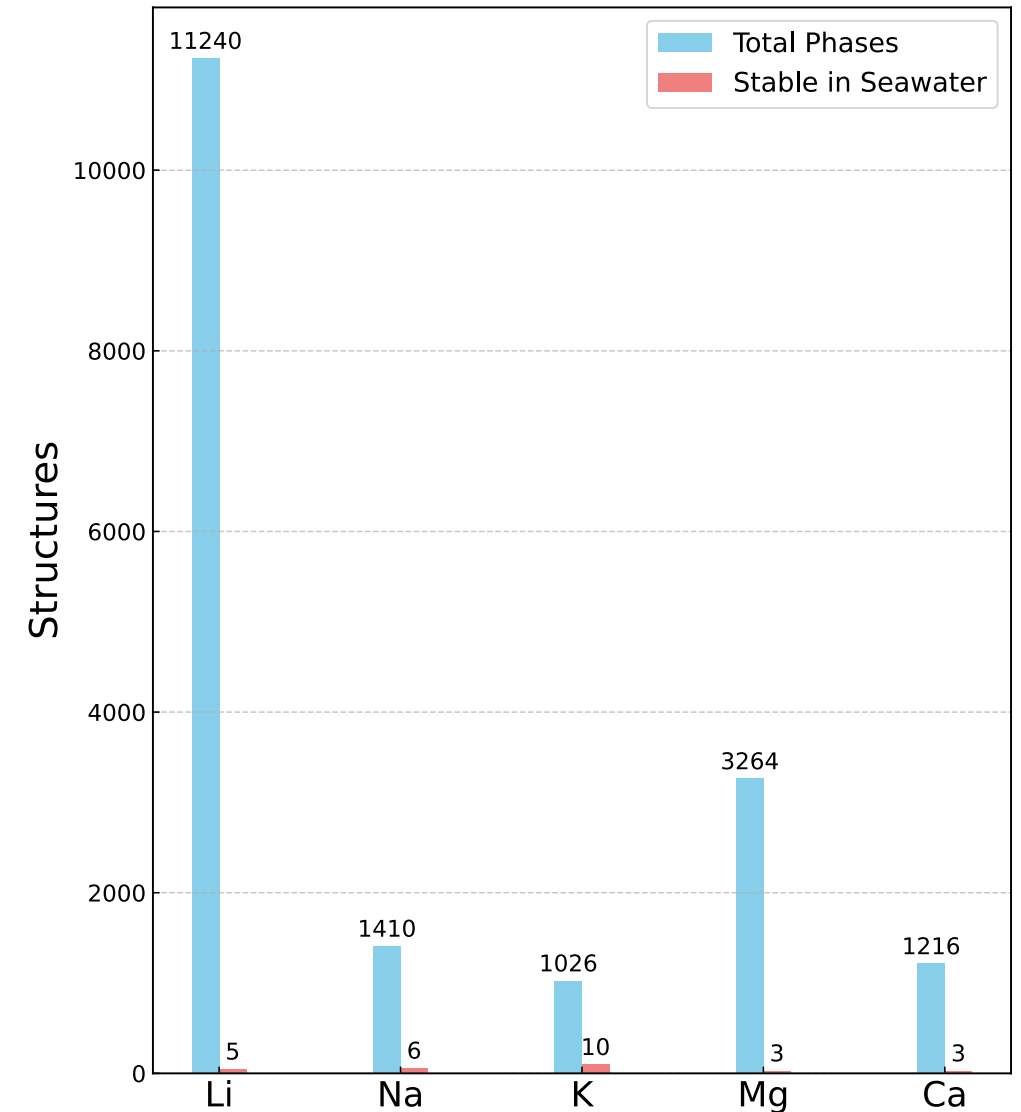


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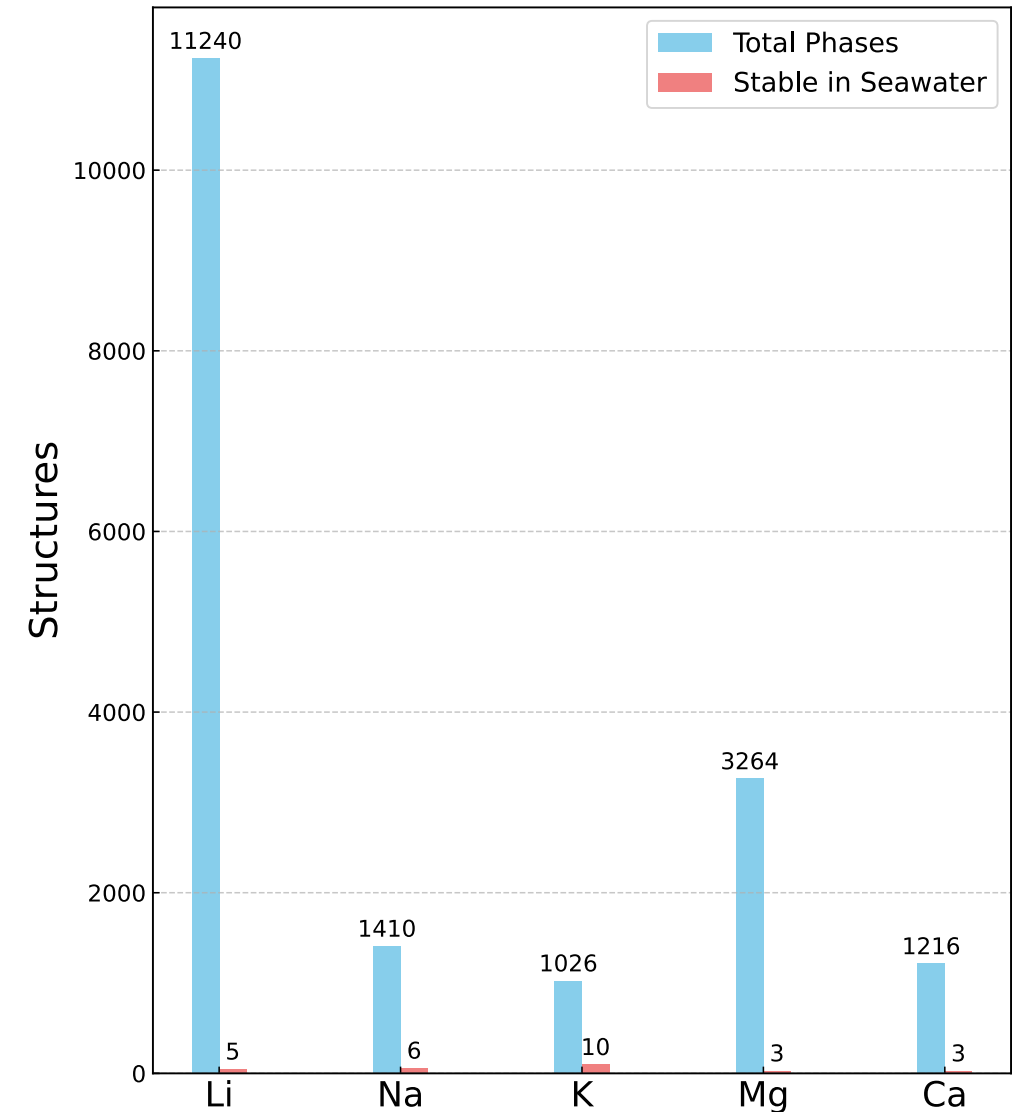
Step 2: Determining aqueous stability of cathodes

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- Quantifying seawater metastability:
Metastable solid 'A', decomposes to stable phases (B, C ...)
$$A \rightarrow B + C + \dots \quad \Delta\Psi \text{ (Decomposition energy)}$$
 1. High energy barriers for bulk solid state transitions
 2. Solid decomposition product can form a self passivating layer

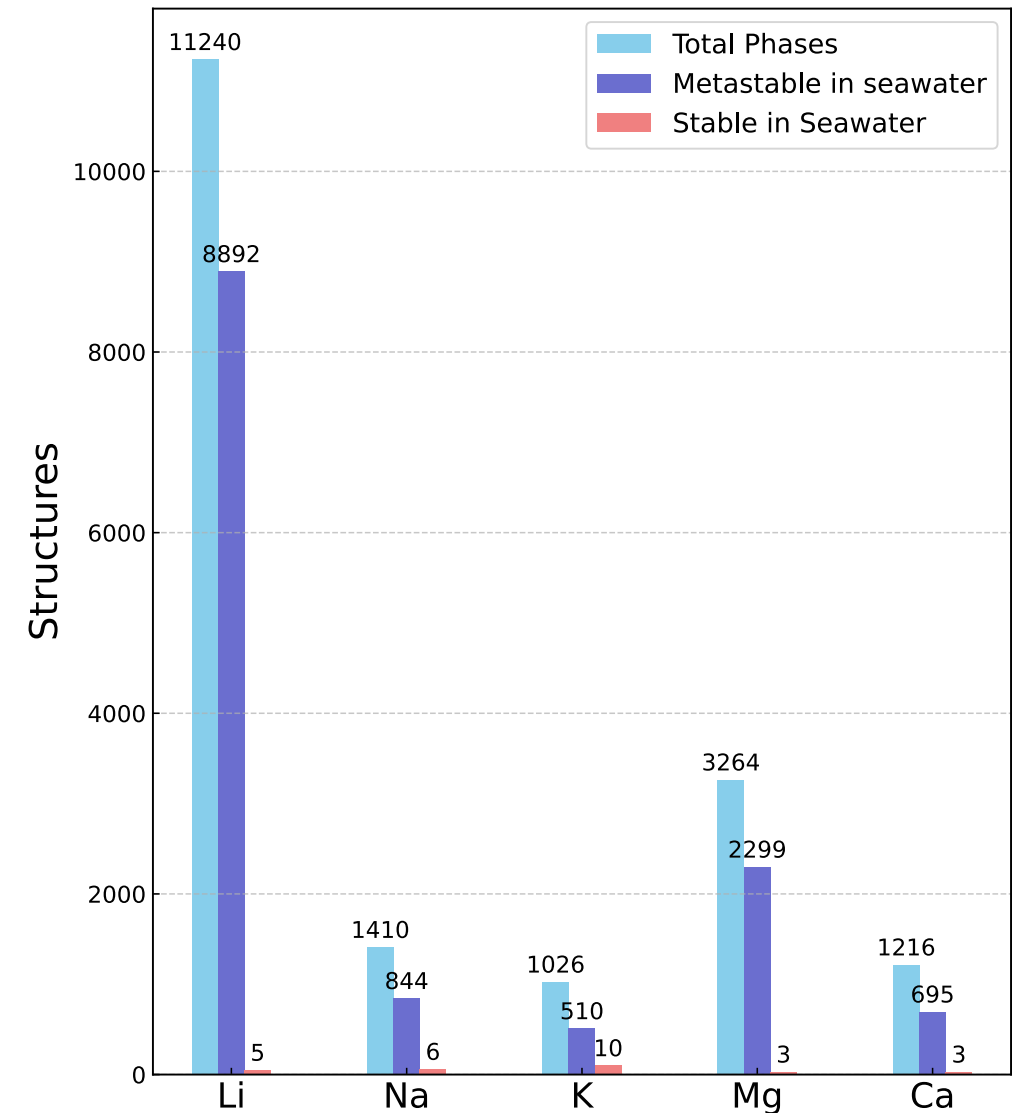


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Metastability criterion for A

