ENGE 2026

Simulations **A**nd **I**nformatics of
MATerials Group



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

17th November 2026

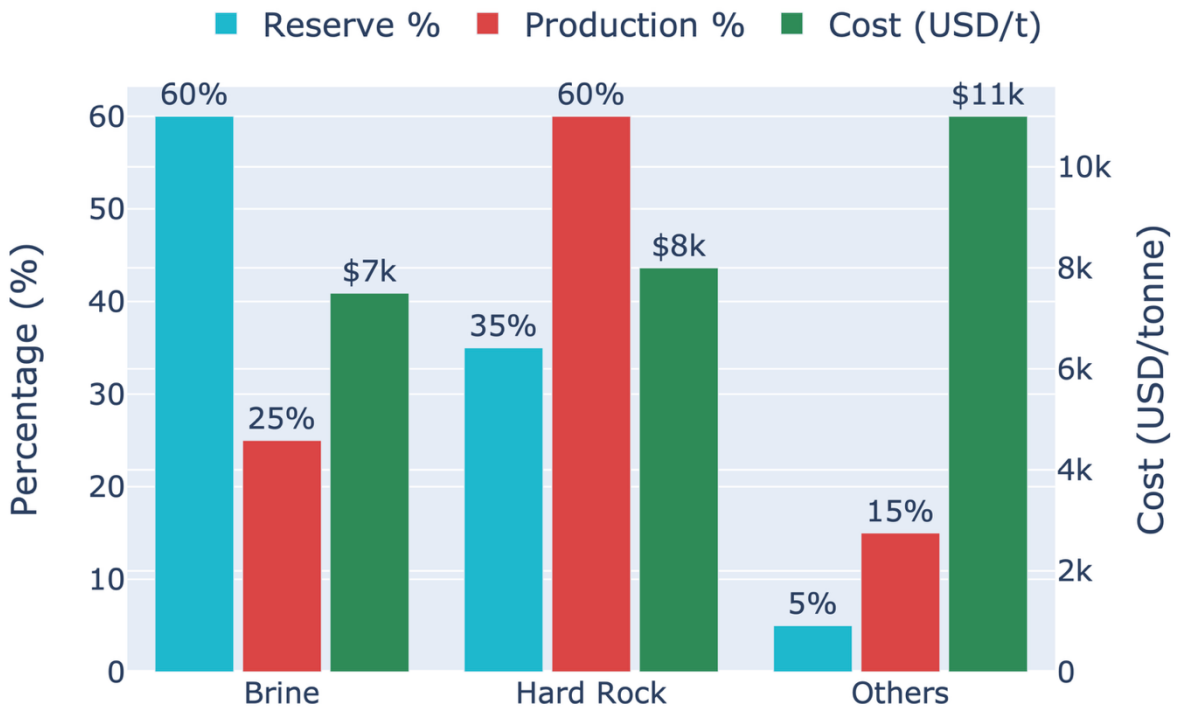
Presenter: **Sougat Purohit**
PhD Scholar, sougatp@iisc.ac.in

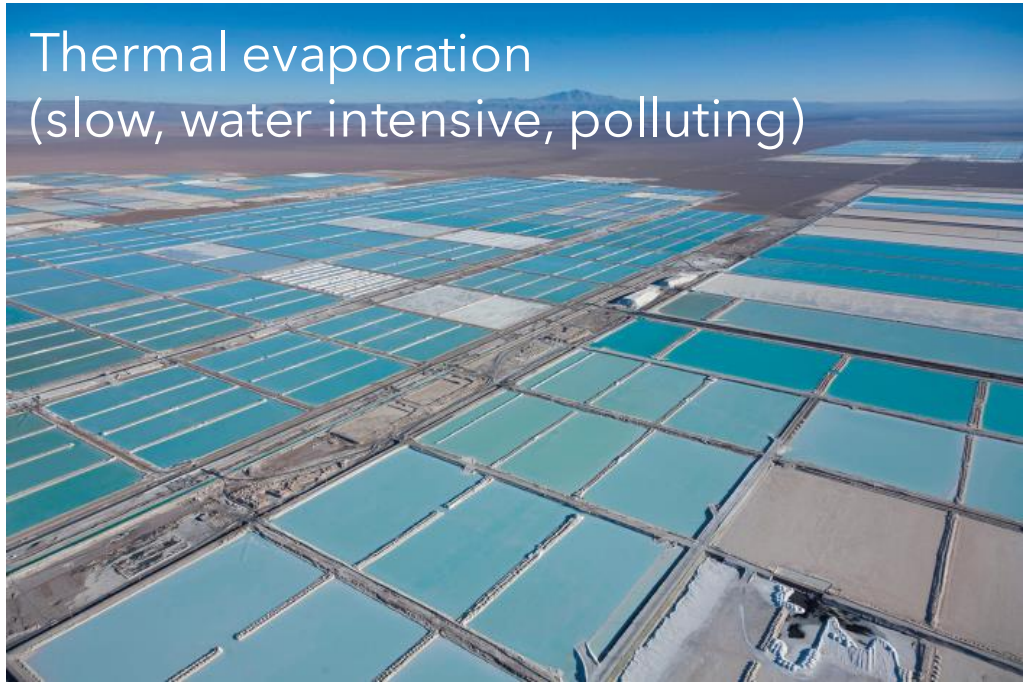
Under the guidance of :
Prof. Sai Gautam Gopalakrishnan



Department of Materials Engineering
Indian Institute of Science, Bengaluru

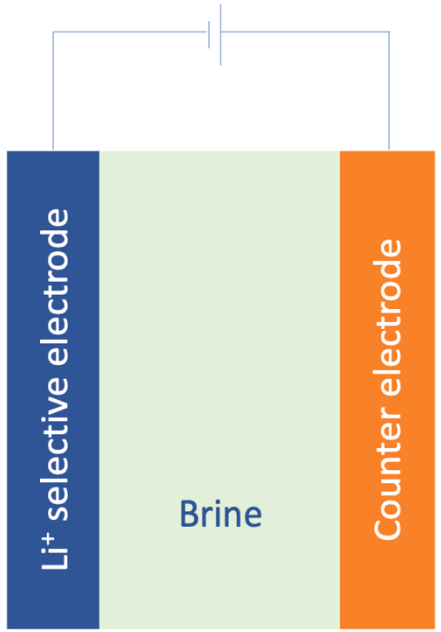
Problem with Li extraction from brines

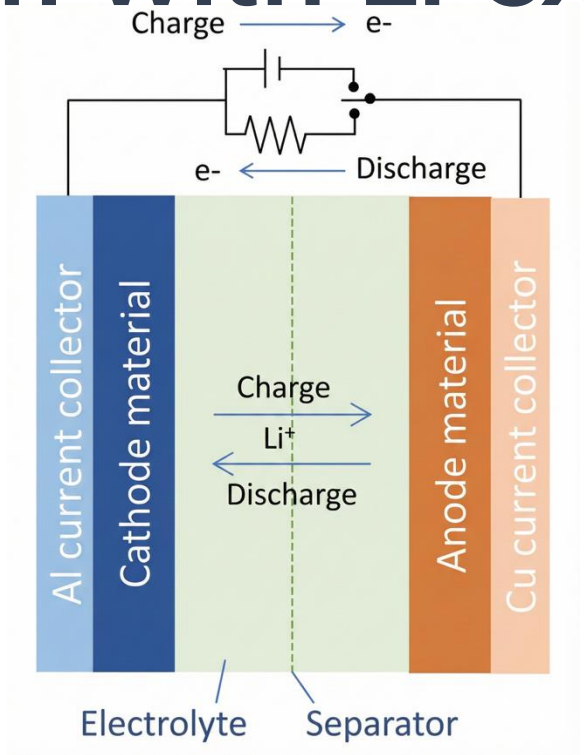


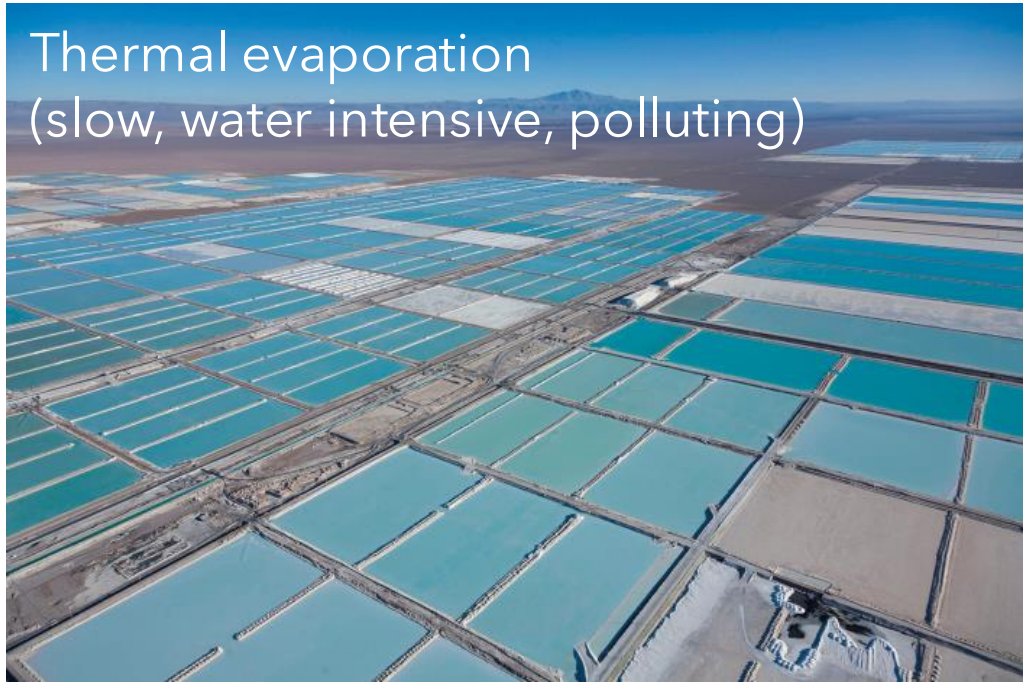


acfequityresearch.com/lithium-extraction-mineral-deposits-vs-salt-brines/
discoveryalert.com.au/news/lithium-prices-2025-production-market-imbalance/

Problem with Li extraction from brines







Electrochemical ion-recovery:

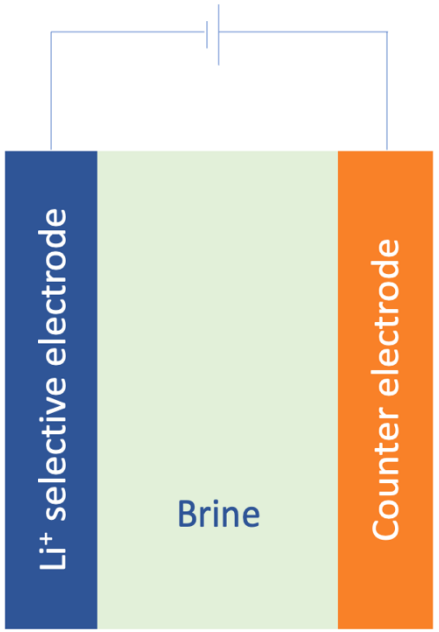
- Faster, low energy consumption
- Handle various brine compositions including **seawater**
- Similar to Li-ion Battery (LIB)

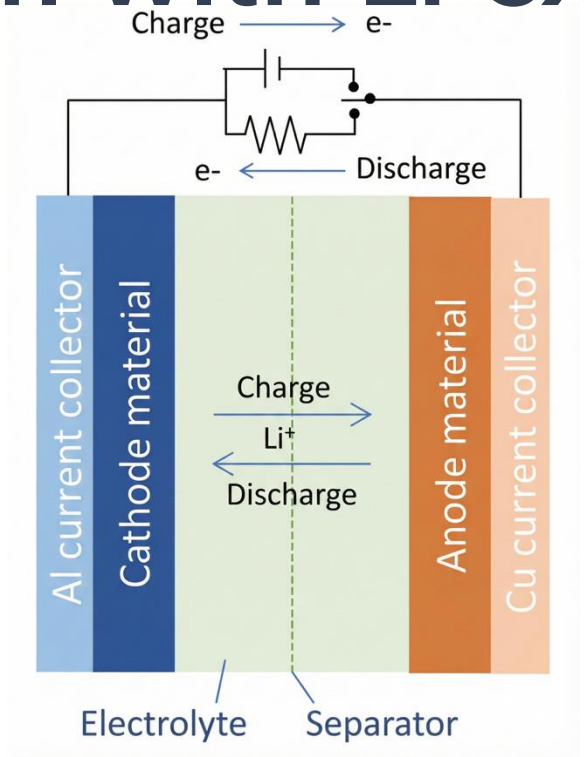
Necessary traits:

