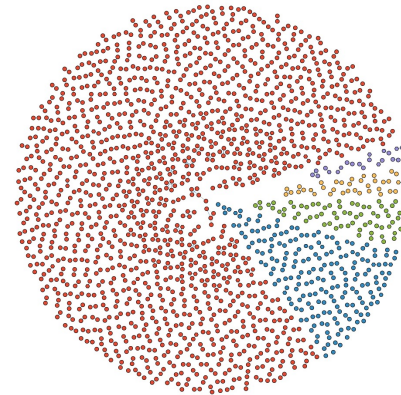




High-throughput screening of intercalation electrodes for electrochemical ion-recovery

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Acknowledgments



Sougat



Hans-Georg



Andreas



Marten

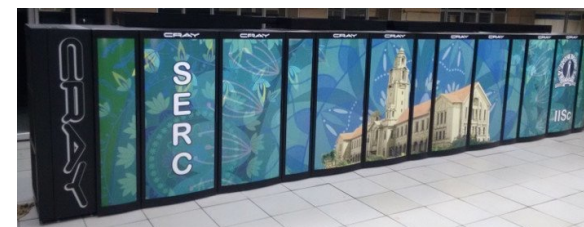
Jun 2026



Ion recovery screening



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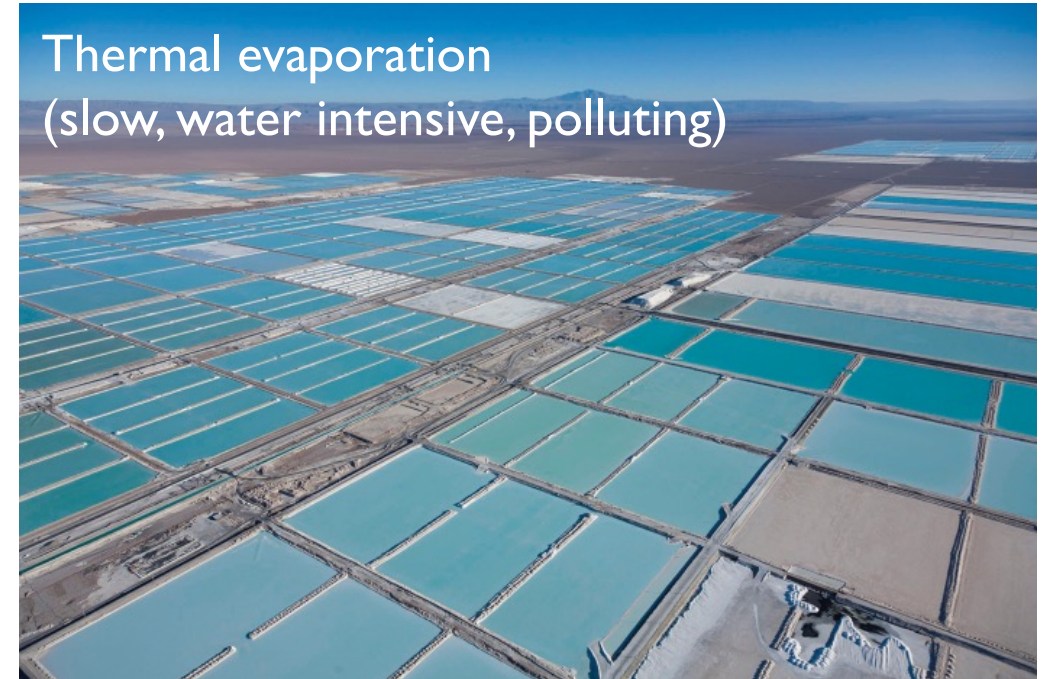
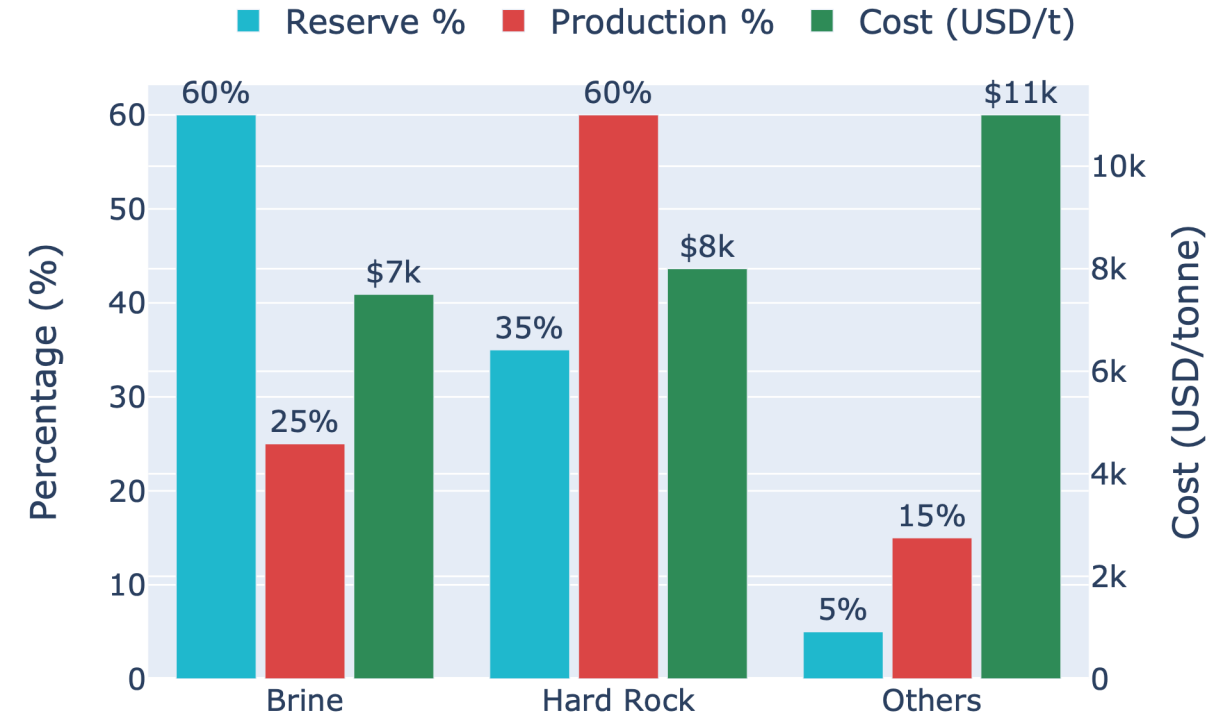