- At least one of B, C ... is a non elemental solid without the mobile ion
- $\Delta\Psi < \text{threshold (0.3 eV atom}^{-1}\text{)}$



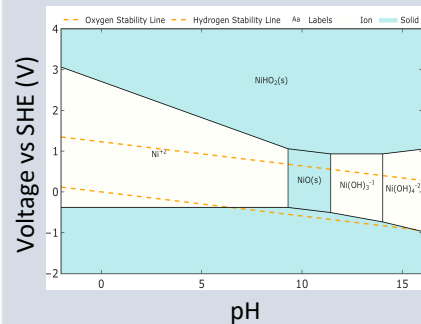
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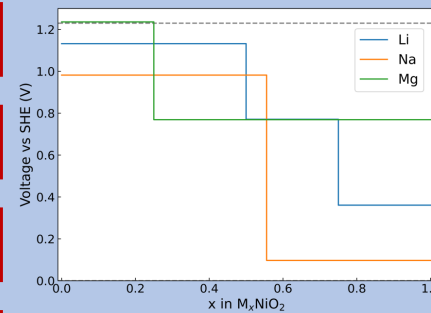
Step 2

Determine aqueous stability of the cathodes



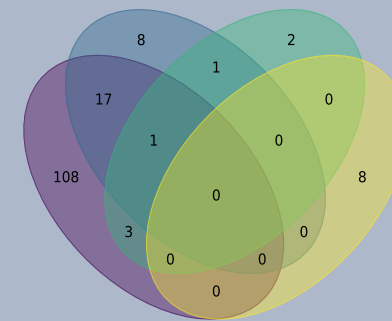
Step 3

Calculate intercalation voltage



Step 4

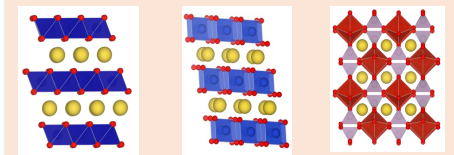
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Step 3: Intercalation voltages

Approximations:

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Metastability scenarios at the intercalation voltage:

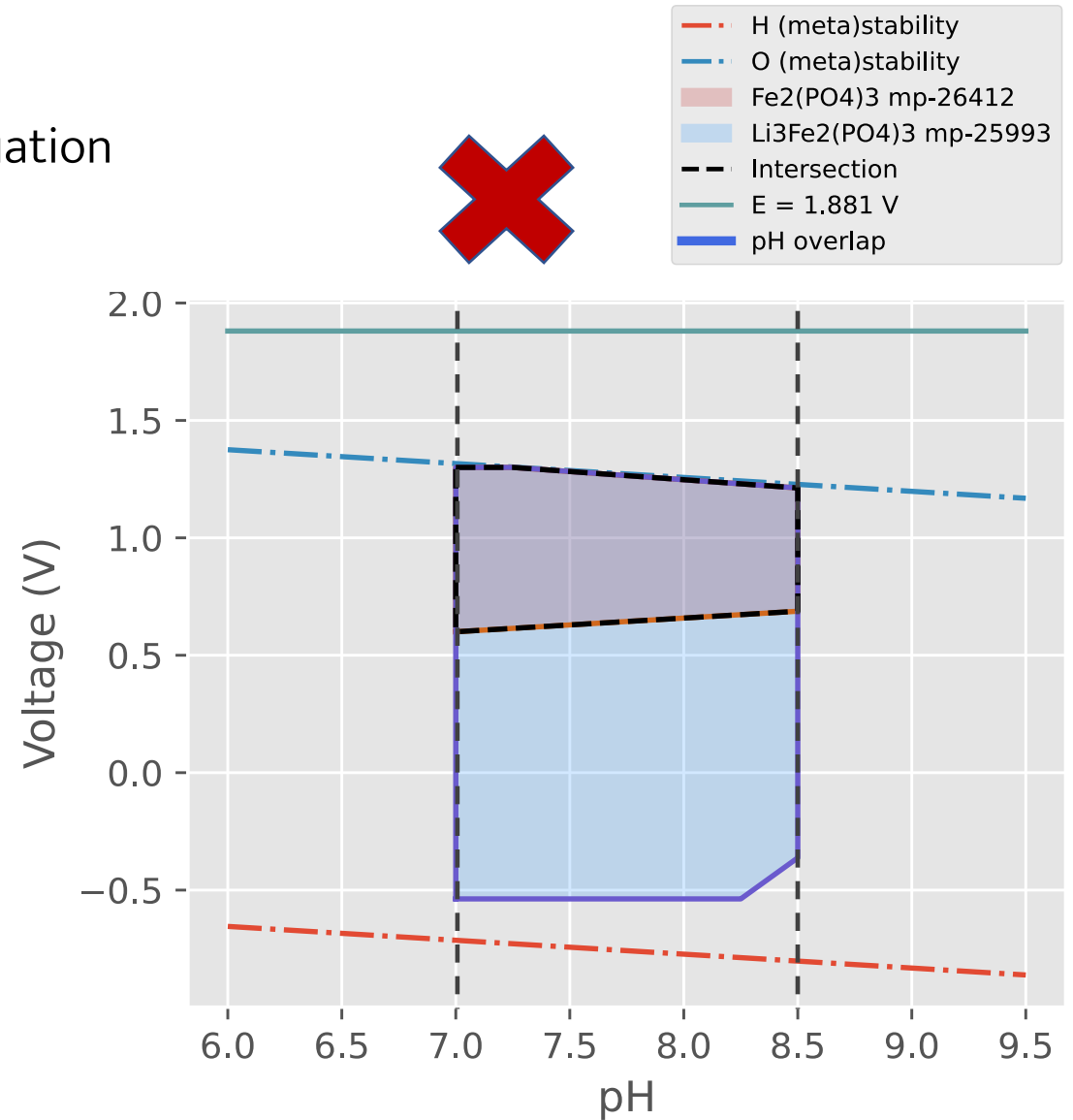
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Metastability scenarios at the intercalation voltage:

- Voltage beyond seawater stability window



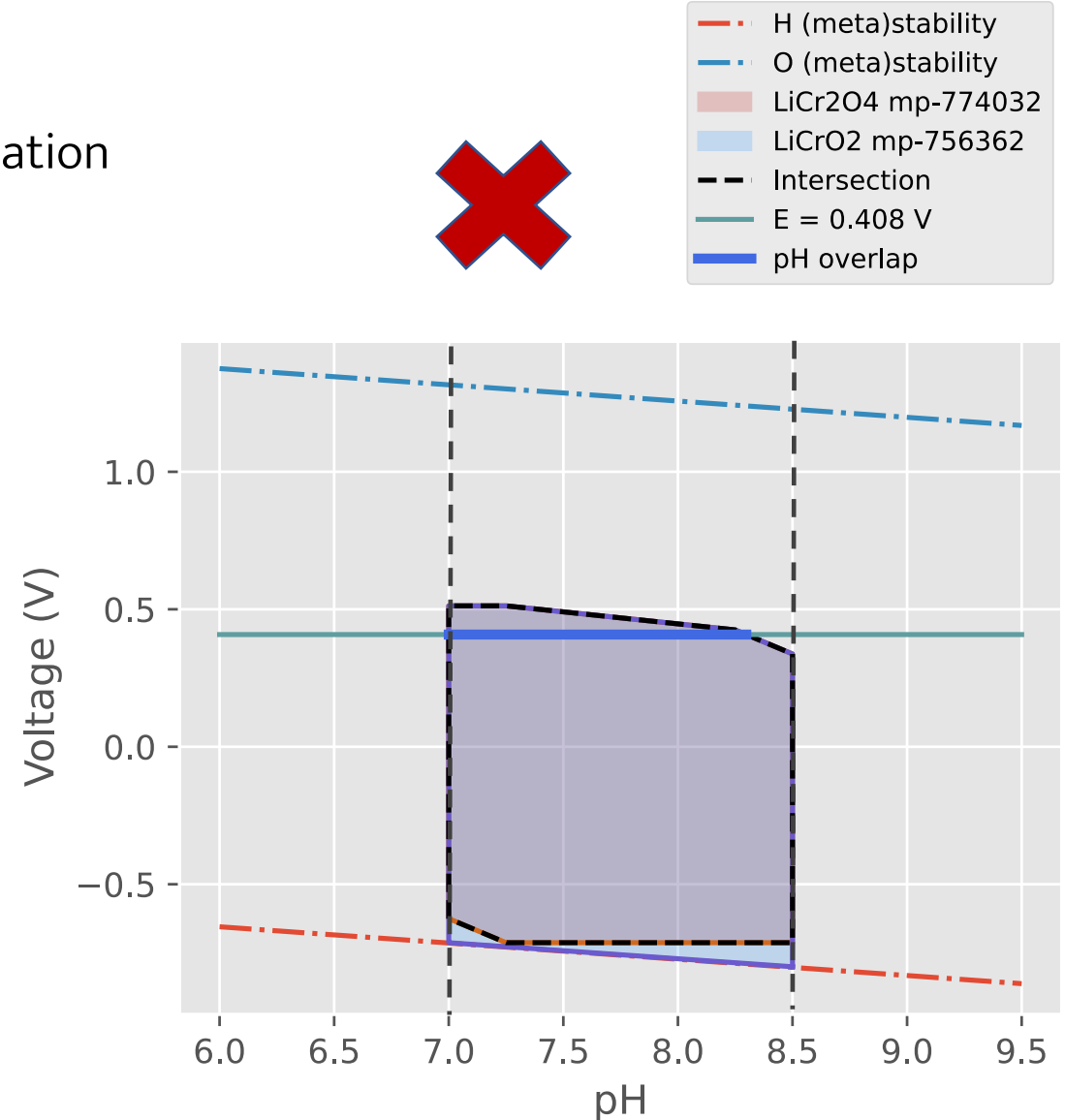
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Metastability scenarios at the intercalation voltage:

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- Electrode not stable throughout pH 7-8.5 at intercalation voltage