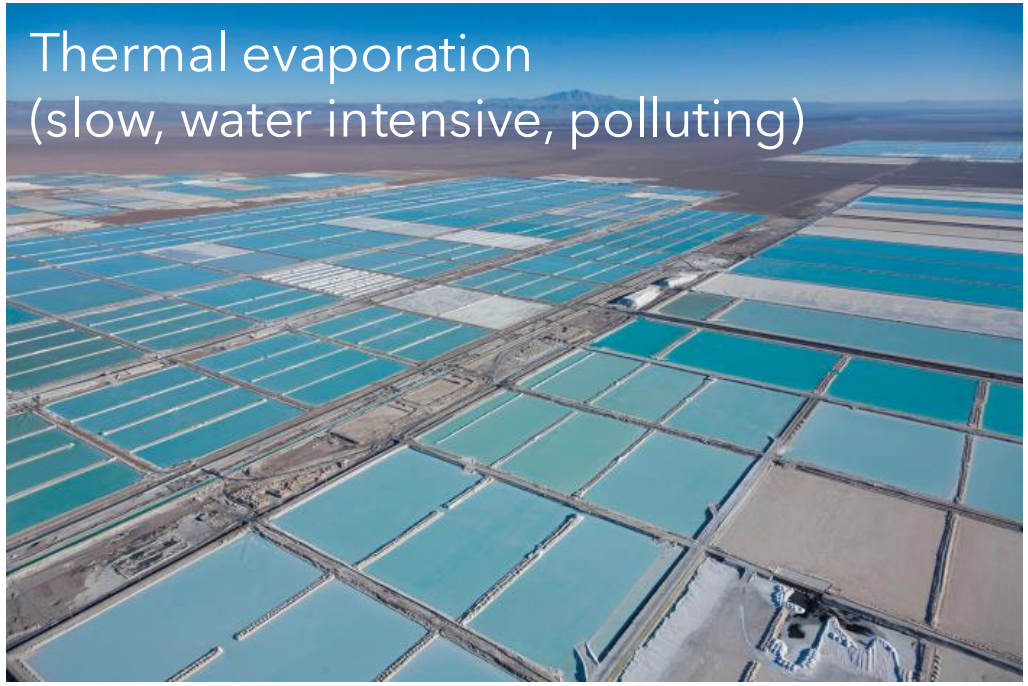
1. Must be **selective towards Li^+** (doesn't intercalate Na^+ K^+ Ca^{+2} Mg^{+2})
2. Must be **stable in the brine**
3. Multi-ions intercalating electrodes: **desalination**

Barranco, C. Nat Sustain 2022, 5, 730 Battistel et. al. Adv. Mater. 2020, 32, 1905440 Xiong et. al. Matter 2022, 5, 1760-1791

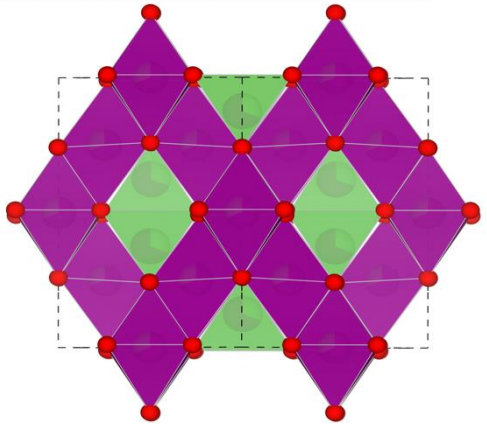
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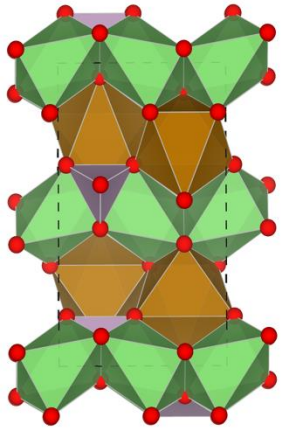




State of the art

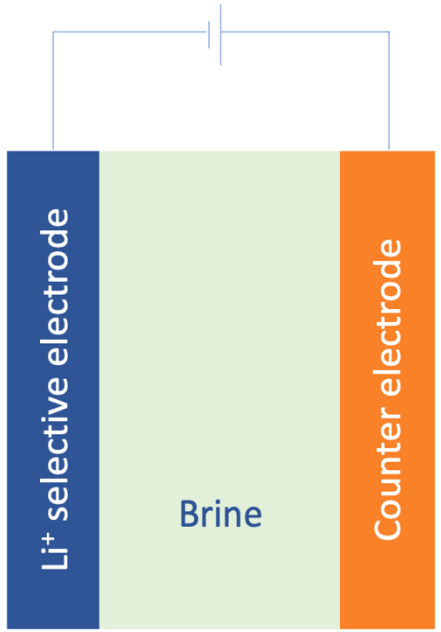


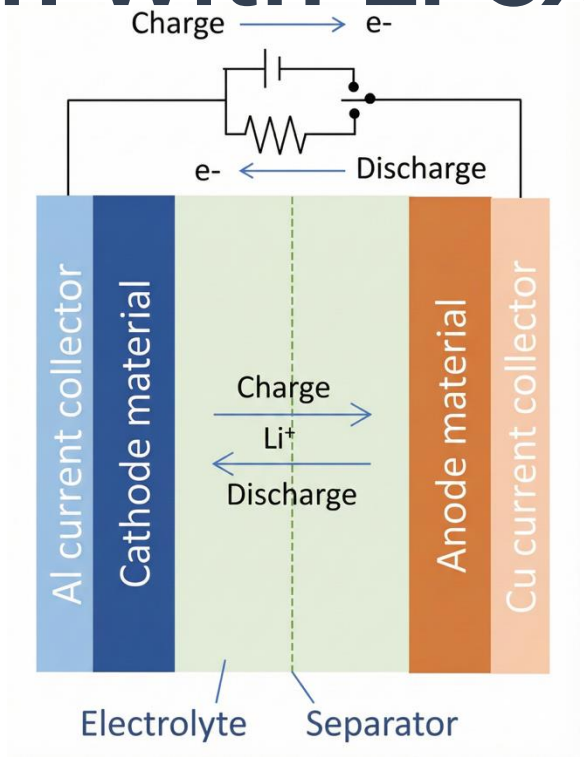
Spinel $LiMn_2O_4$

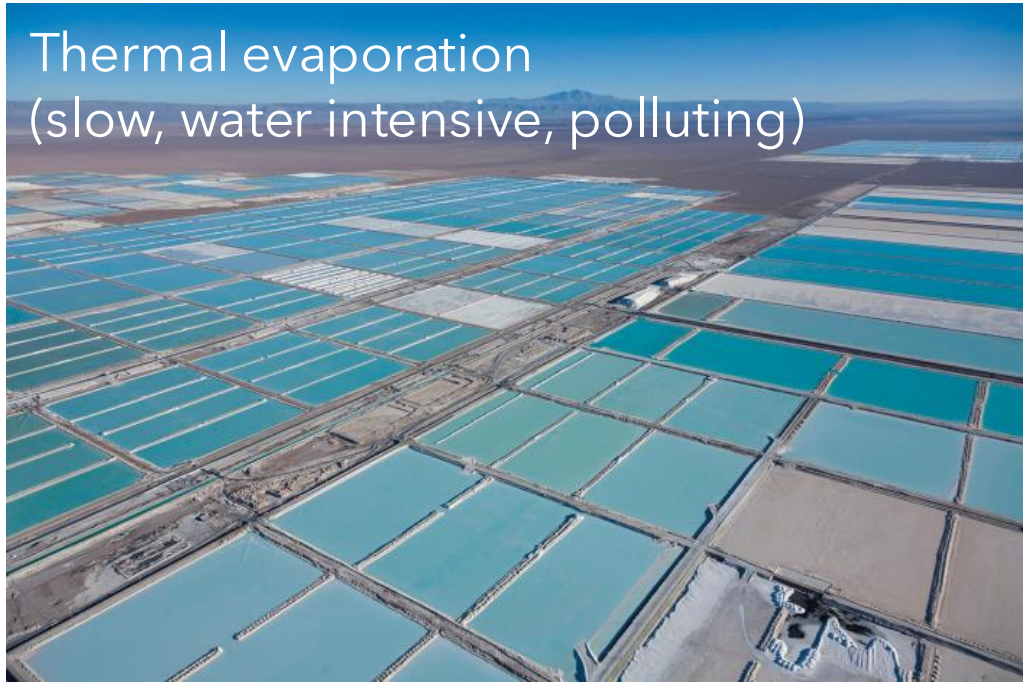


Olivine $LiFePO_4$

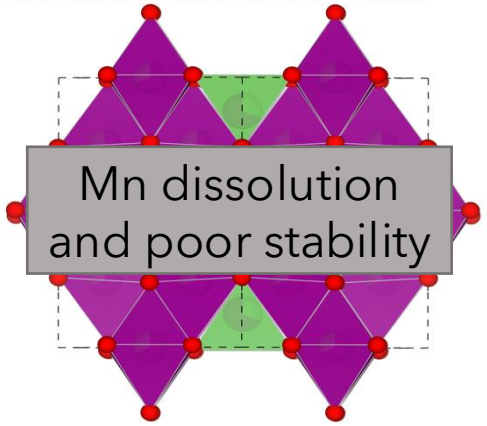
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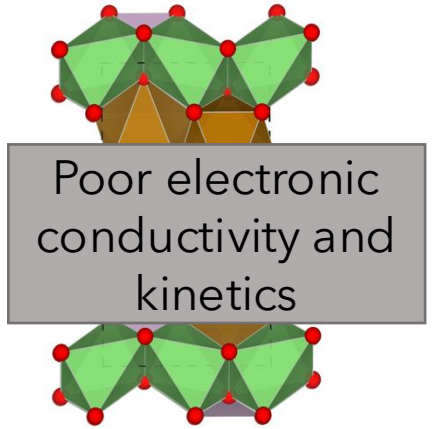




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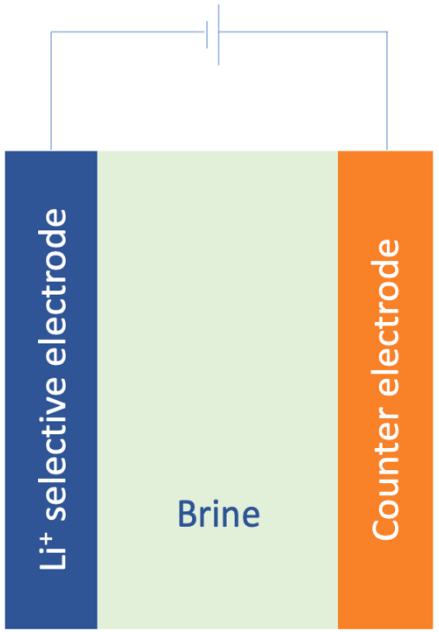