SERC (IISc)

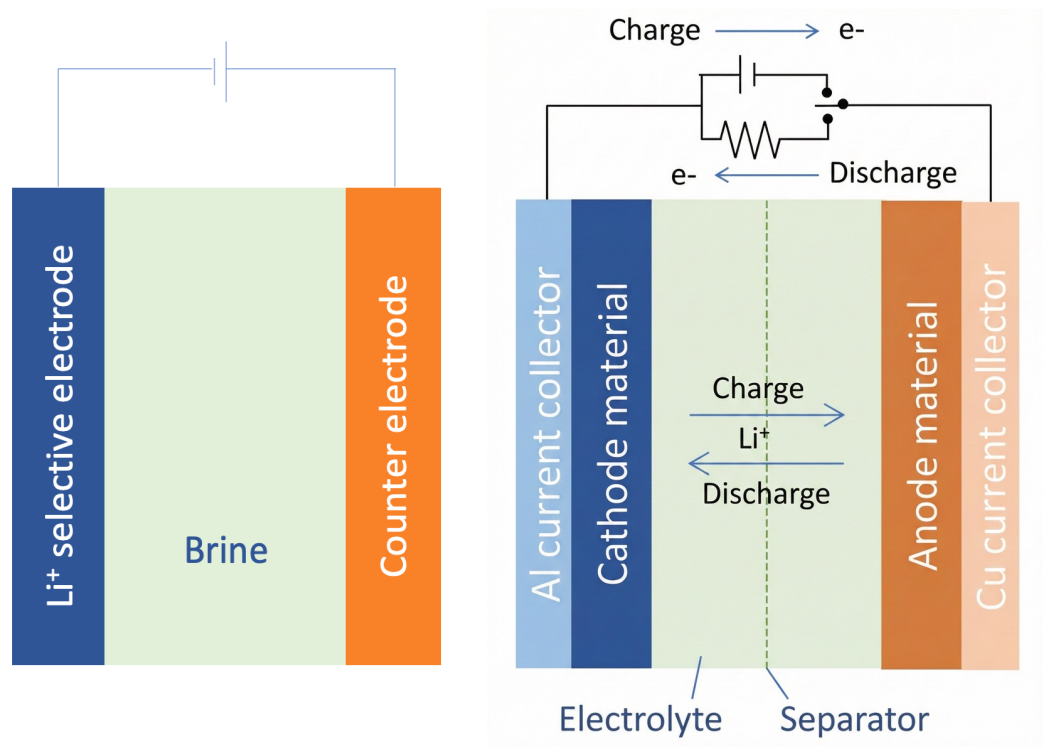


Jureca
(Germany)

(Li) Extraction from brines...and desalination

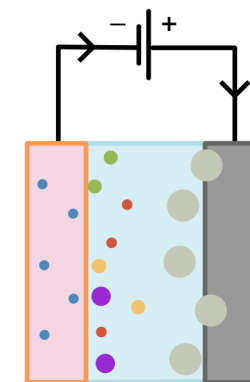
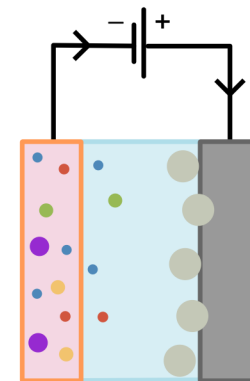
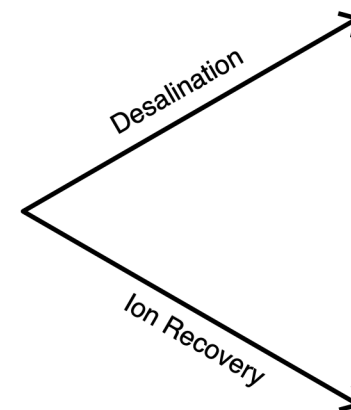
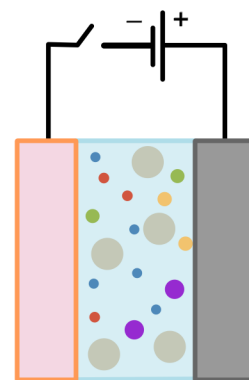
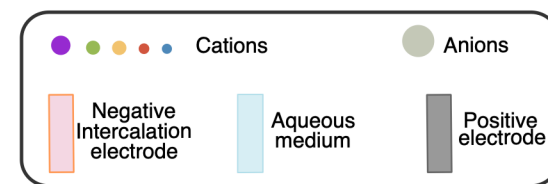


(Li) Extraction from brines...and desalination



Electrochemical ion-recovery:

- Faster, low energy consumption
- Can handle various brine compositions including **seawater**
- Similar to Li-ion battery



State-of-the-art

- Olivine-FePO₄
- Spinel-Mn₂O₄

Can we computationally identify (better) intercalation electrodes for electrochemical ion recovery?

Workflow

Step 1

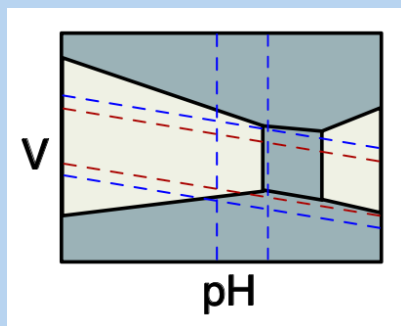
Query first-principles cathodes data across ions



Ion recovery screening

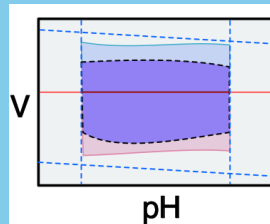
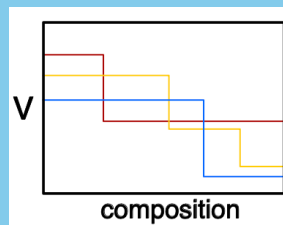
Step 2