Step 3: Intercalation voltages

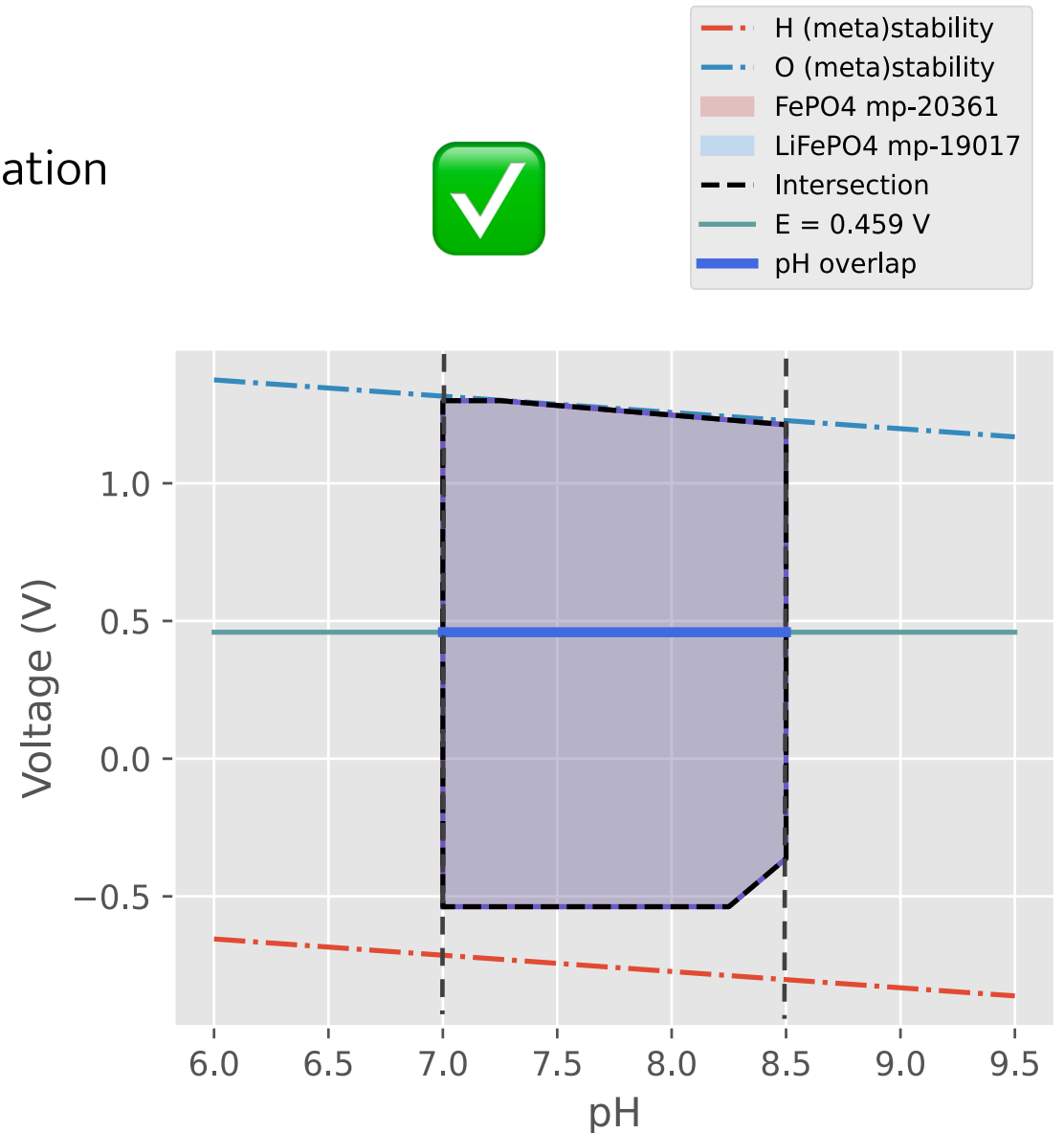
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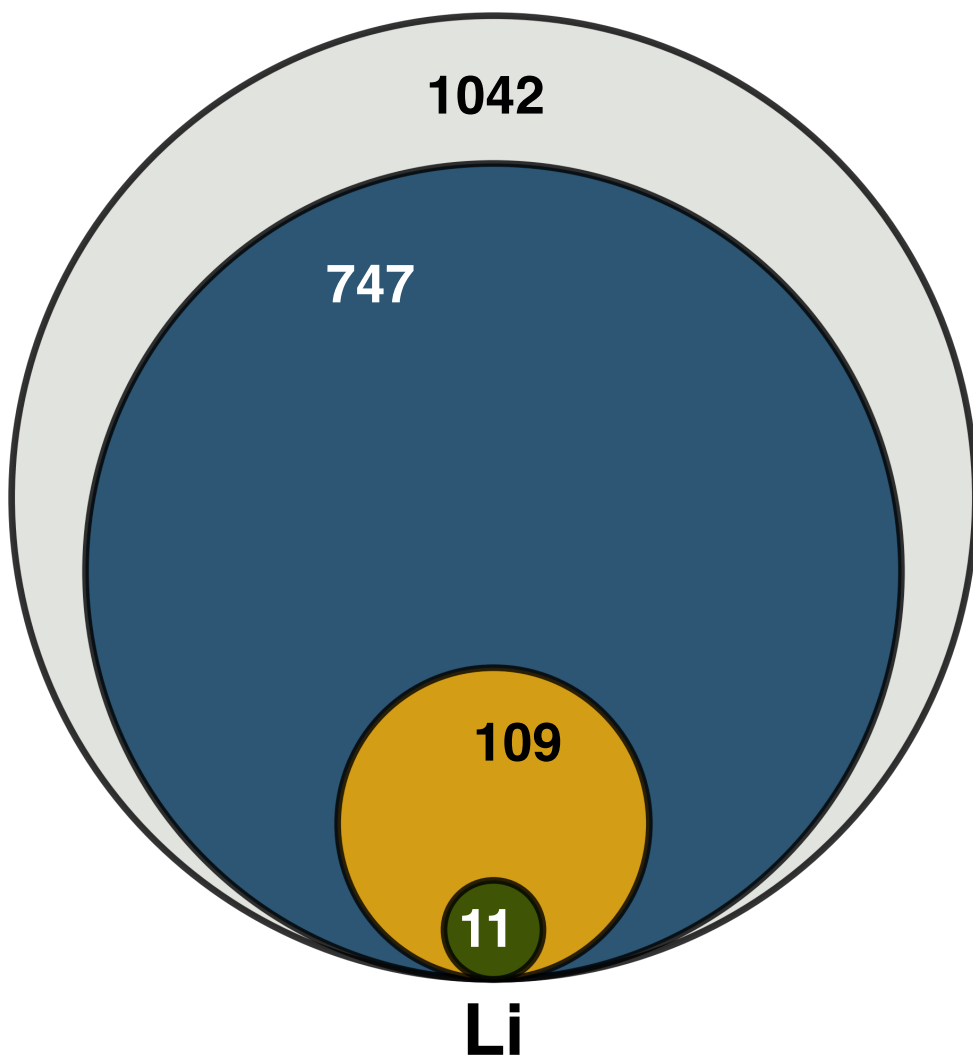


Metastability scenarios at the intercalation voltage:

- Voltage beyond seawater stability window
- Electrode not stable throughout pH 7-8.5 at intercalation voltage
- Electrode stable throughout pH 7-8.5 and occupies > 80% area of seawater stability



Filtered electrodes

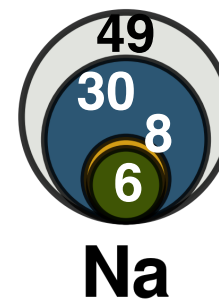
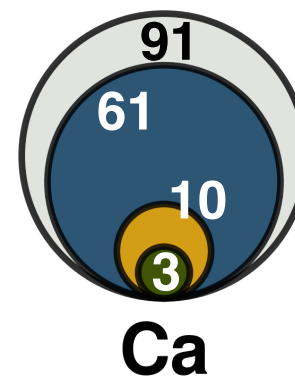
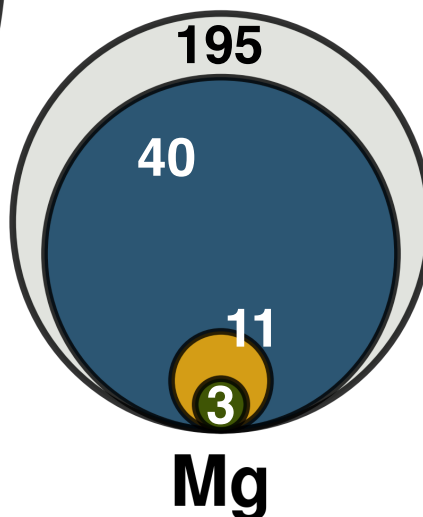


Metastable at
intercalation voltage

Metastable throughout
pH 7-8.5

Metastability area $\geq 80\%$

At least one experimental
(dis)charged electrode



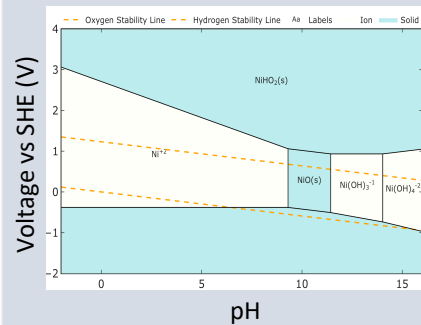
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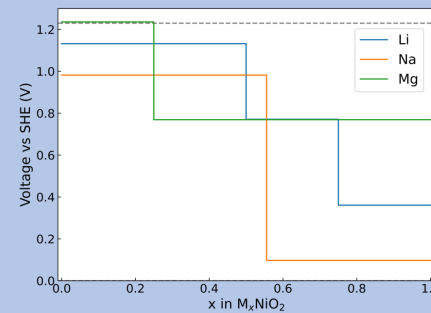
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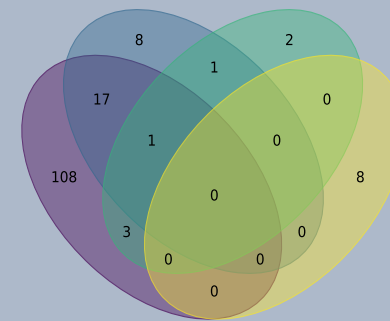
Step 3