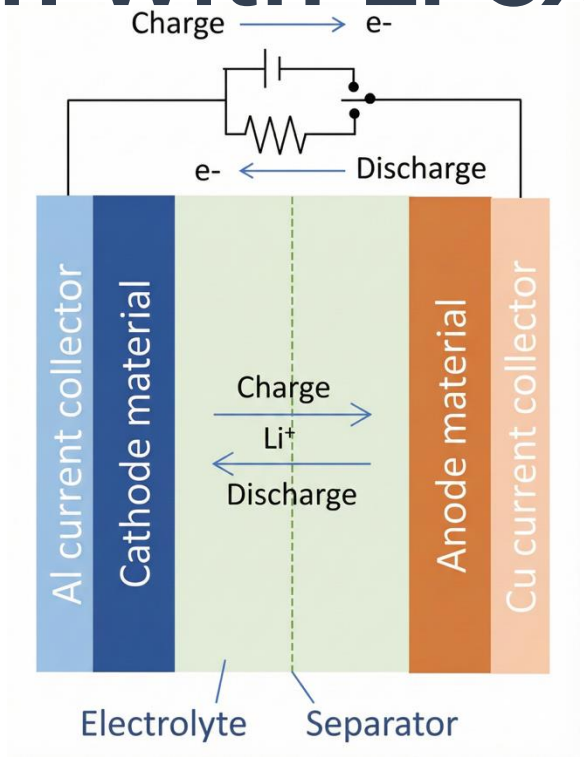
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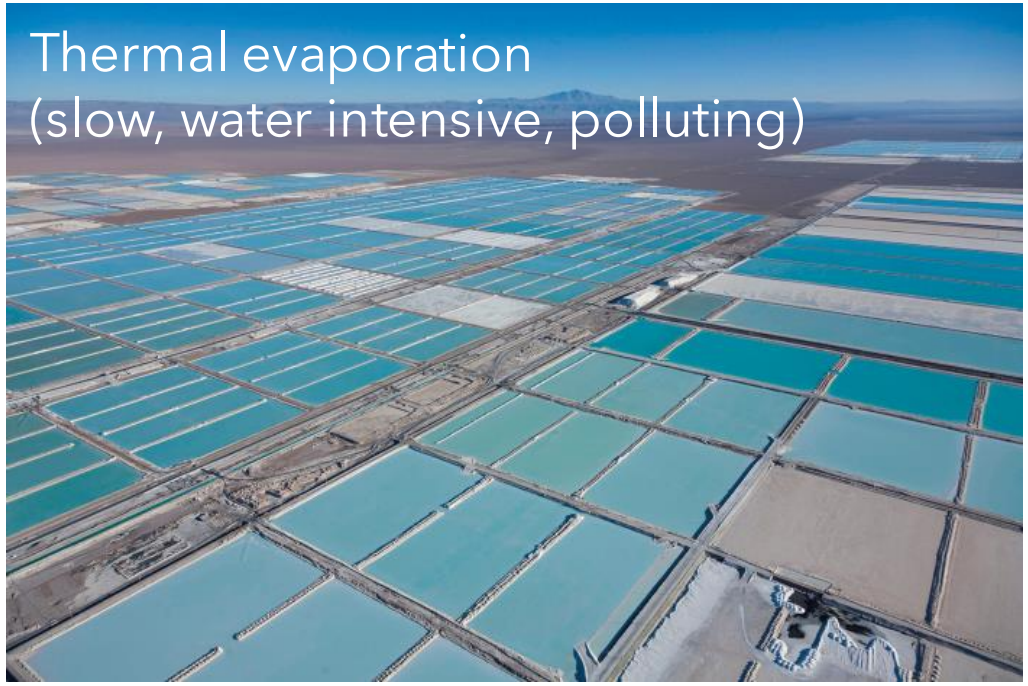


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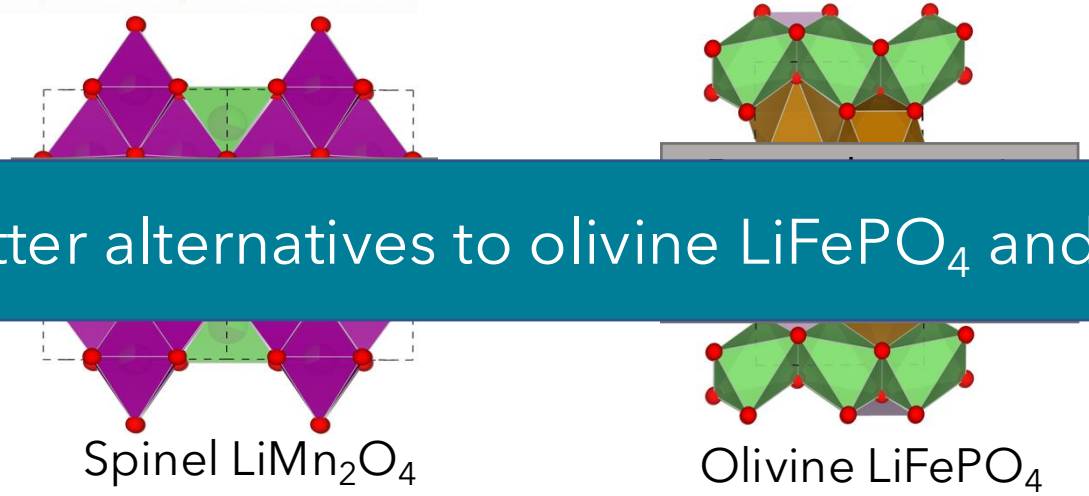
Problem with Li extraction from brines







State of the art



Spinel $LiMn_2O_4$ Olivine $LiFePO_4$

Objective: Find better alternatives to olivine $LiFePO_4$ and spinel $LiMn_2O_4$

High-throughput screening workflow

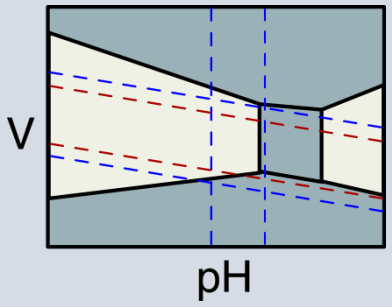
Step 1

Query first-principles cathodes' data across ions

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materialsproject.org

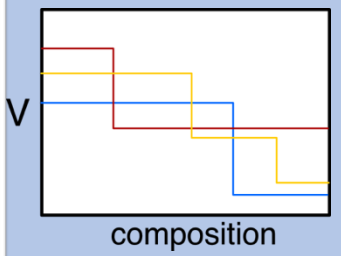
Step 2

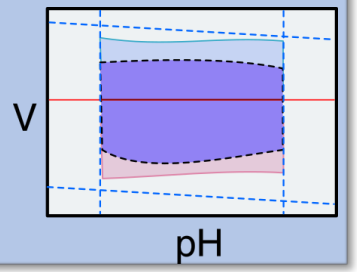
Determine aqueous stability of the cathodes



Step 3

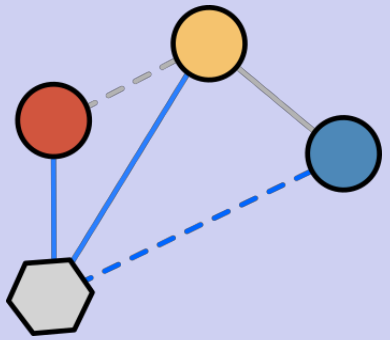
Calculate intercalation voltage





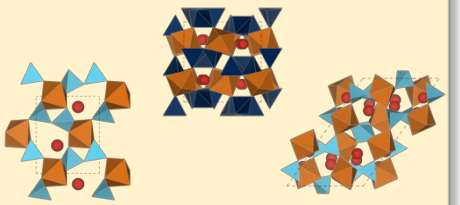
Step 4

Compare structures across ions

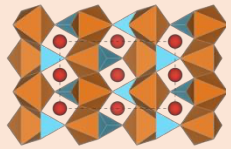


Candidates

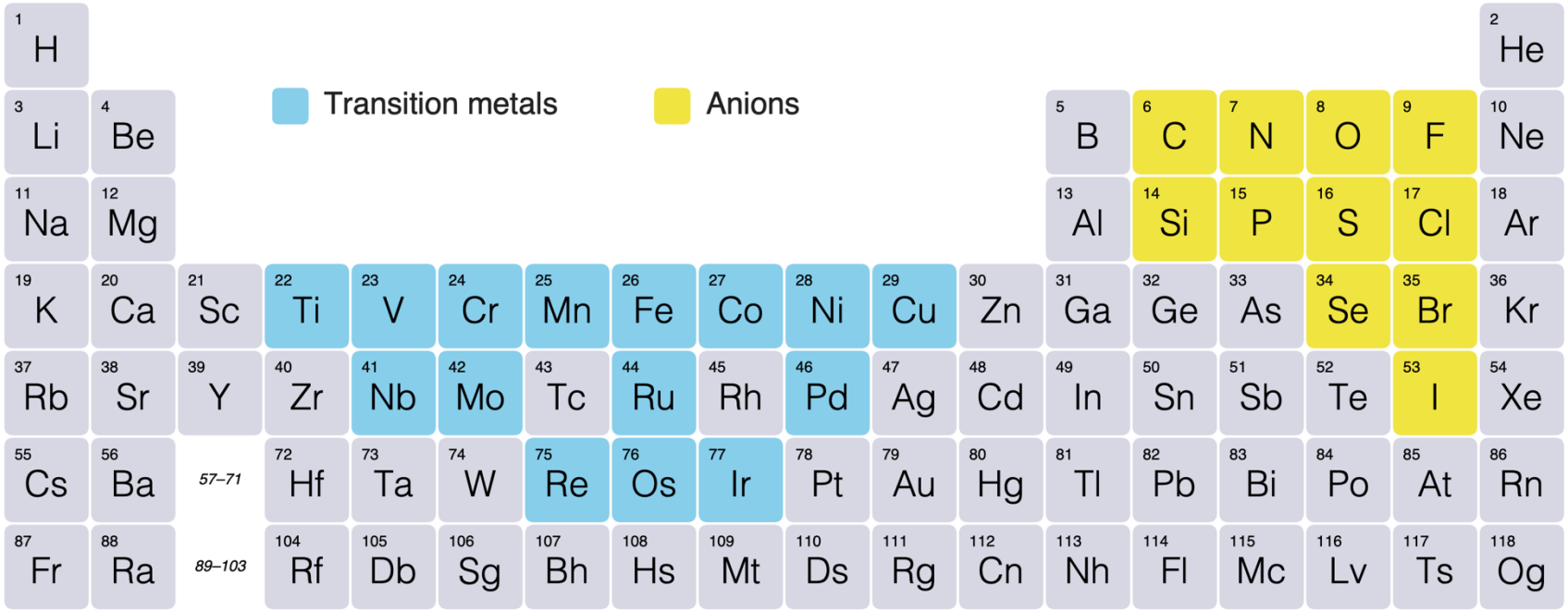
Selective ion recovery



Non-selective desalination



Step 1: Querying Cathodes' data



5 electro-active ions Li/Mg/Ca/Na/K

+

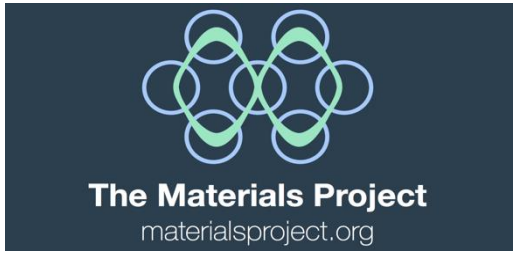
At most 3 out of 15 Transition Metals

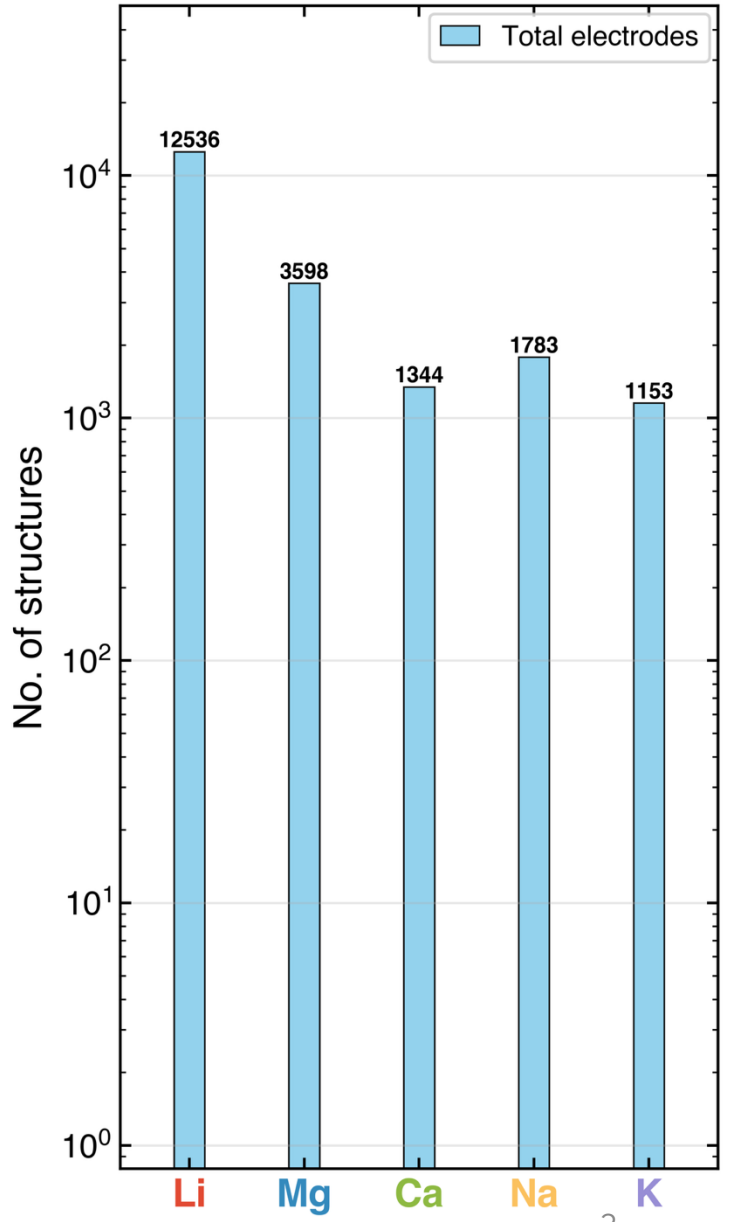
+

At most 3 out of 11 Anions

+

= **20,414** structures





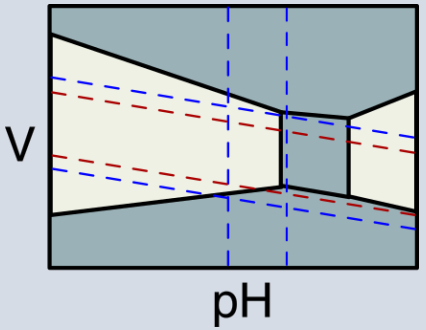
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Query first-principles cathodes' data across ions