Determine aqueous stability of the cathodes



Step 3

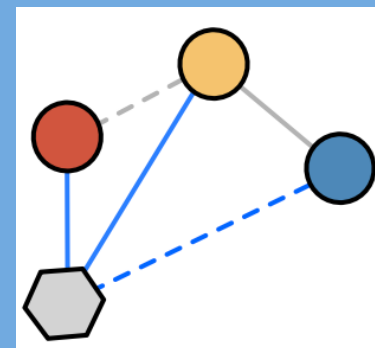
Calculate intercalation voltage and metastability overlap



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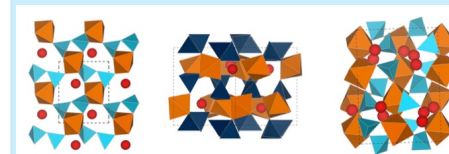
Step 4

Compare structures across ions

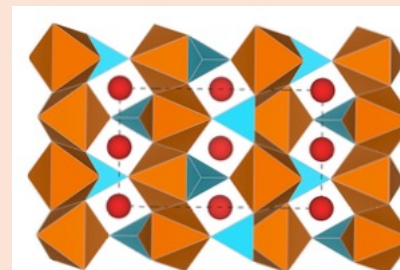


Candidates

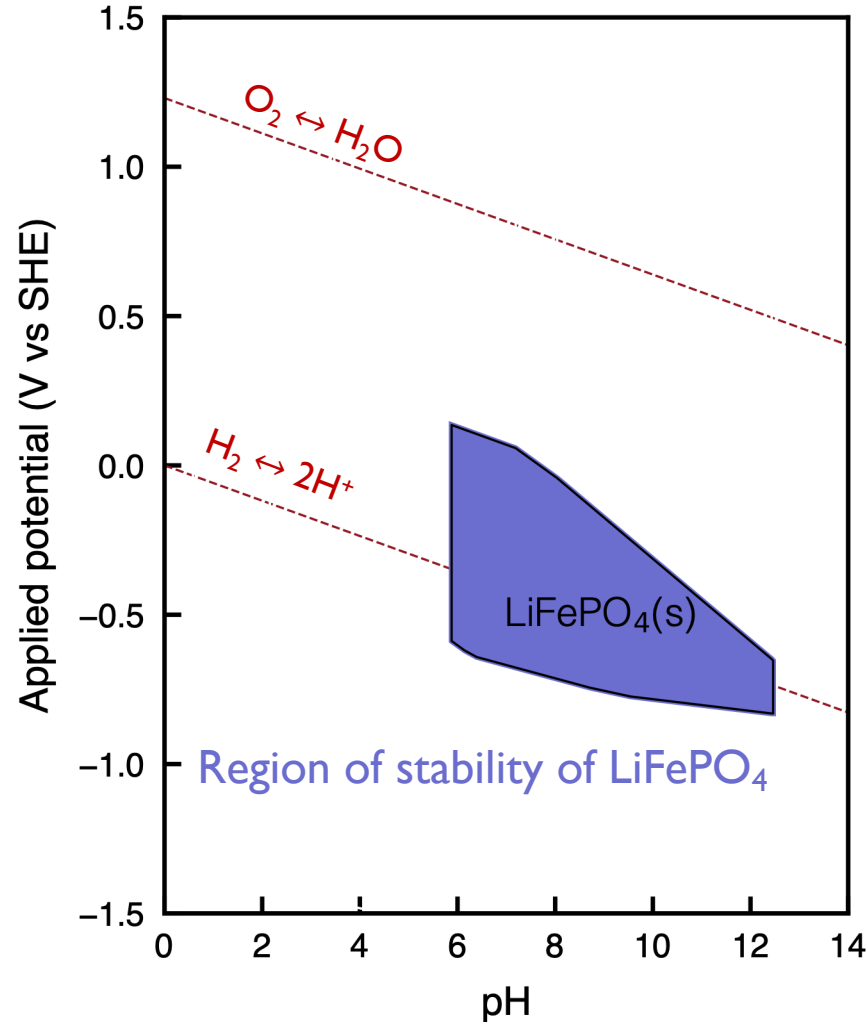
Selective ion recovery



Non-selective desalination