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Step 4

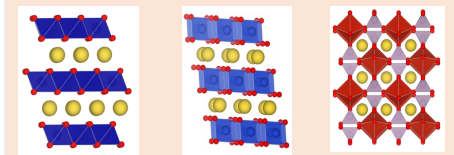
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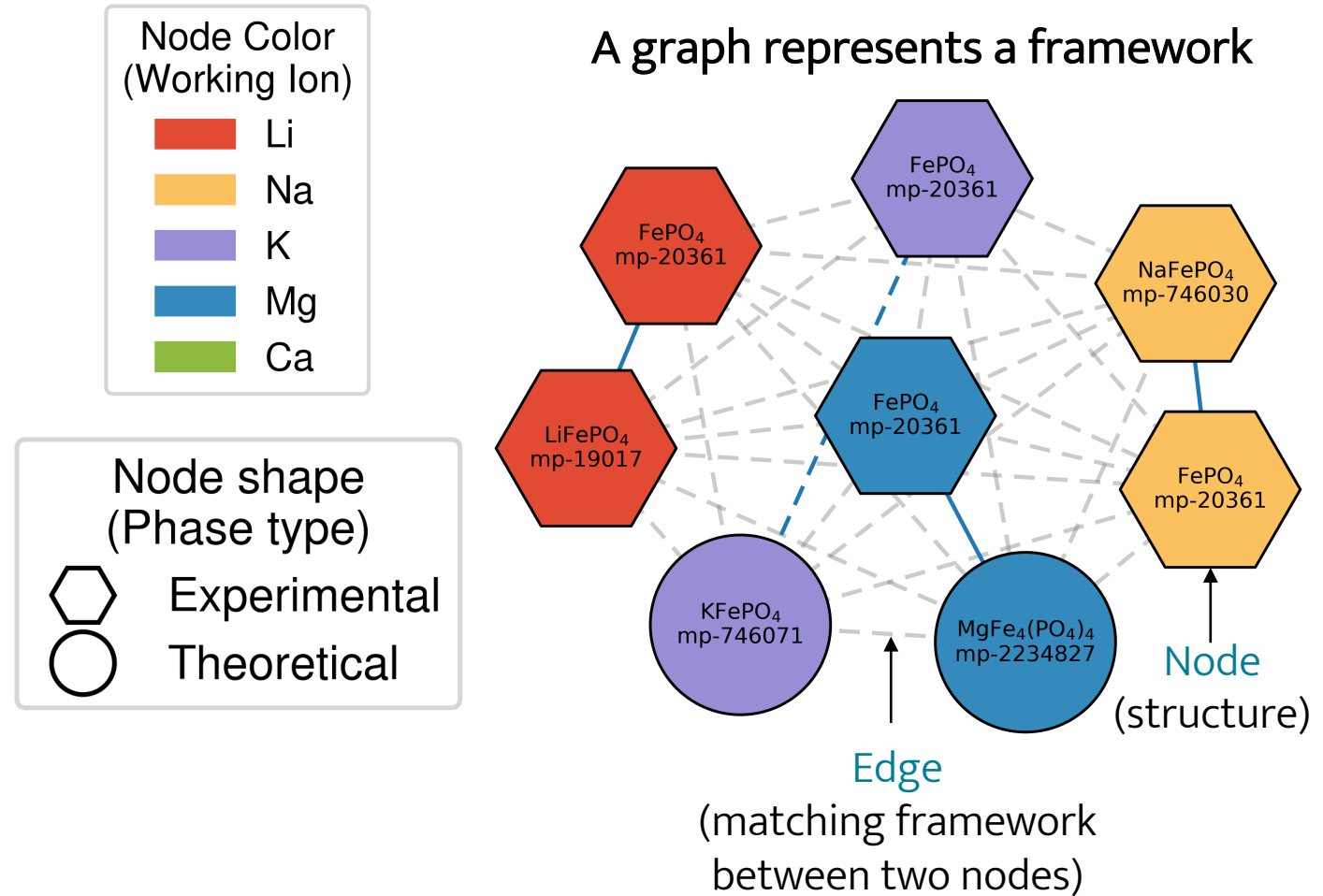
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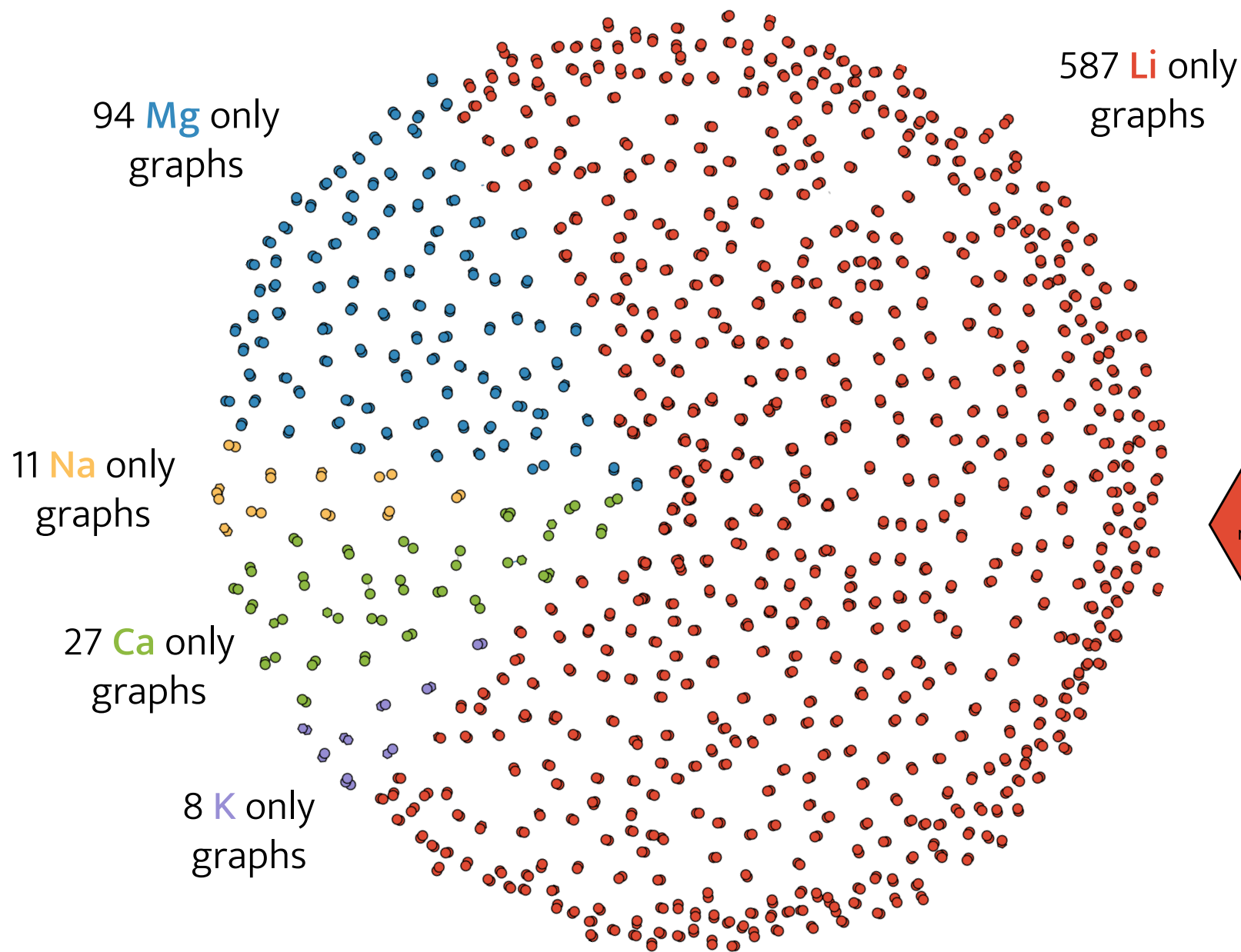
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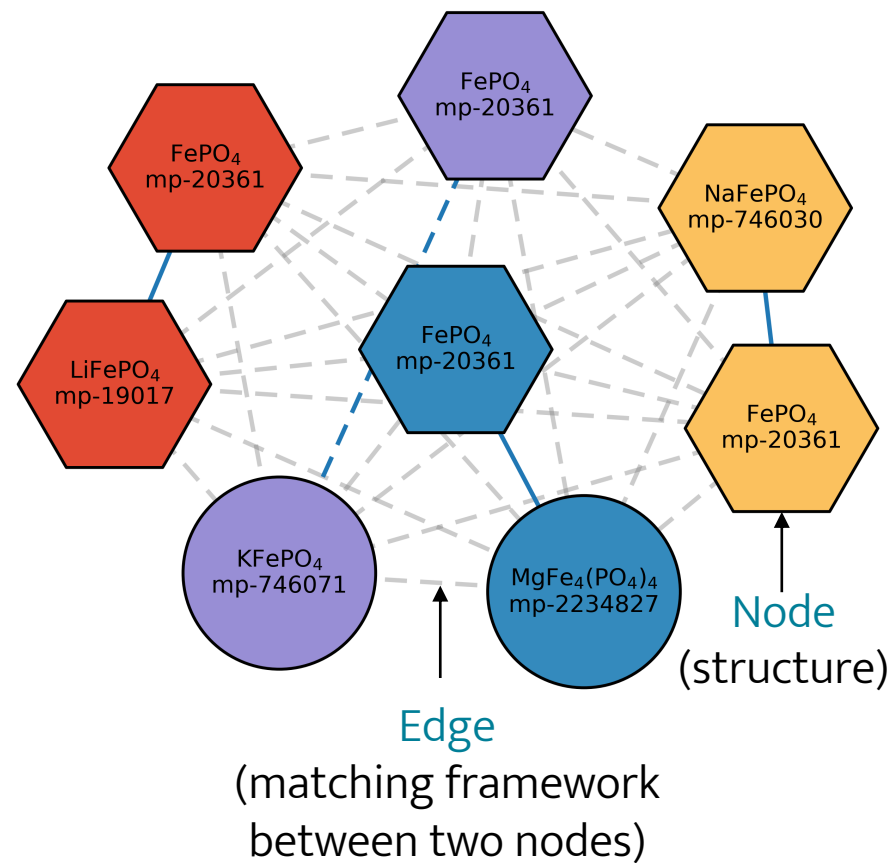
Step-4a Ion selective frameworks



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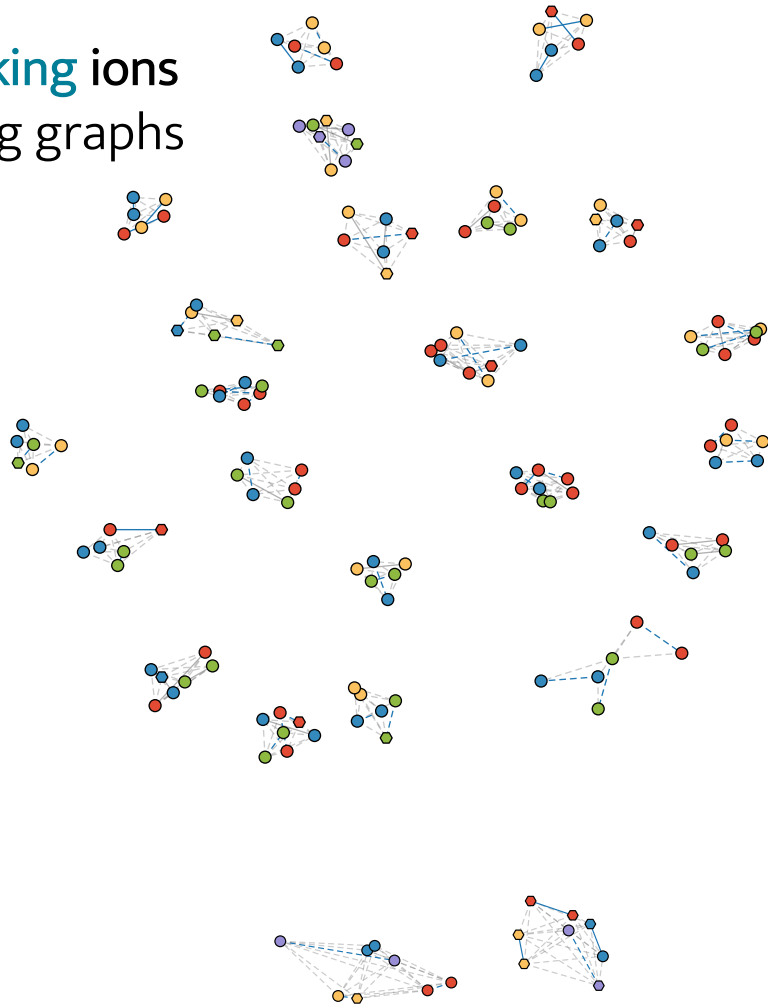