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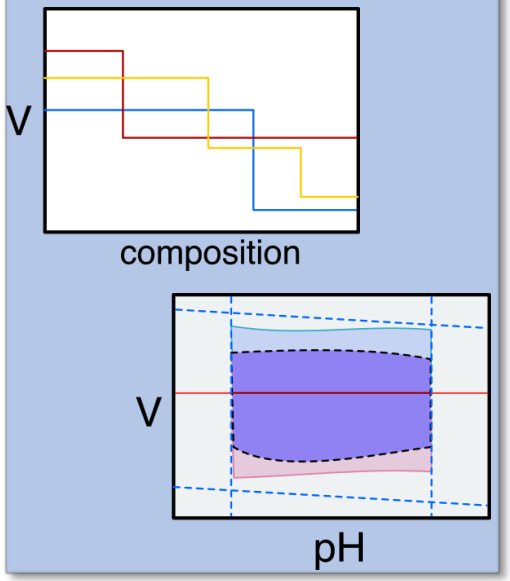
Step 2

Determine aqueous stability of the cathodes



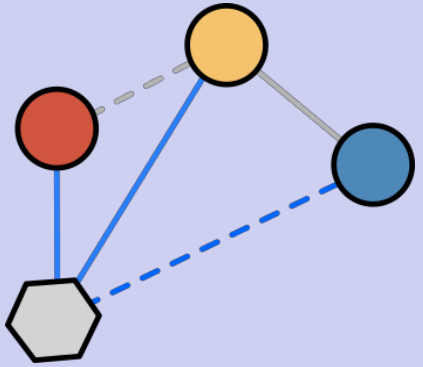
Step 3

Calculate intercalation voltage



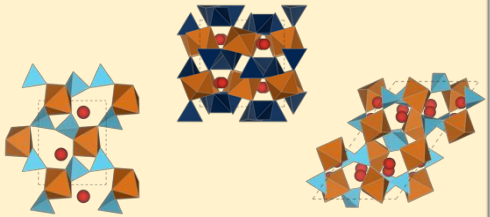
Step 4

Compare structures across ions

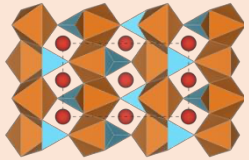


Candidates

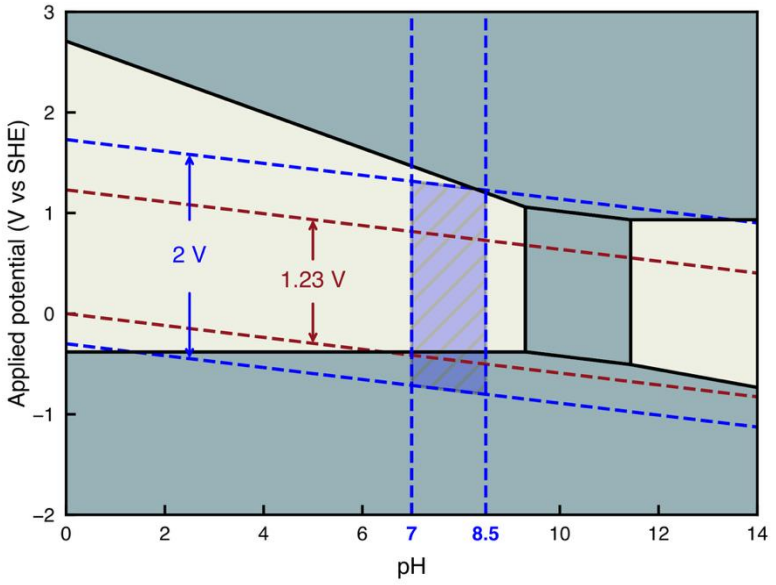
Selective ion recovery



Non-selective desalination



Step 2: Aqueous stability of cathodes

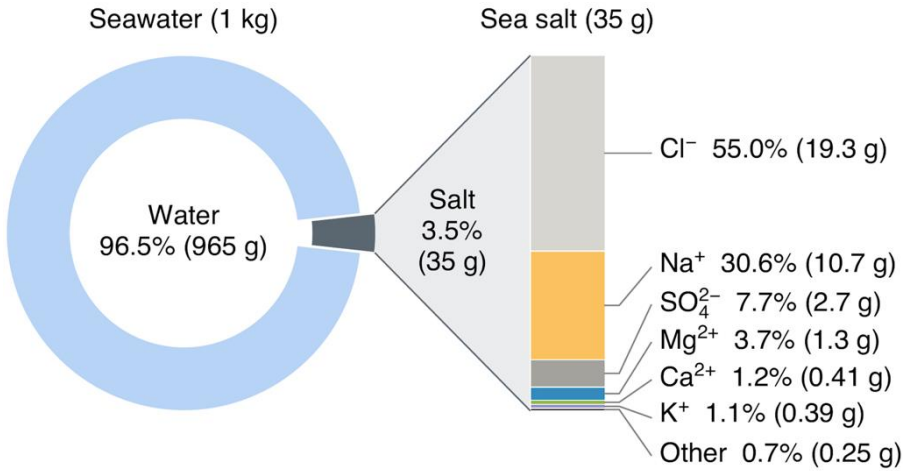


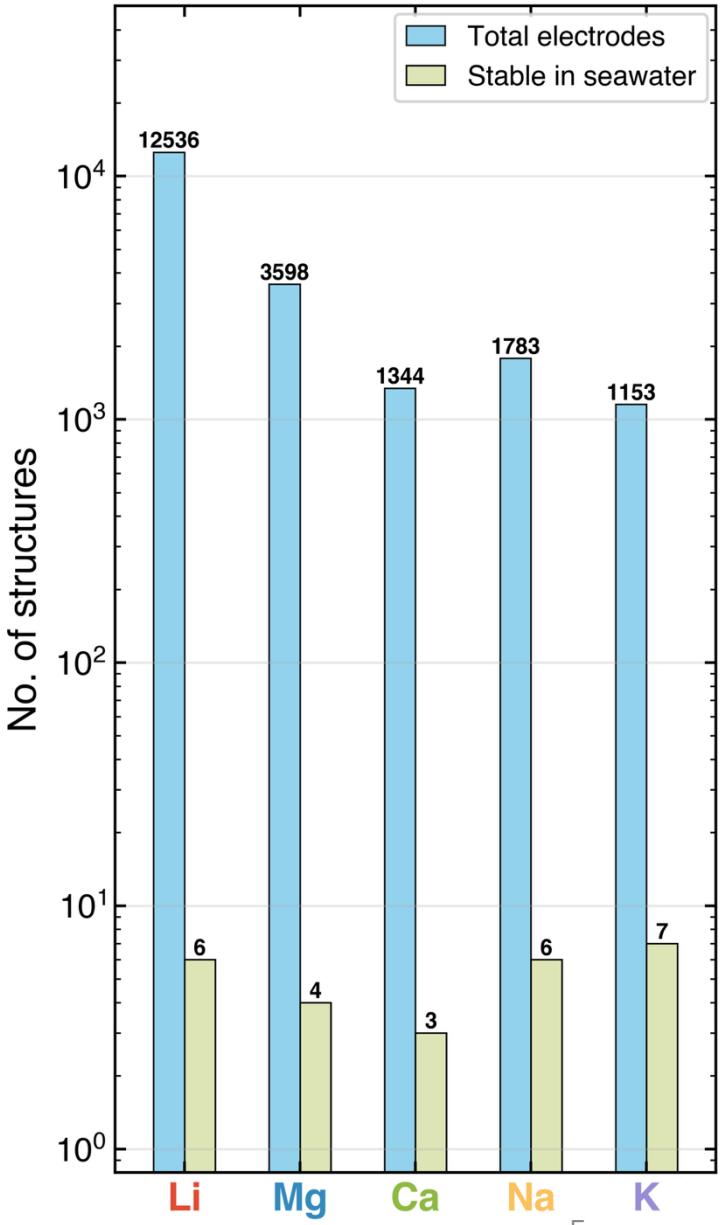
Multi-component Pourbaix Diagrams with

- Top 4 seawater elements
  Cl, Na, S, Mg

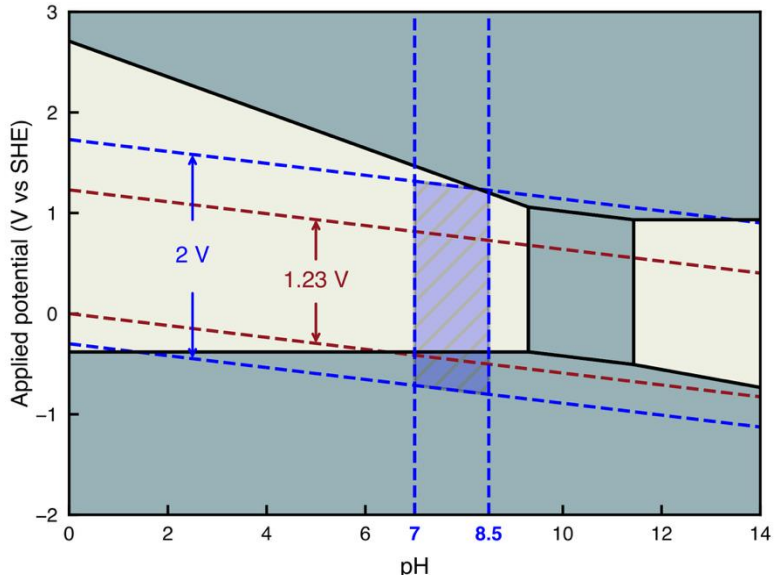
- If already present in the electrode
  Ca, K

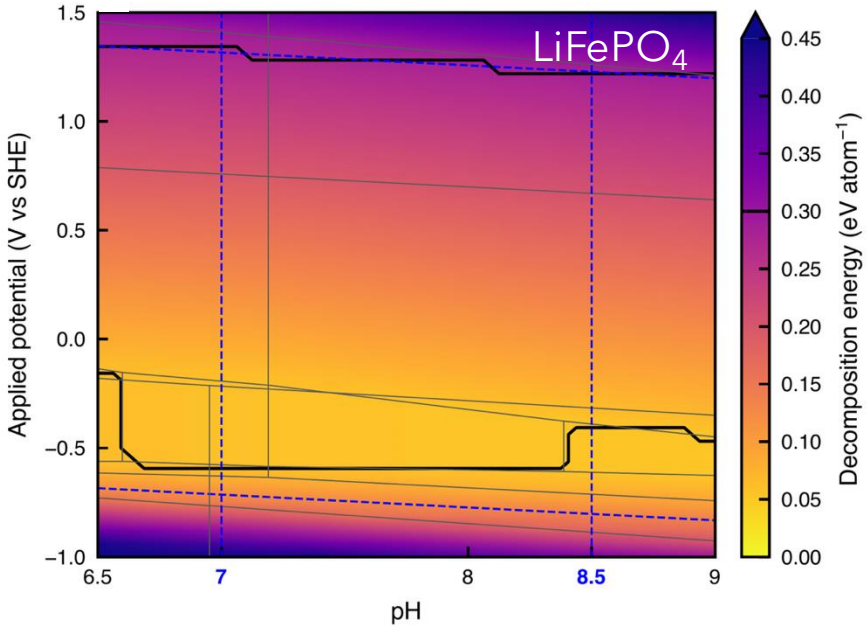
Widely used olivine $LiFePO_4$ and spinel $LiMn_2O_4$ are not seawater stable – probably metastable





Step 2: Aqueous stability of cathodes





Multi-component Pourbaix Diagrams with

- Top 4 seawater elements
  Cl, Na, S, Mg

- If already present in the electrode
  Ca, K

Widely used olivine $LiFePO_4$ and spinel $LiMn_2O_4$ are not seawater stable – probably metastable