Pourbaix diagrams and aqueous (meta)stability

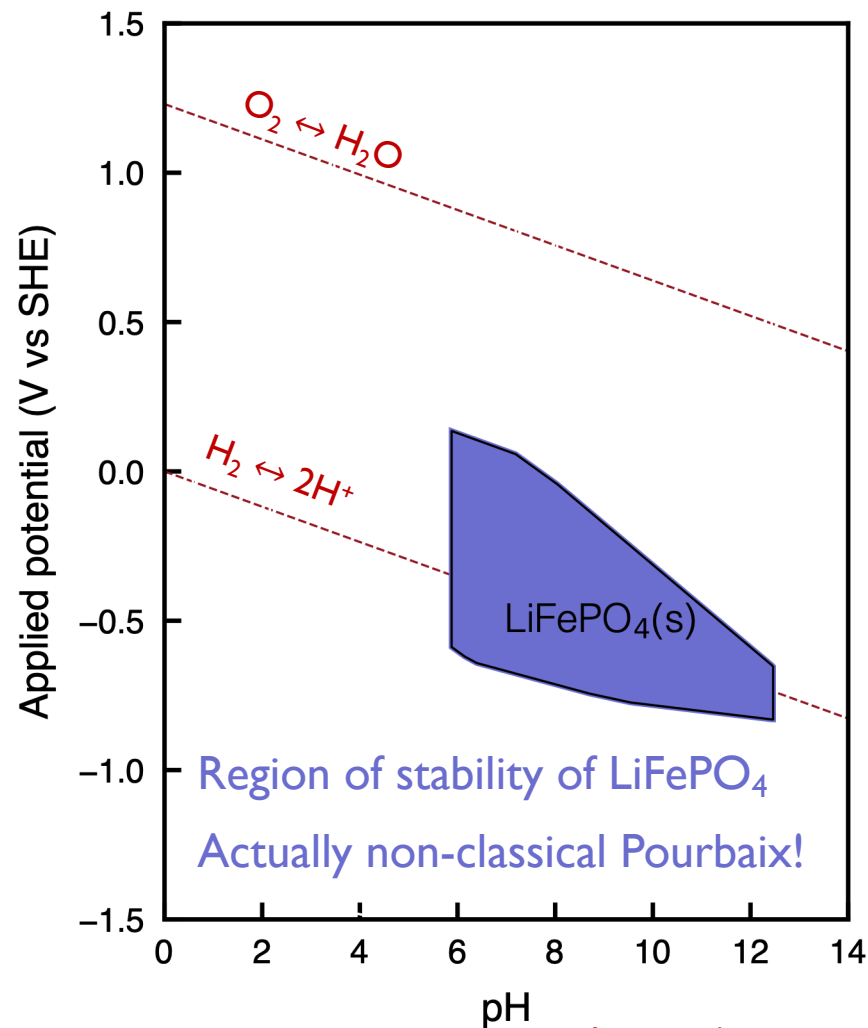


Potential-pH phase diagrams indicating stability of a solid phase against an aqueous reservoir

- Define a Pourbaix potential, Ψ^α , and identify potential-pH regions where Ψ^α is minimum for a given α solid
- $\Psi^\alpha = G^\alpha - \mu_O^\alpha N_O^\alpha - \mu_H^\alpha N_H^\alpha - E q^\alpha$

Classic Pourbaix: reservoir is water with dilute concentrations ($\leq 10^{-6}$ M) of ions