A graph represents a framework

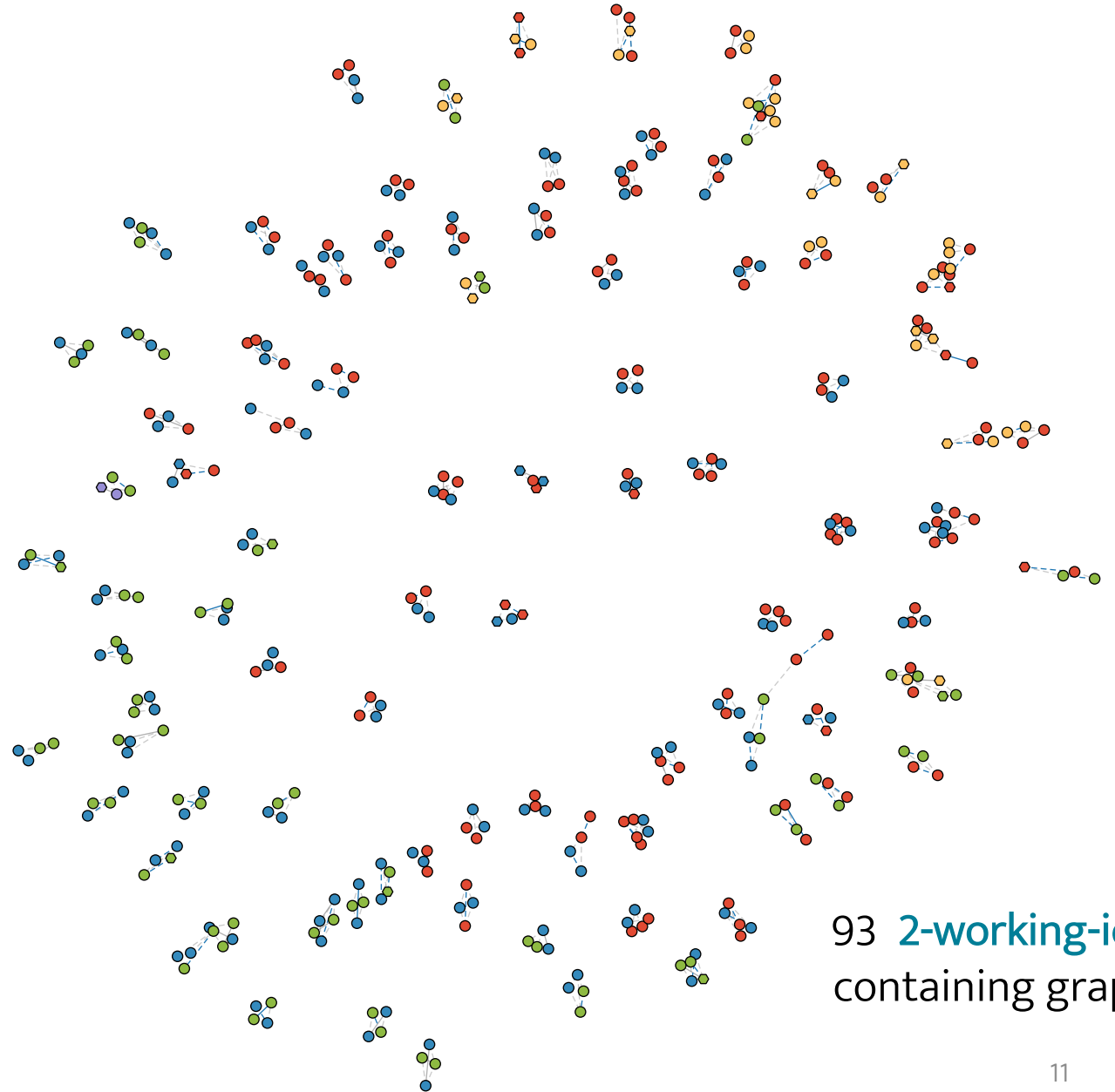
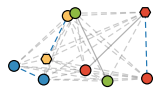


Step-4b Multiple-ions intercalating frameworks

22 **3-working** ions
containing graphs



3 **4-working** ions
containing graphs



93 **2-working-ions**
containing graphs

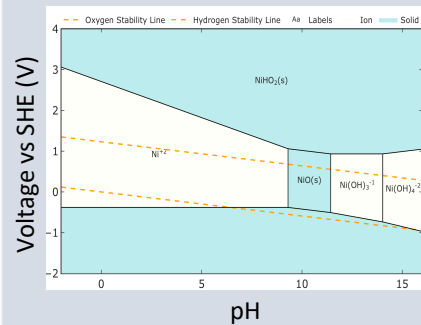
Step 1

Query first-principles cathodes' data across ions



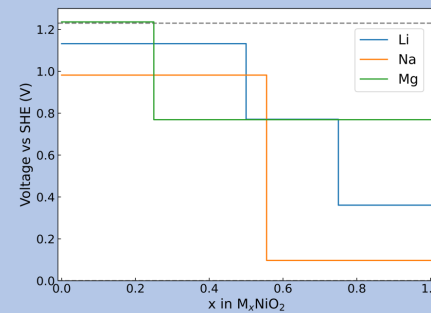
Step 2

Determine aqueous stability of the cathodes



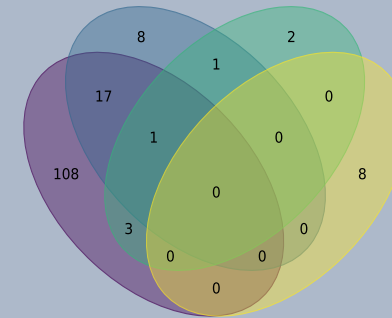
Step 3

Calculate intercalation voltage



Step 4

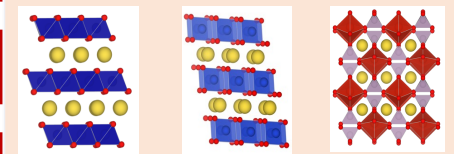
Compare structures across ions



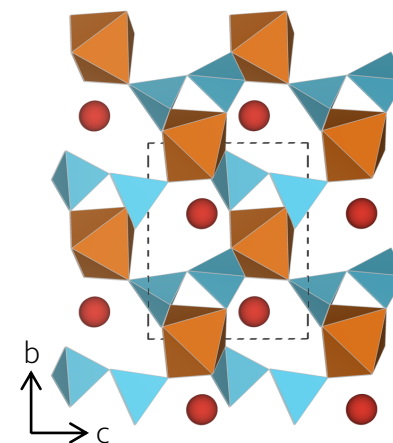
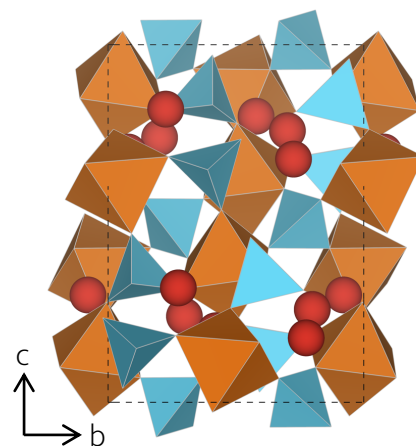
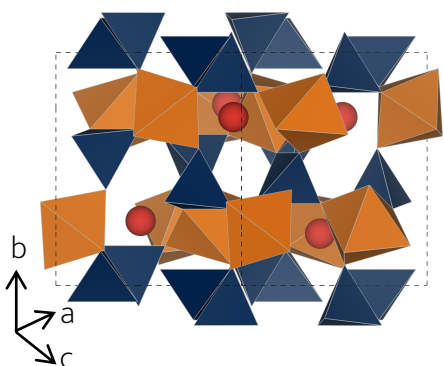
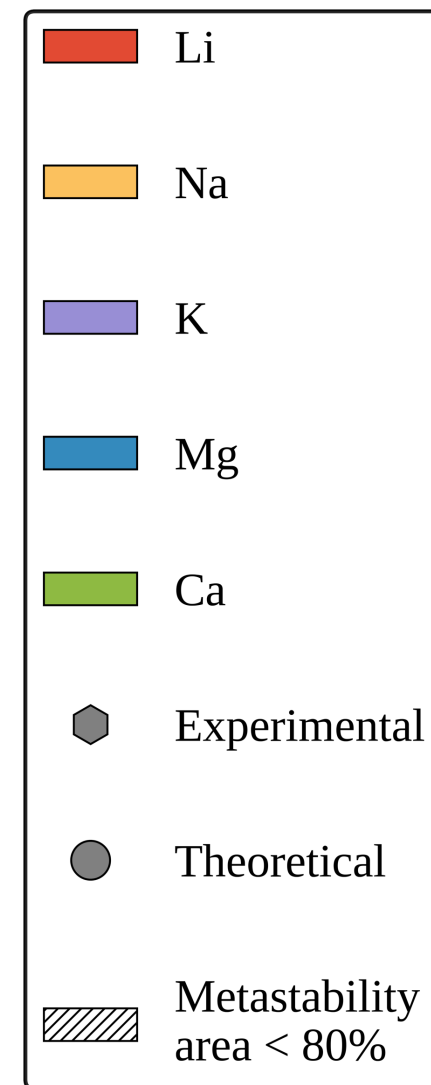
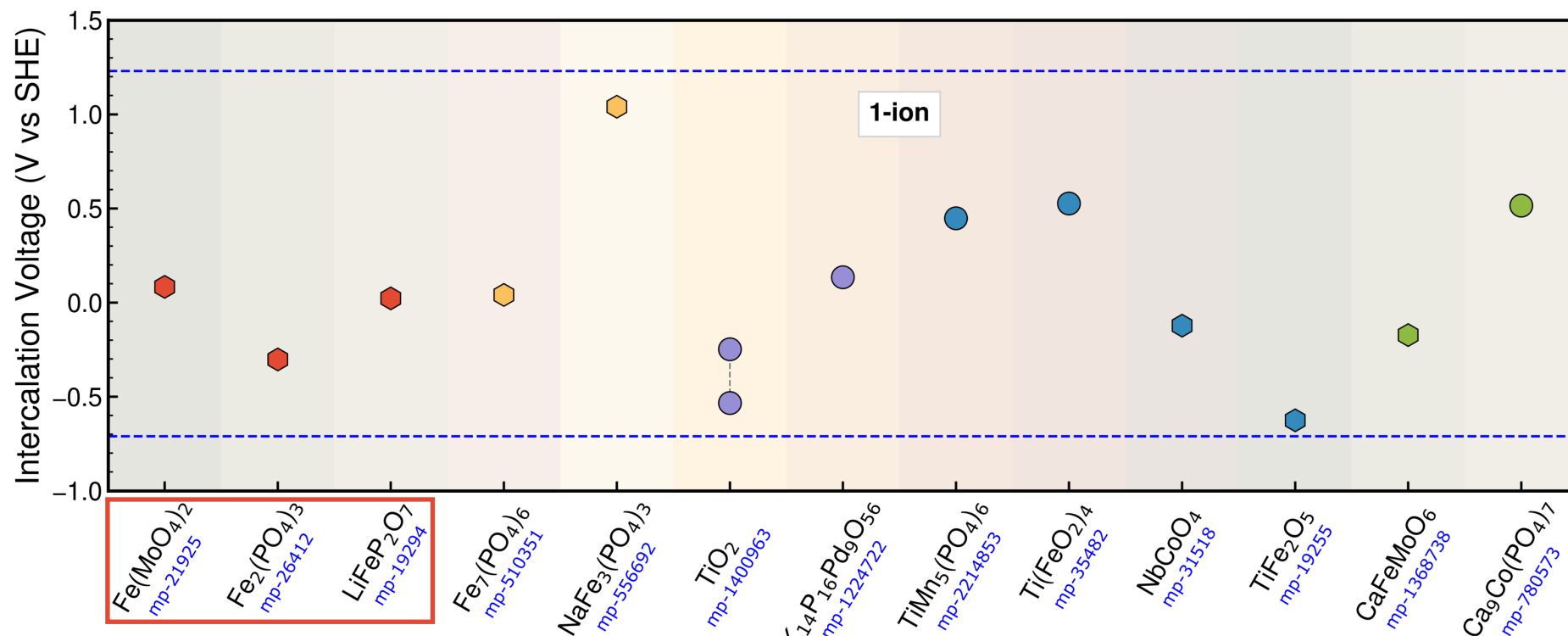
Results