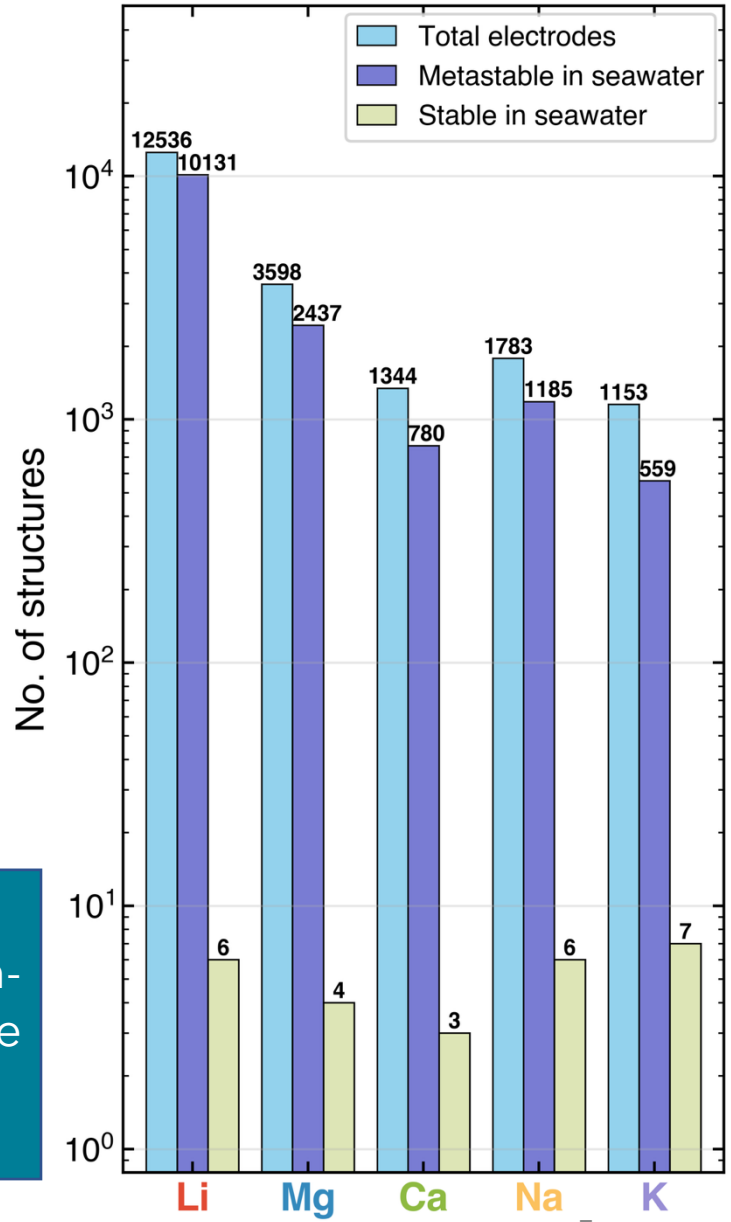
$$A \longrightarrow B + C + \ldots$$

$\Delta\Psi$ (Decomposition energy)

A is metastable if

. Atleast one of B, C . . . is a non-elemental solid without the mobile ion

. $\Delta\Psi <$ threshold (0.3 eV atom^{-1})



Singh et. al. Chem Mater, 29, 10159-10167 (2017)

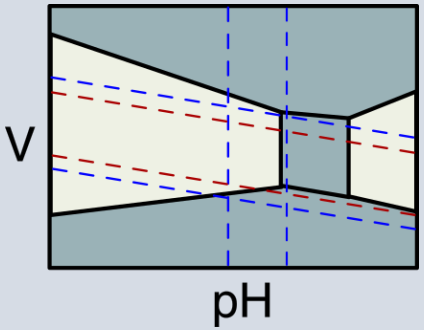
Step 1

Query first-principles cathodes' data across ions

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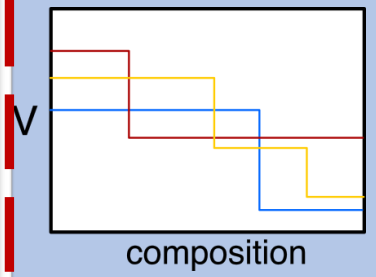
Step 2

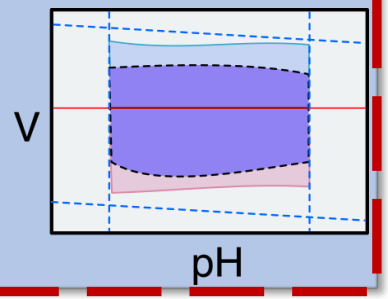
Determine aqueous stability of the cathodes



Step 3

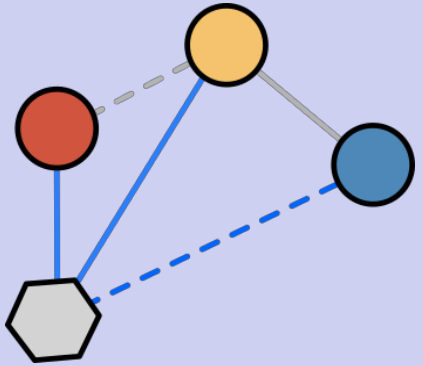
Calculate intercalation voltage





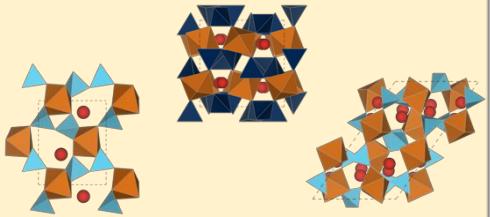
Step 4

Compare structures across ions

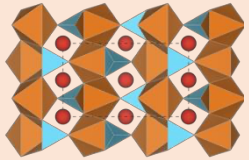


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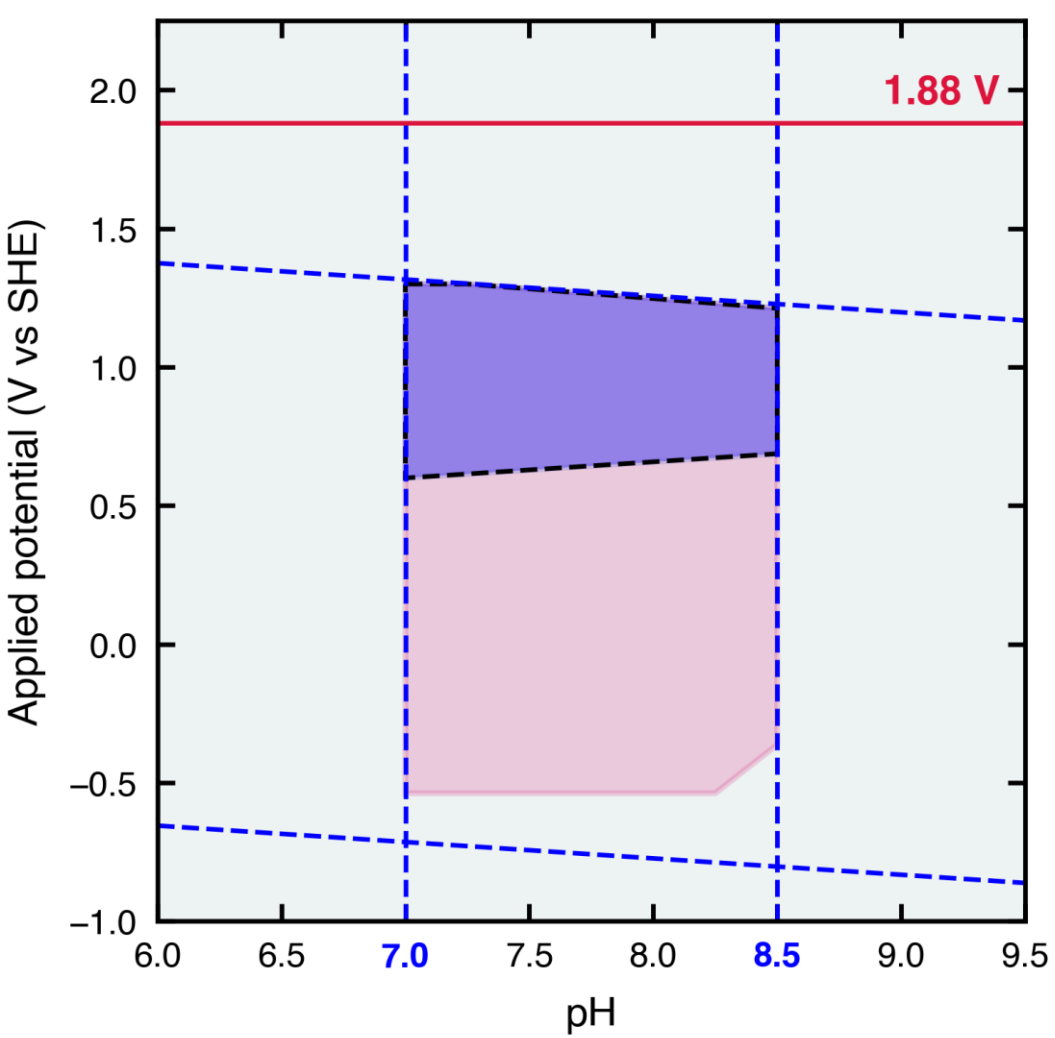
Selective ion recovery



Non-selective desalination



Step 3: Intercalation voltages



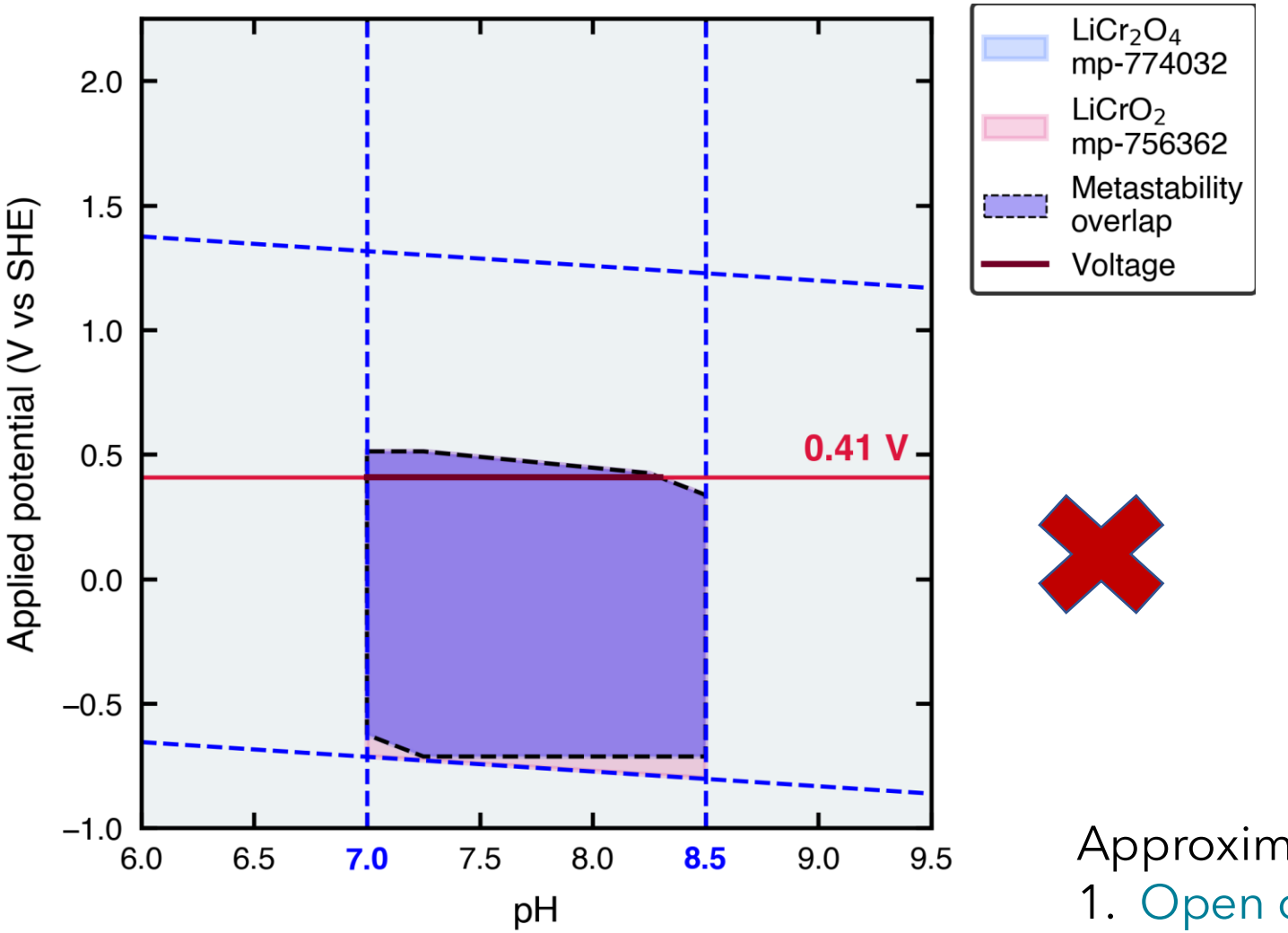
Metastability scenarios at the intercalation voltage:

- Voltage beyond seawater stability window

Approximations:

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

Step 3: Intercalation voltages



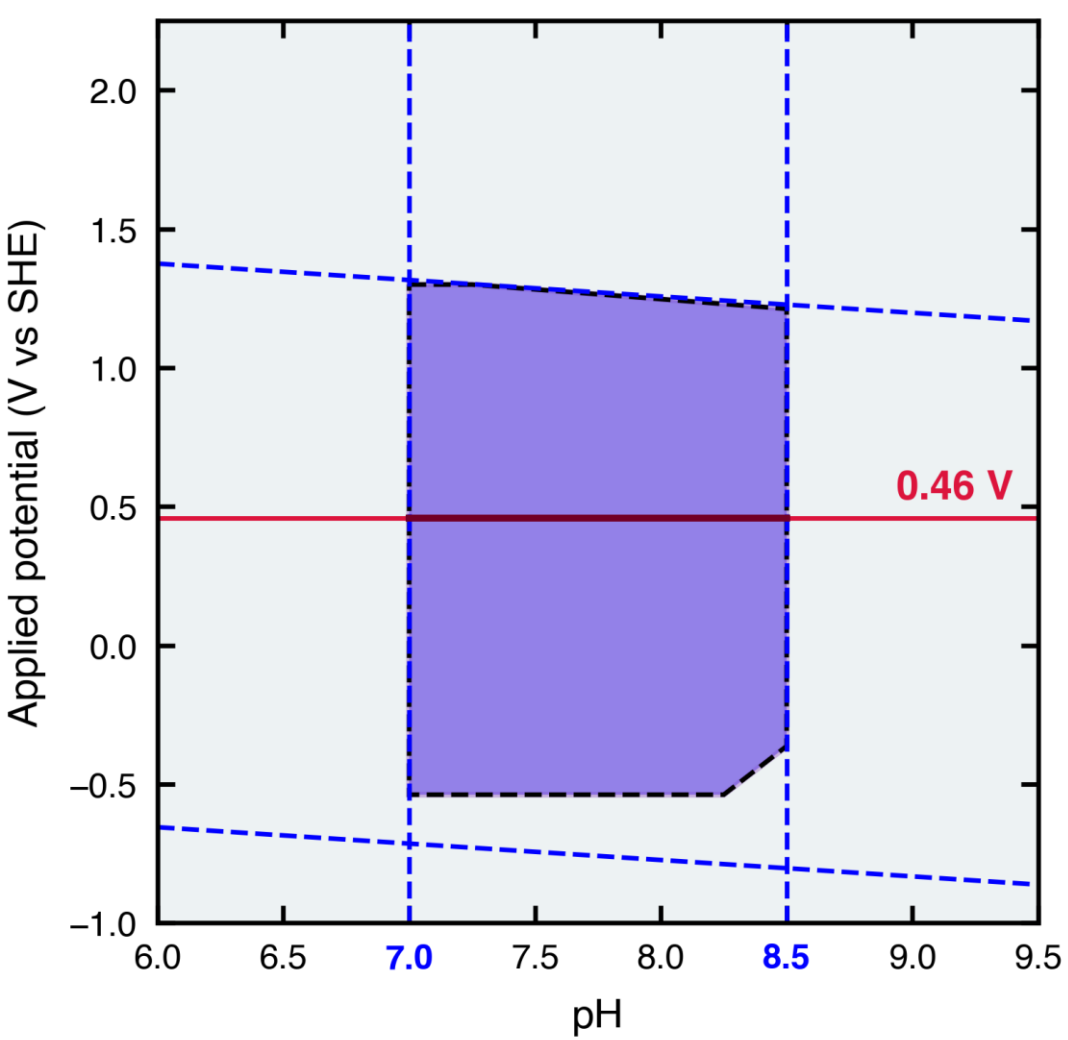
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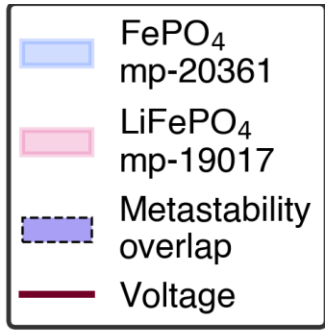
- Voltage beyond seawater stability window
- Electrode not stable throughout pH 7-8.5 at intercalation voltage

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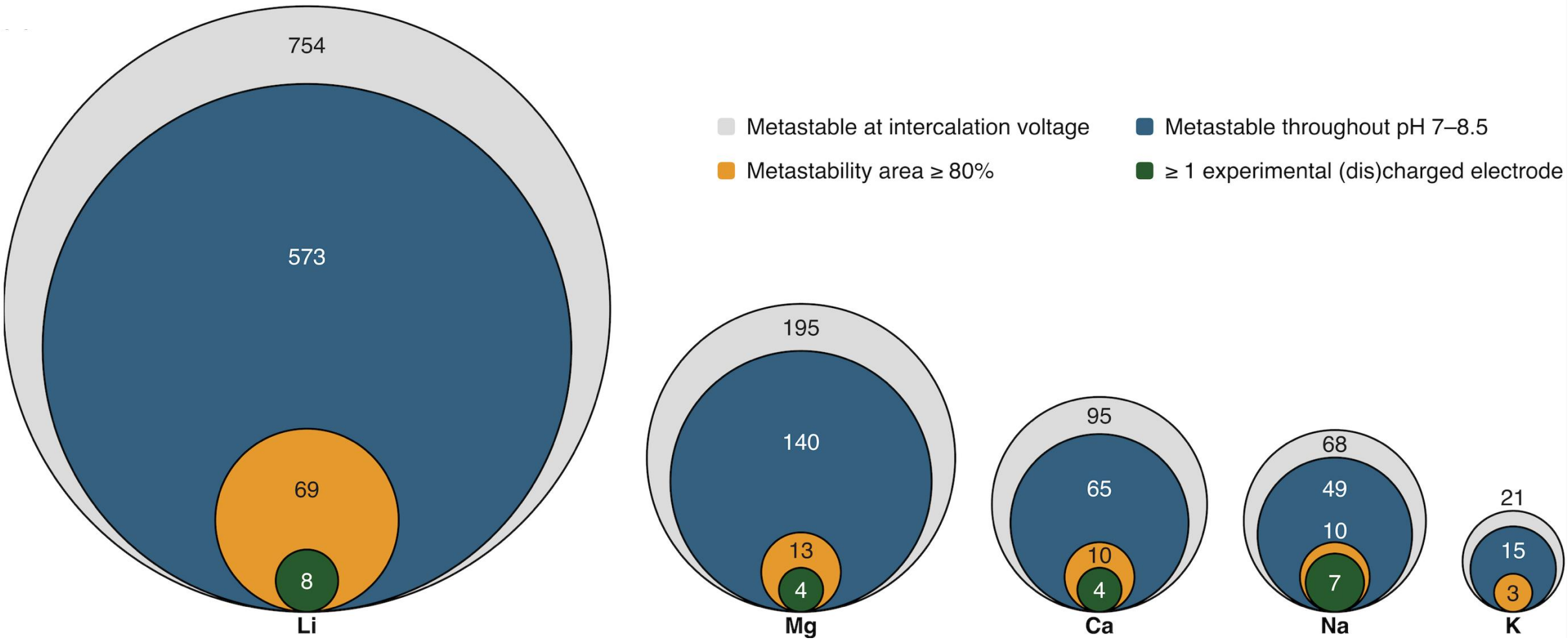
Metastability scenarios at the intercalation voltage:

- 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

Approximations:

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

Filtered electrodes



Total queried structures:	12,536	3,598	1,344	1,783	1,153

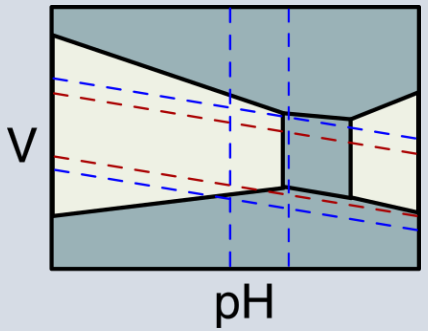
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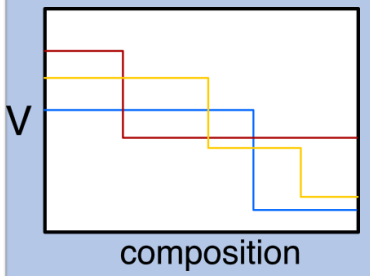
Step 2

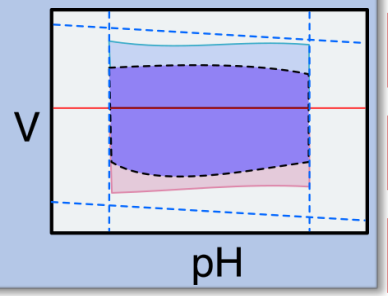
Determine aqueous stability of the cathodes