Li-capturing electrodes
(Selective-ion extraction)

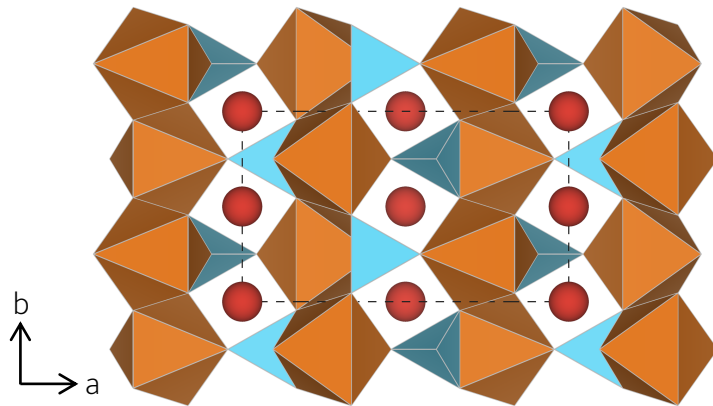
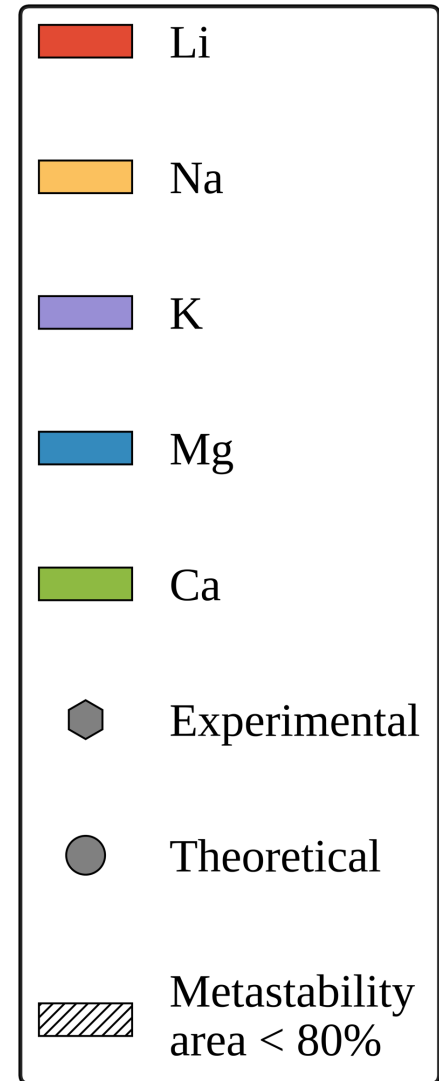
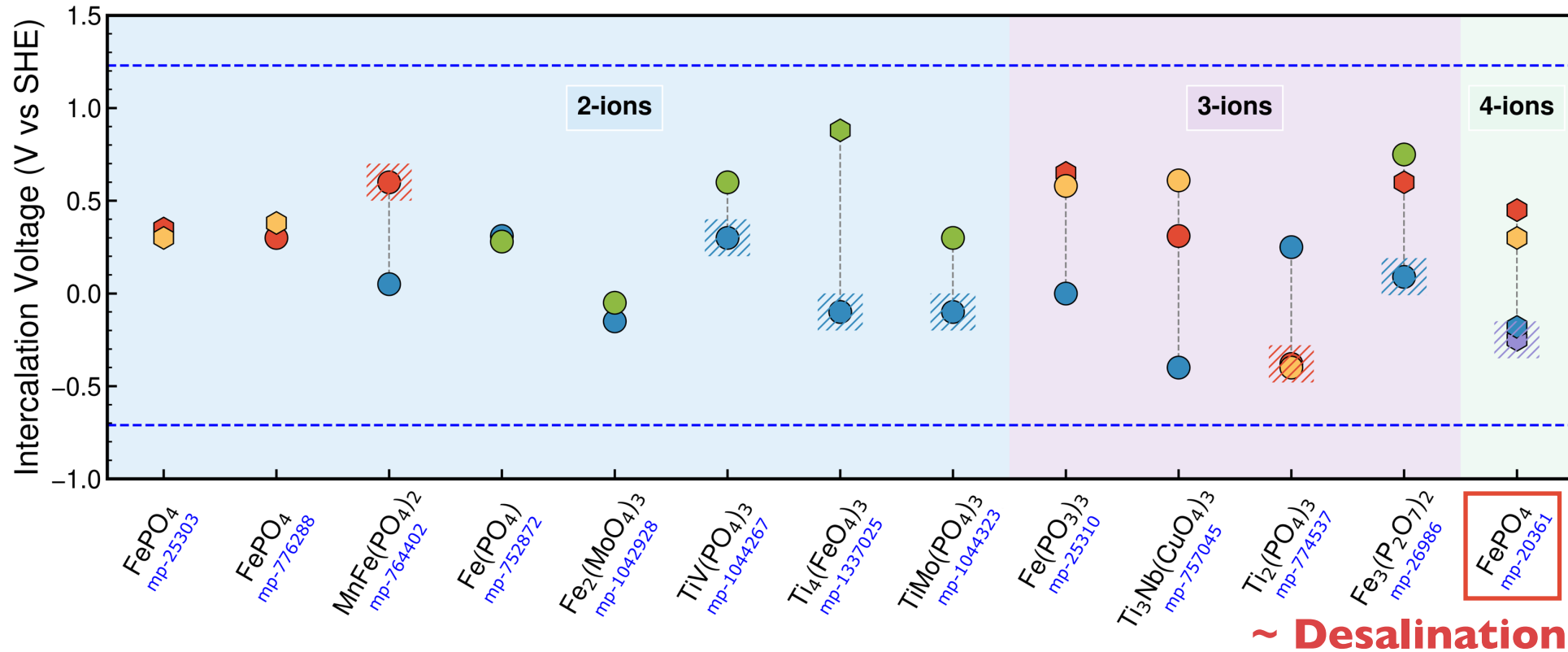
All-ions-capturing electrodes
(Desalination)



Single-ion-selective frameworks



Multi-ions-selective frameworks

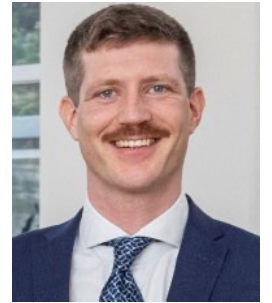


Conclusions and Acknowledgement

- Objective: identify novel electrodes for Li^+ recovery and desalination
- Developed a high-throughput workflow to
 - Evaluate aqueous (meta)stability of electrodes
 - Calculate voltages
 - Compare electrode frameworks
- Identified novel electrodes for:
 - Li extraction: LiFeP_2O_7 , $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ and $\text{Fe}_2(\text{MoO}_4)_3$
 - Desalination: FePO_4

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To be submitted:

High-throughput screening of intercalation electrodes for electrochemical ion-capture and desalination

Sougat Purohit¹, Andreas Kuhlmann², Marten Huck², Hans-Georg Steinrück², Sai Gautam Gopalakrishnan^{1,3}

¹Department of Materials Engineering, Indian Institute of Science, Bengaluru, India,

²Institute for a Sustainable Hydrogen Economy (INW), Forschungszentrum Jülich GmbH, Jülich, Germany

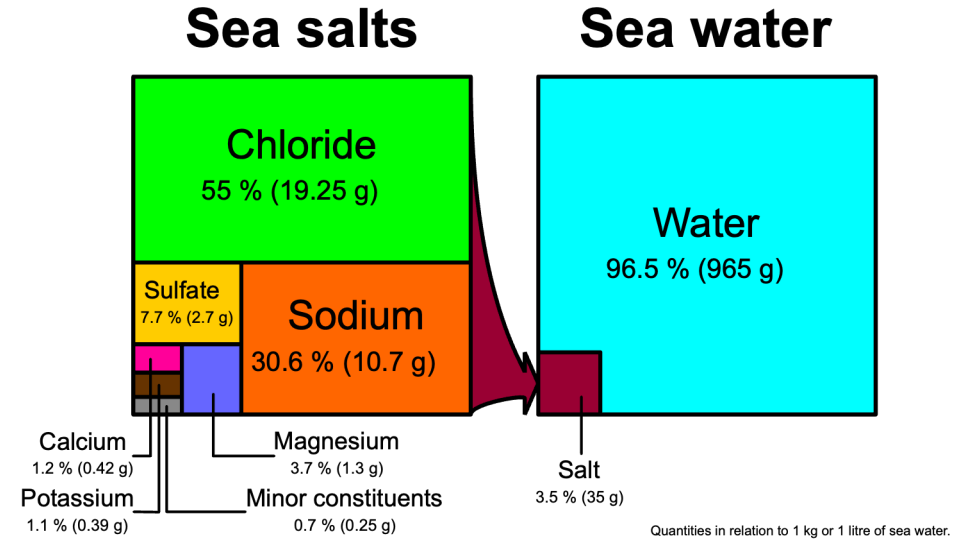
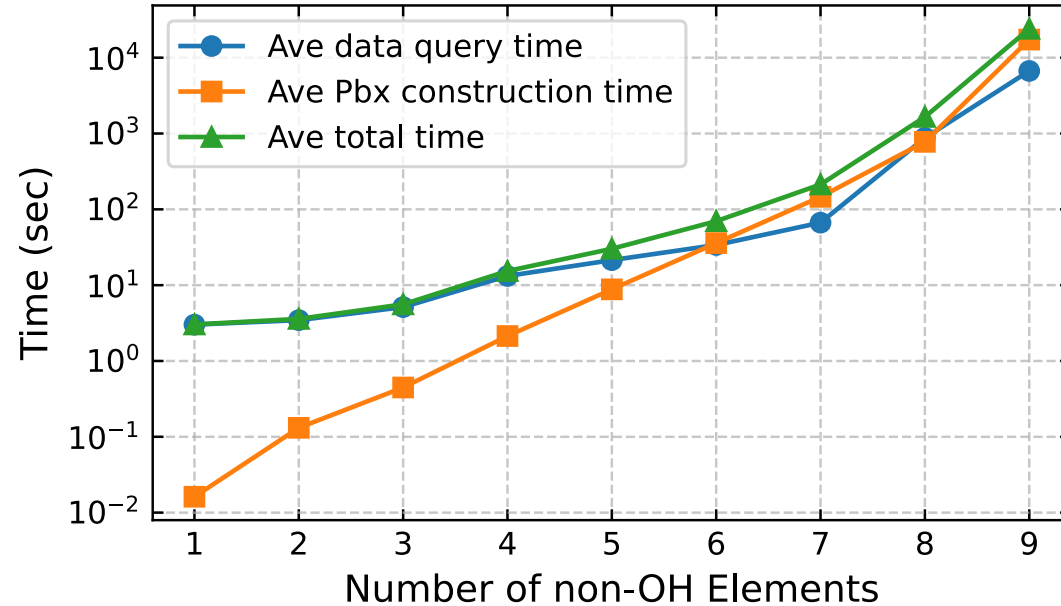
email: sougatp@iisc.ac.in