Step 3

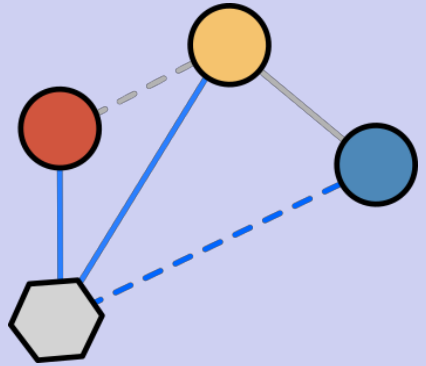
Calculate intercalation voltage





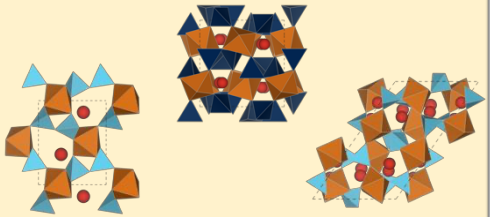
Step 4

Compare structures across ions

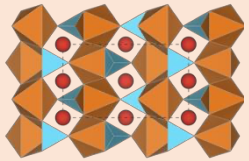


Candidates

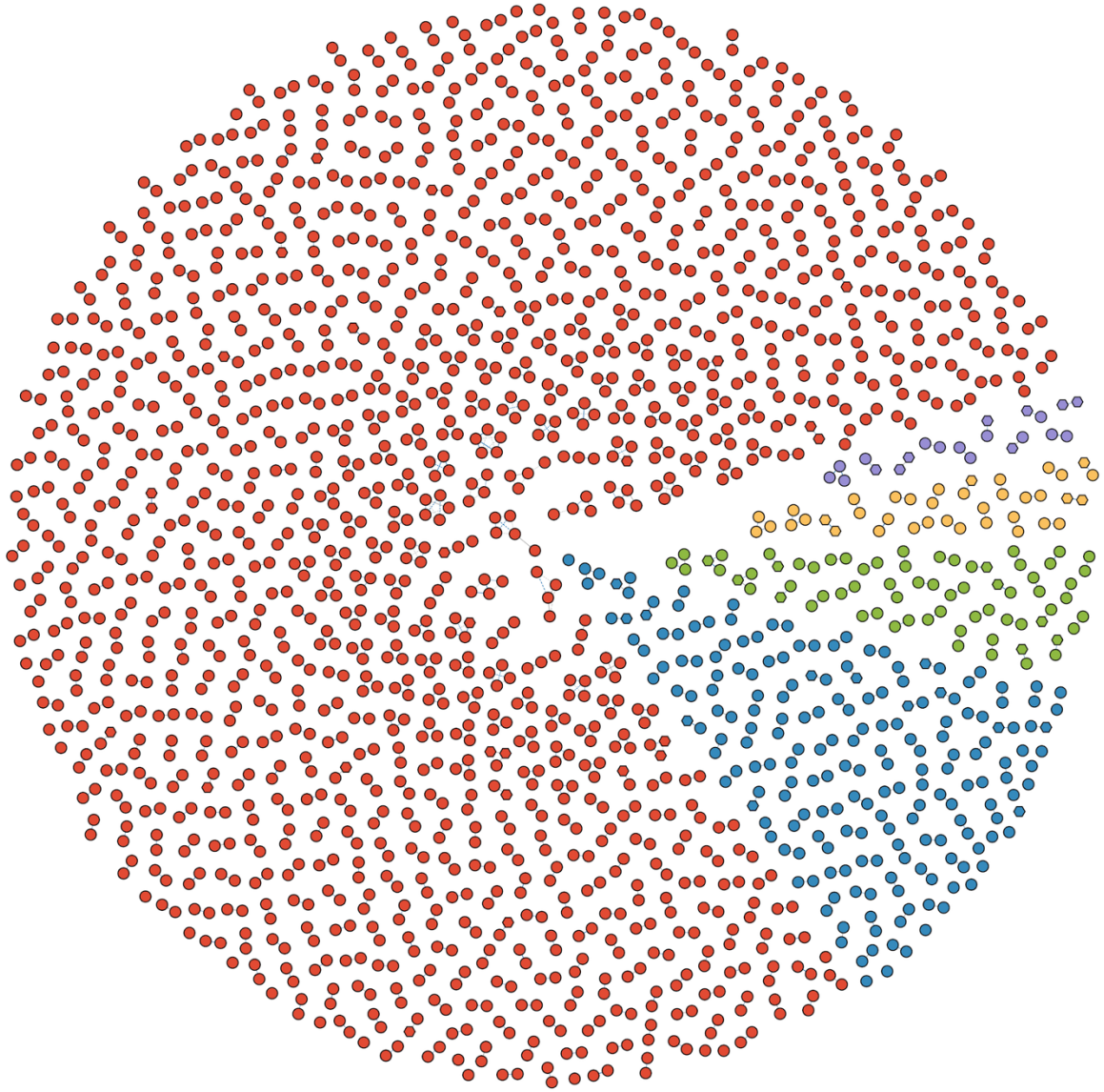
Selective ion recovery



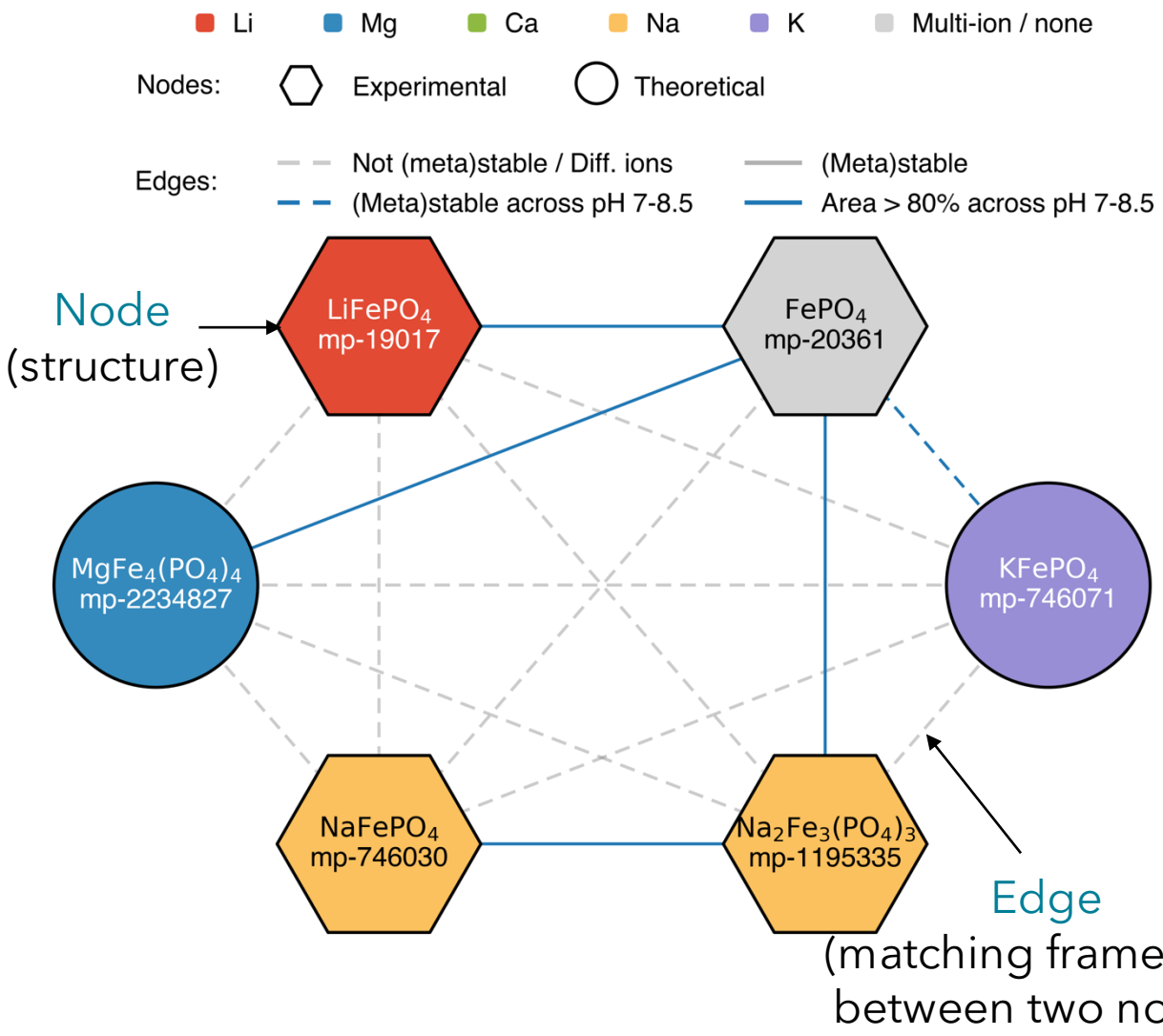
Non-selective desalination



Ion-selective hosts (graphs)

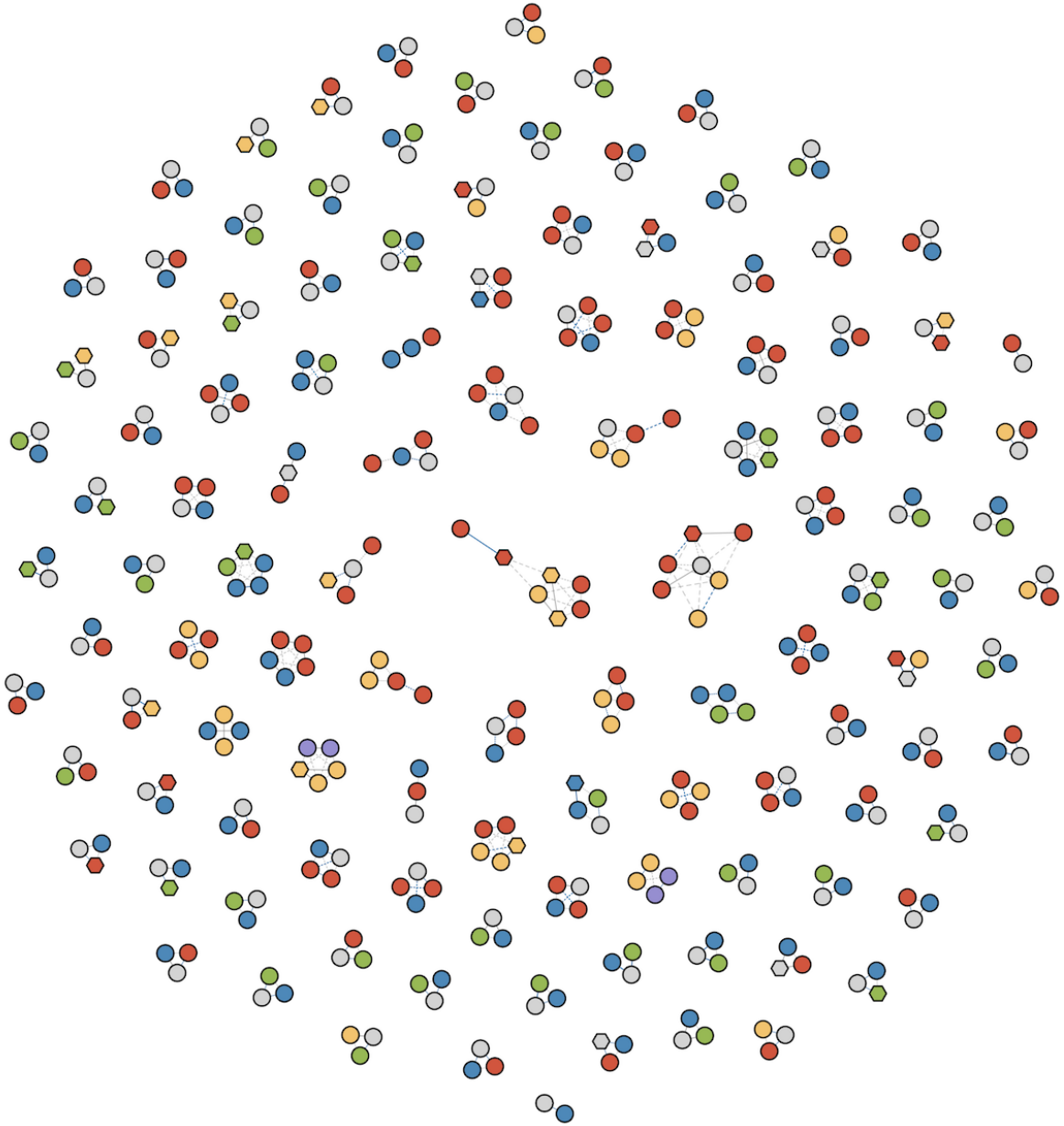


859 ion-selective hosts (690 **Li**, 108 **Mg**, 33 **Ca**, 18 **Na** and 10 **K**)



A graph represents a host

Non-selective hosts (graphs)

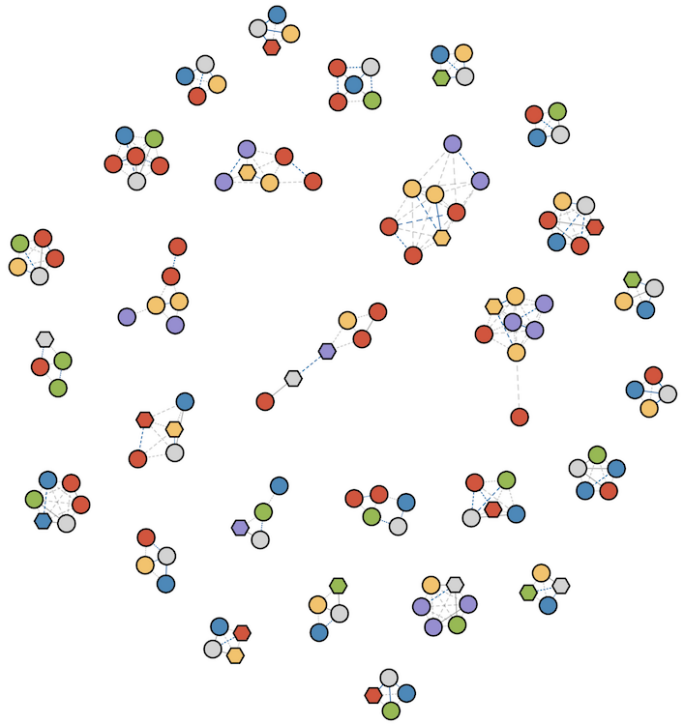


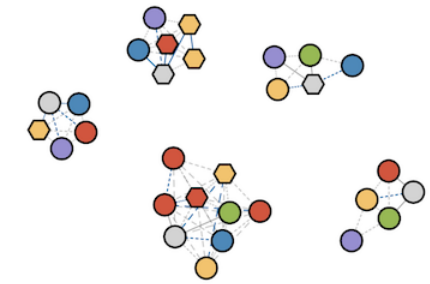
115 2-ions intercalating hosts

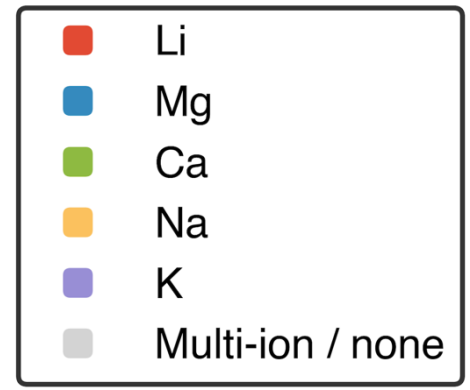
28 3-ion intercalating hosts

5 4-ion intercalating hosts

0 5-ion intercalating hosts







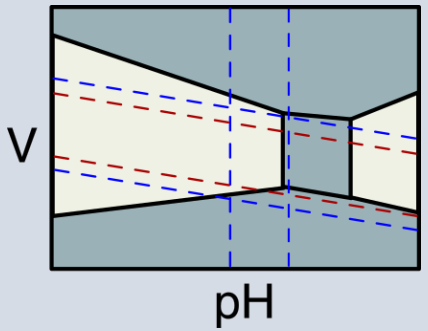
Step 1

Query first-principles cathodes' data across ions

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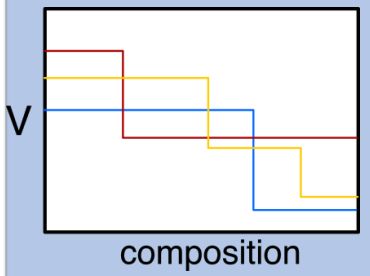
Step 2