Group-webiste: <https://sai-mat-group.github.io/>

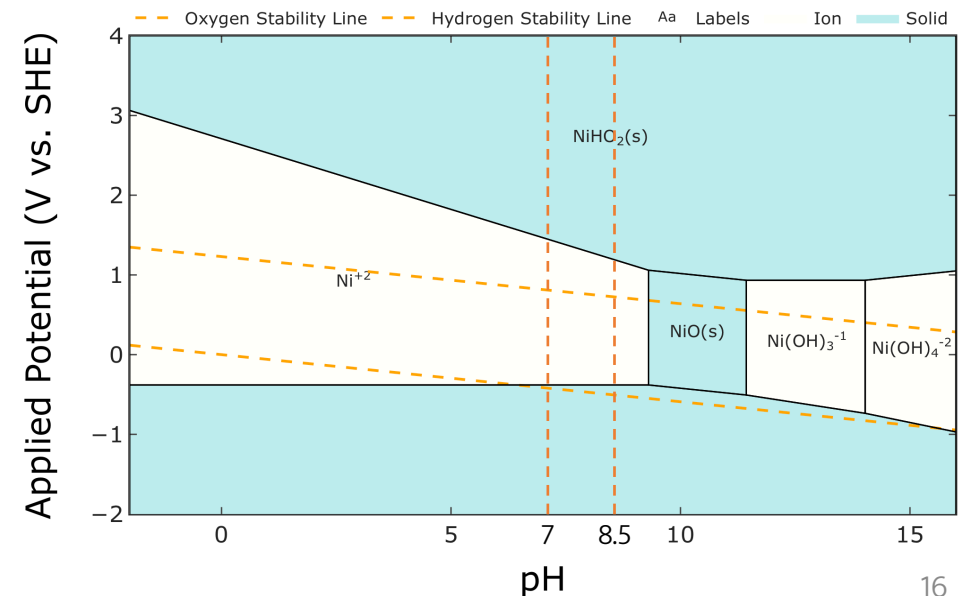


Constructing Seawater Pourbaix Diagrams

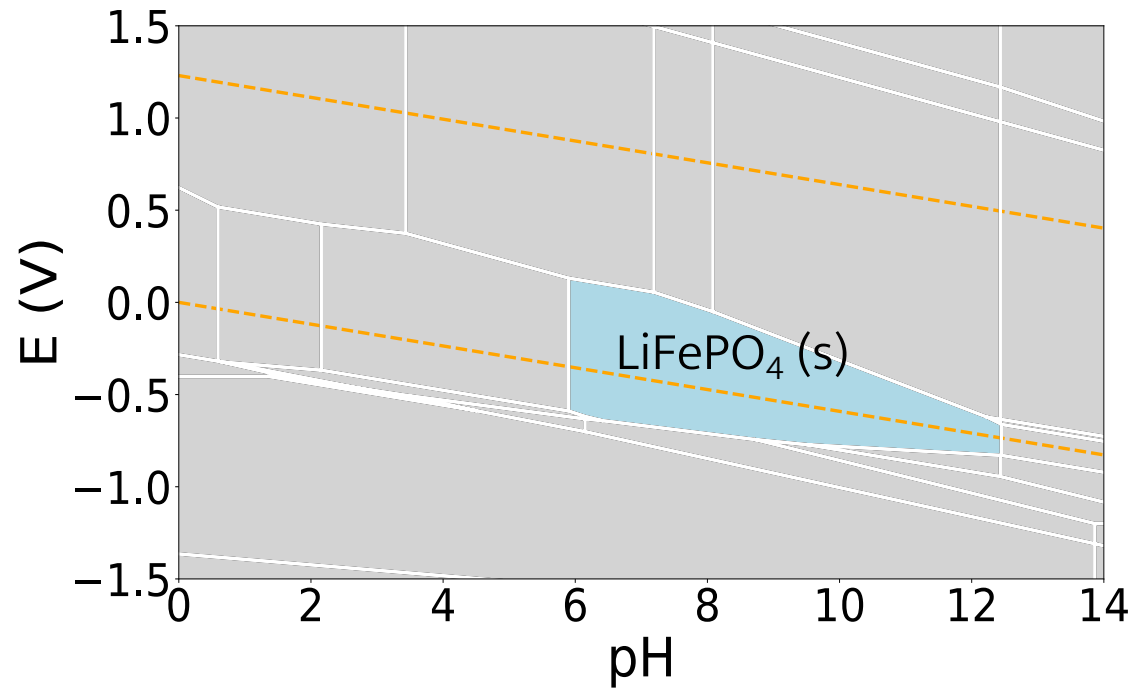
- We consider average seawater concentrations for the aqueous medium



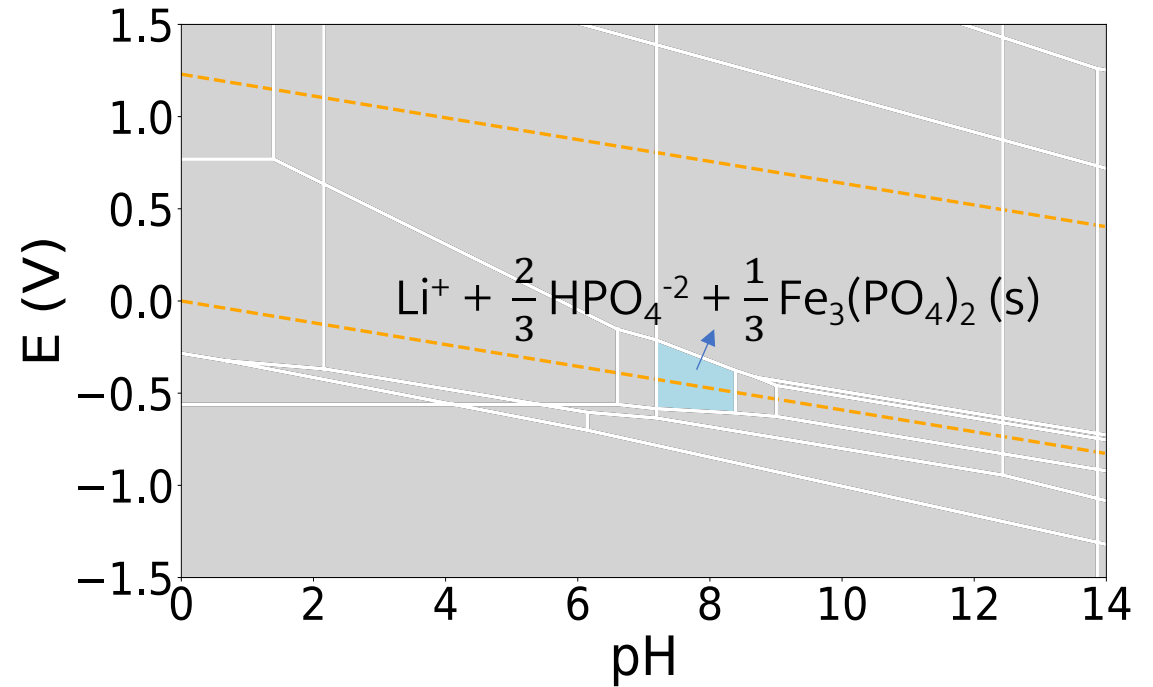
- Seawater Pourbaix Diagram approximation:
 - Ψ remains unmodified
 - Extended water metastability window of 2 V
 - pH range of 7 - 8.5
 - Only Cl^- , Na^+ , Mg^{+2} and SO_4^{-2} added to all systems
 - K^+ and Ca^{+2} added only to K, Ca-ion cathodes
 - Any other ions have 10^{-6} M concentrations



Aqueous composition affects phase stability



$[\text{Li}] = 0.75\text{M}$ $[\text{Fe}] = 0.25\text{M}$ $[\text{P}] = 0.33\text{M}$

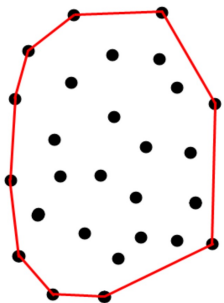
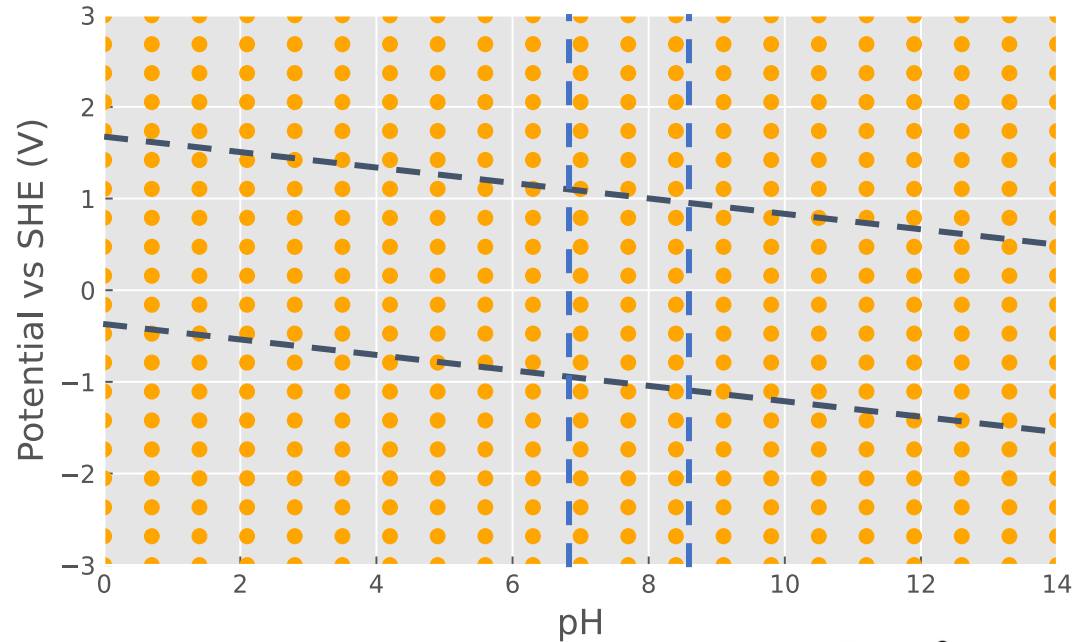


$[\text{Li}] = [\text{Fe}] = [\text{P}] = 10^{-6} \text{ M}$

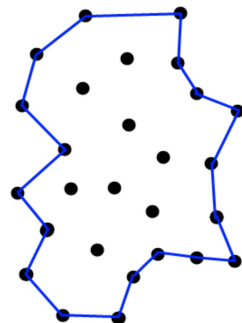
Solid phase stability = f (aqueous composition)

Checking metastability at the intercalation voltage

1. Store the area of metastability instead of booleans

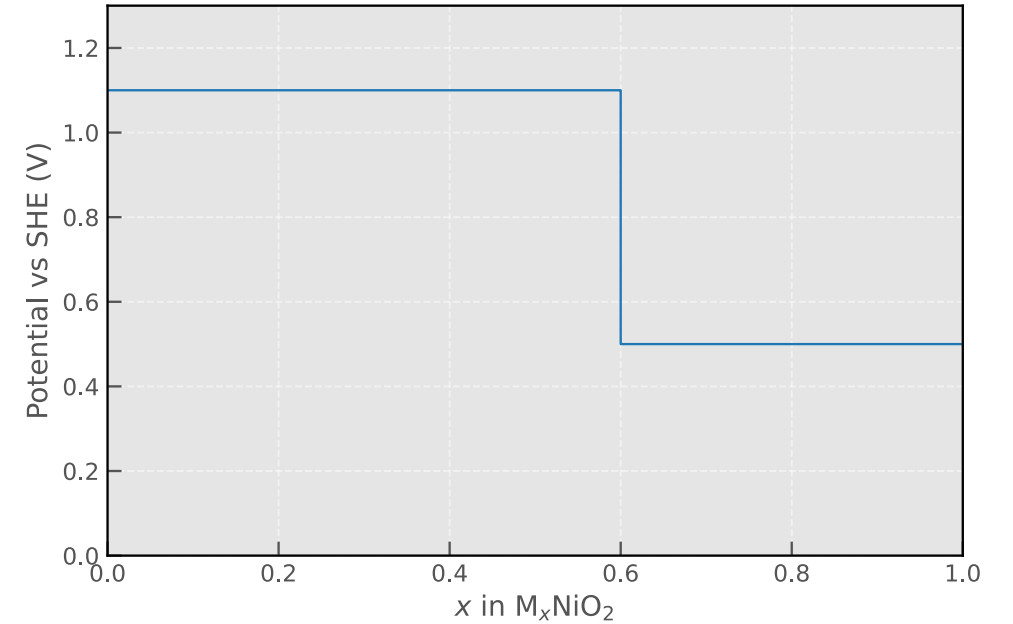


Convex hull of points



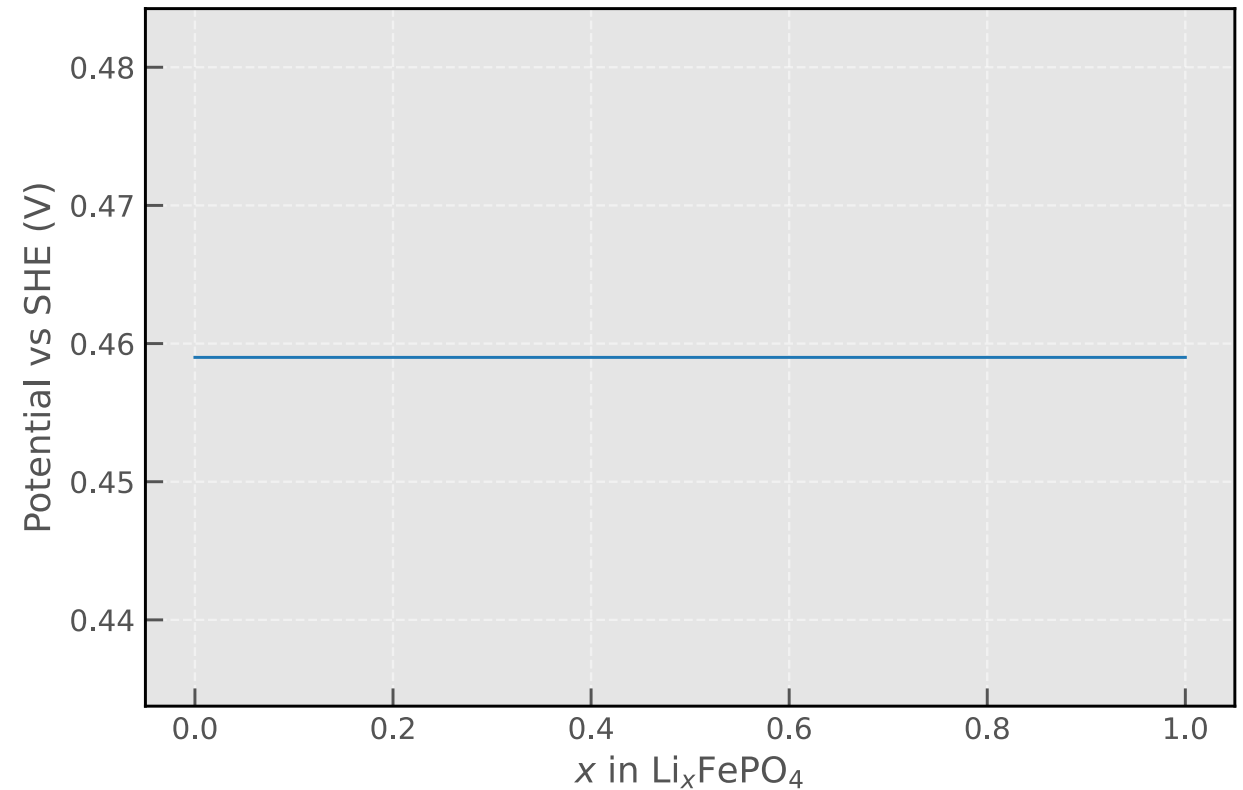
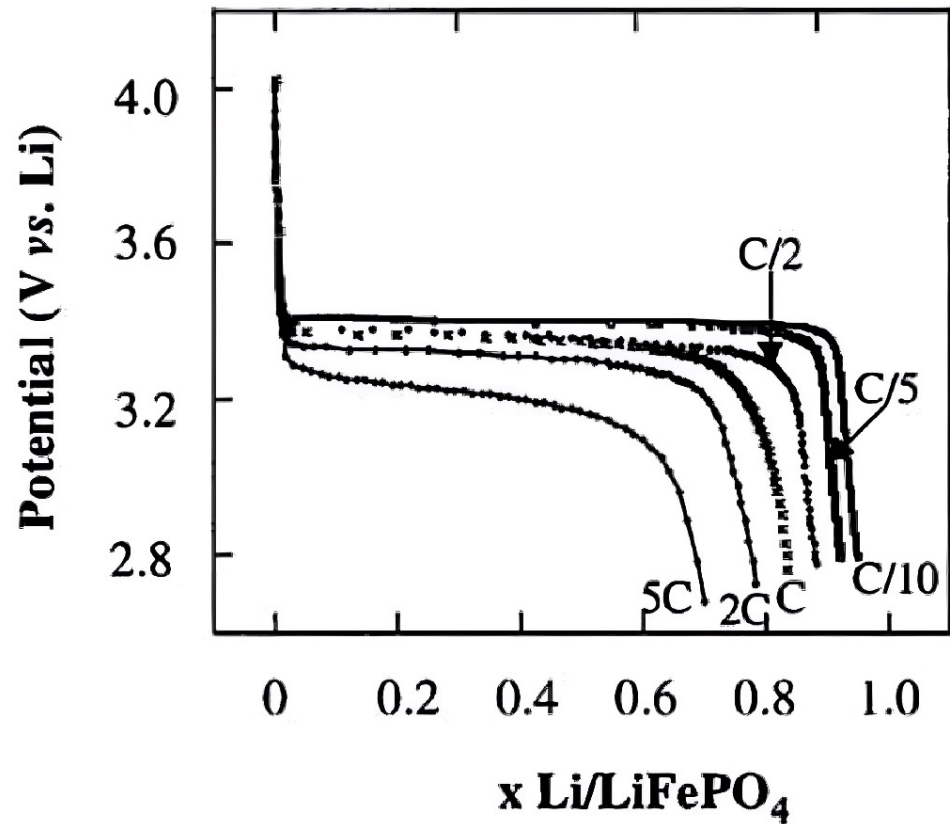
Concave hull of points

2. Calculate all possible voltage plateaus from the queried frameworks



3. Check whether both the phases contributing to a plateau are metastable at that voltage

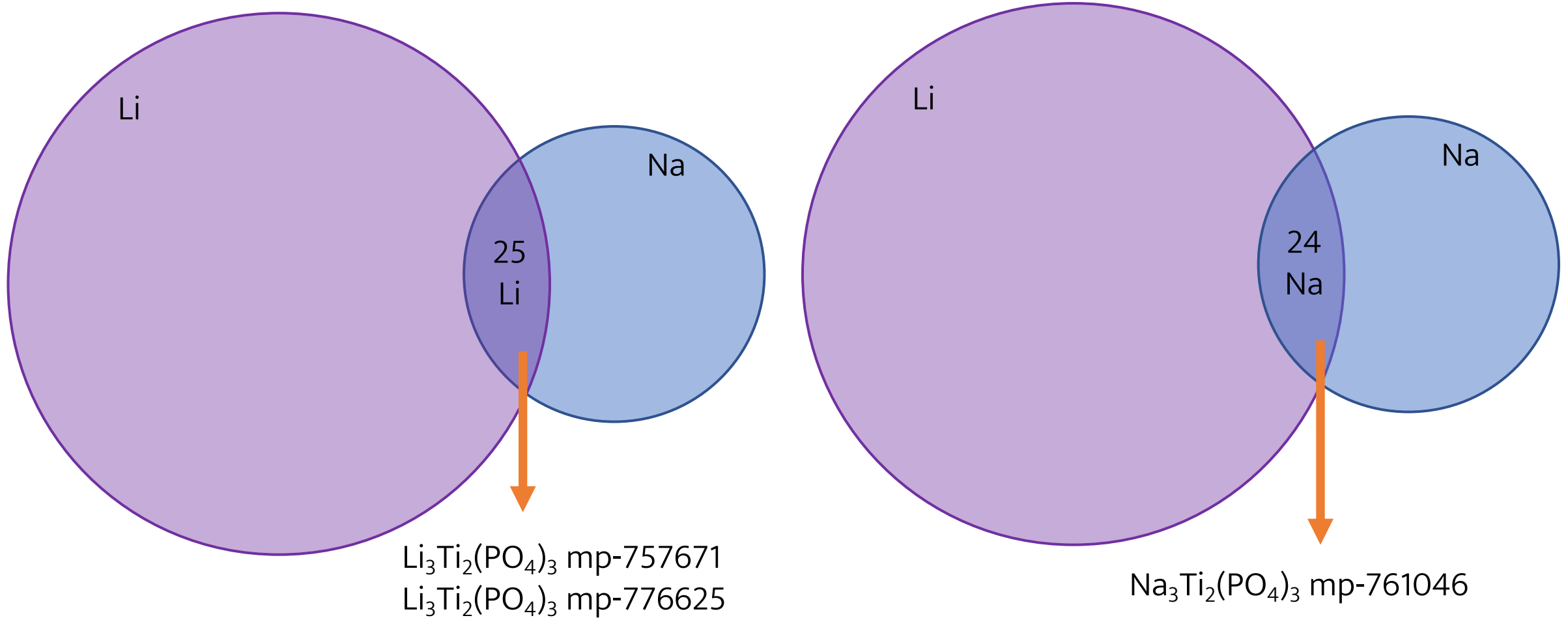
Intercalation voltage from first-principles data



Approximations:

1. Open circuit voltage, calculated using the Nernst equation
2. Only topotactic voltages are calculated

Comparing frameworks



Finite tolerances in the StructureMatcher make framework comparisons tricky