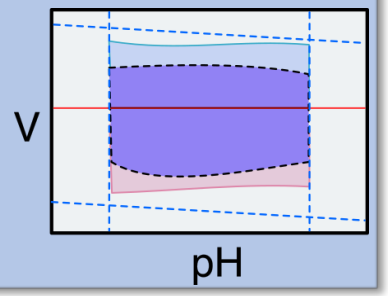
Determine aqueous stability of the cathodes



Step 3

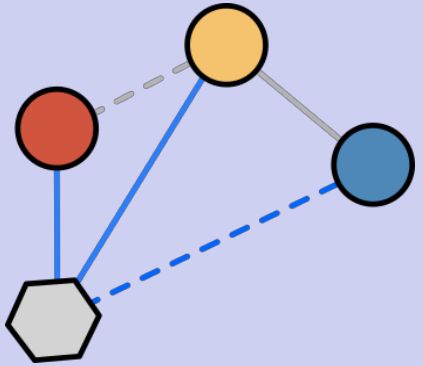
Calculate intercalation voltage





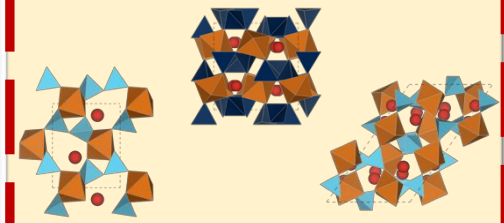
Step 4

Compare structures across ions

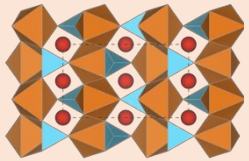


Candidates

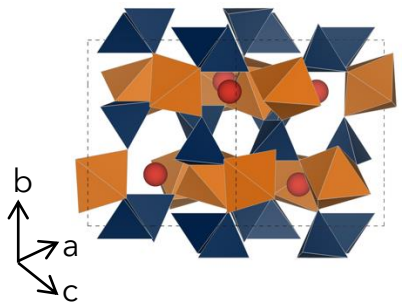
Selective ion recovery



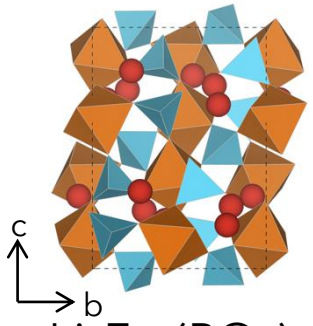
Non-selective desalination



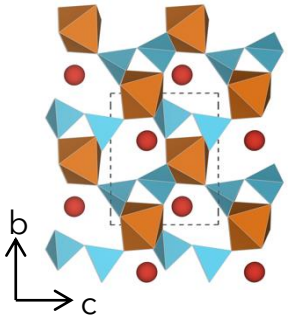
Final Candidates



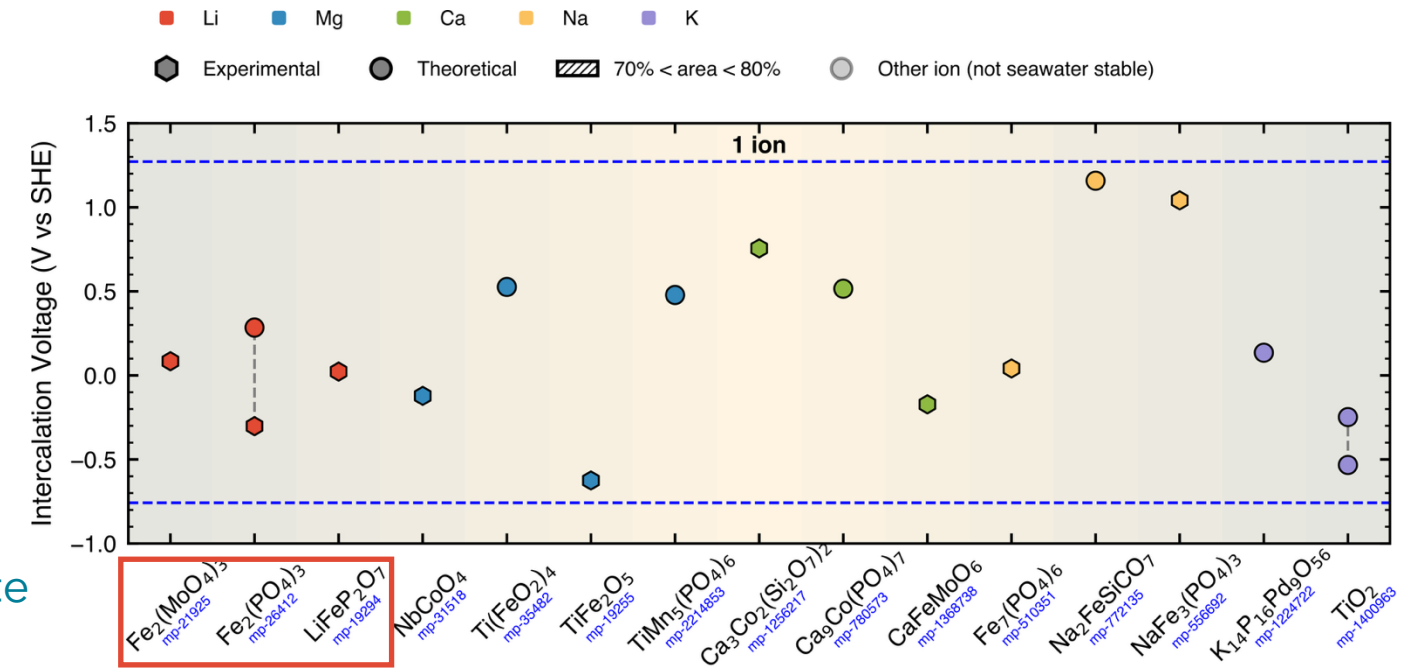
$Fe_2(MoO_4)_3$
Garnet-like



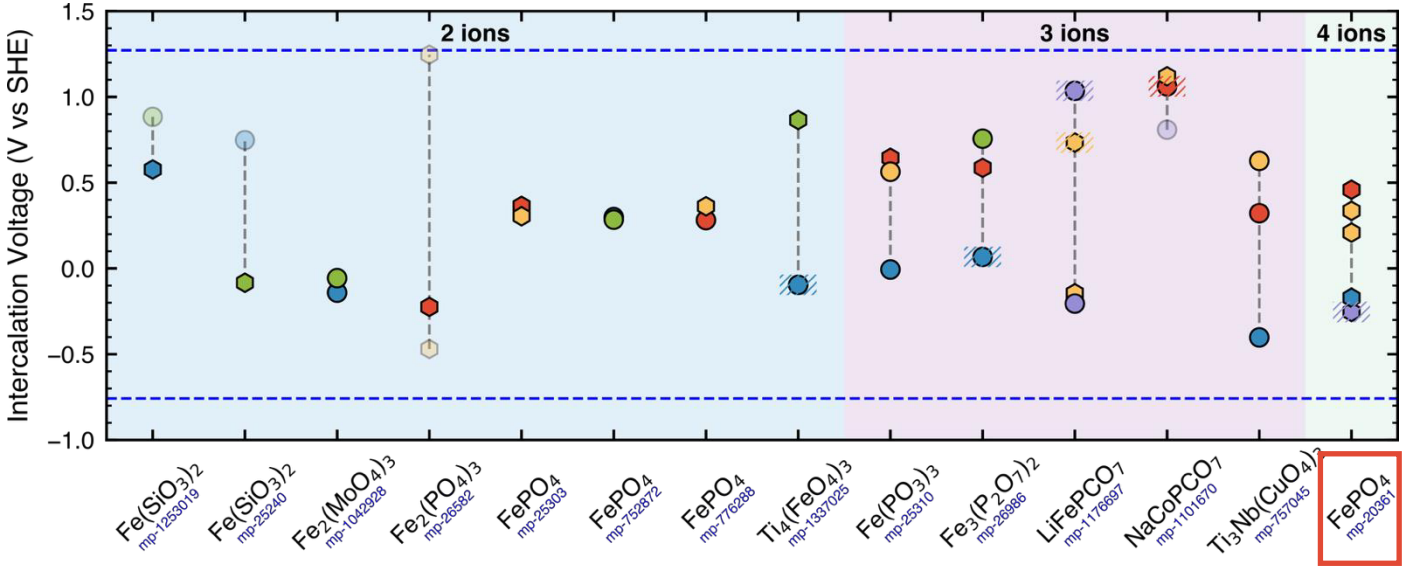
$Li_3Fe_2(PO_4)_3$
Anti- NASICON



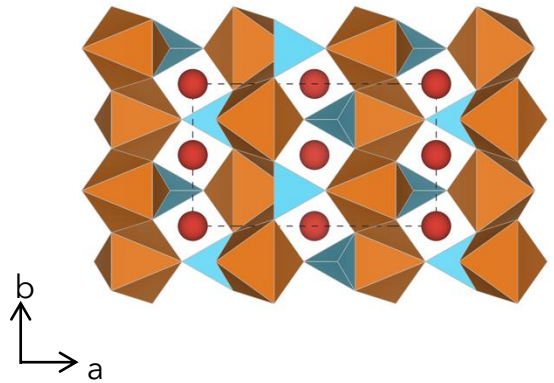
$LiFeP_2O_7$
Pyrophosphate



Li-selective



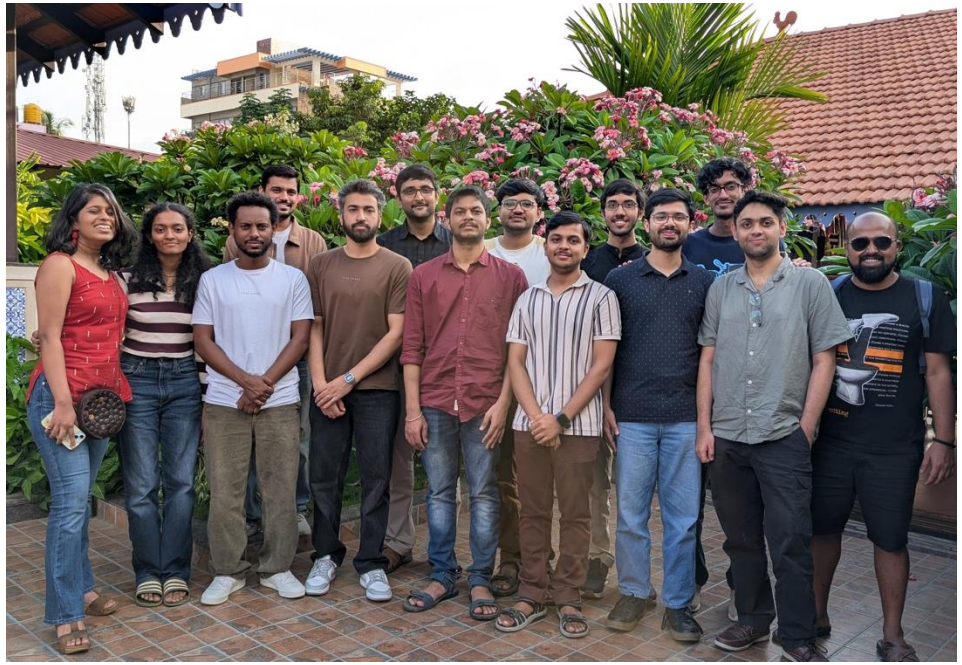
~ Desalination



FePO4
Olivine

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: $LiFeP_2O_7$, $Li_3Fe_2(PO_4)_3$ and $Fe_2(MoO_4)_3$
  - Desalination: $FePO_4$







Under Review (arXiv:2610.20834):

Identifying intercalation electrodes for electrochemical ion recovery and desalination

Sougat Purohit, Andreas Kuhlmann, Marten Huck, Hans-Georg Steinrück, Gopalakrishnan Sai Gautam



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