Pourbaix diagrams and aqueous (meta)stability

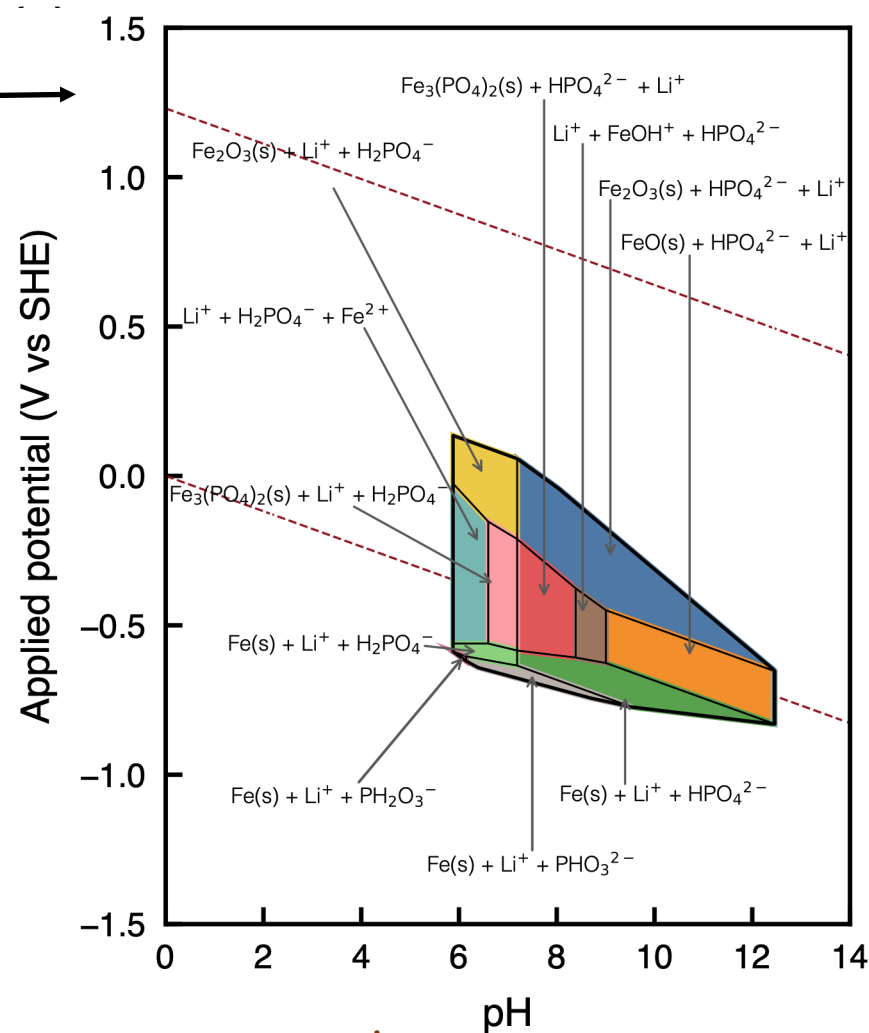


Classical Pourbaix
[Li]=[Fe]=[P]=10⁻⁶ M

Need an 'appropriate'
aqueous reservoir for
ion recovery

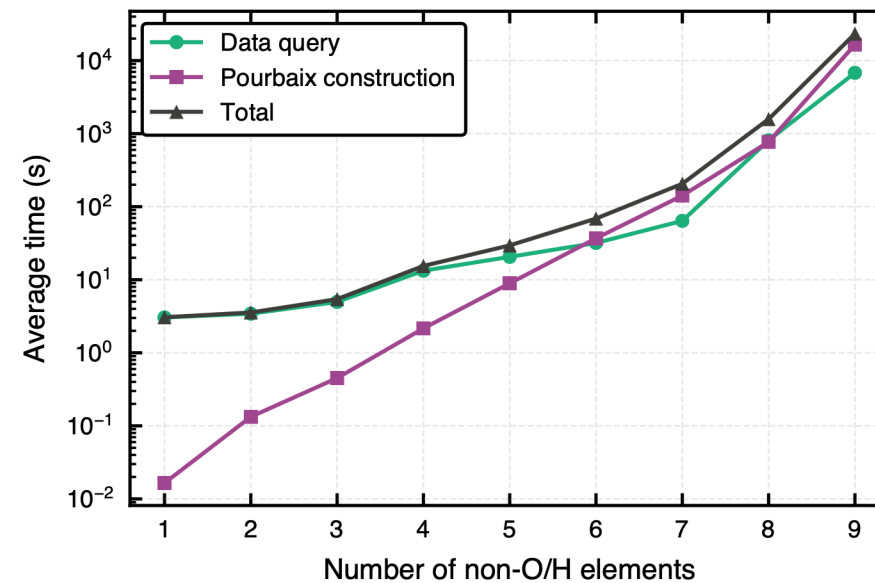
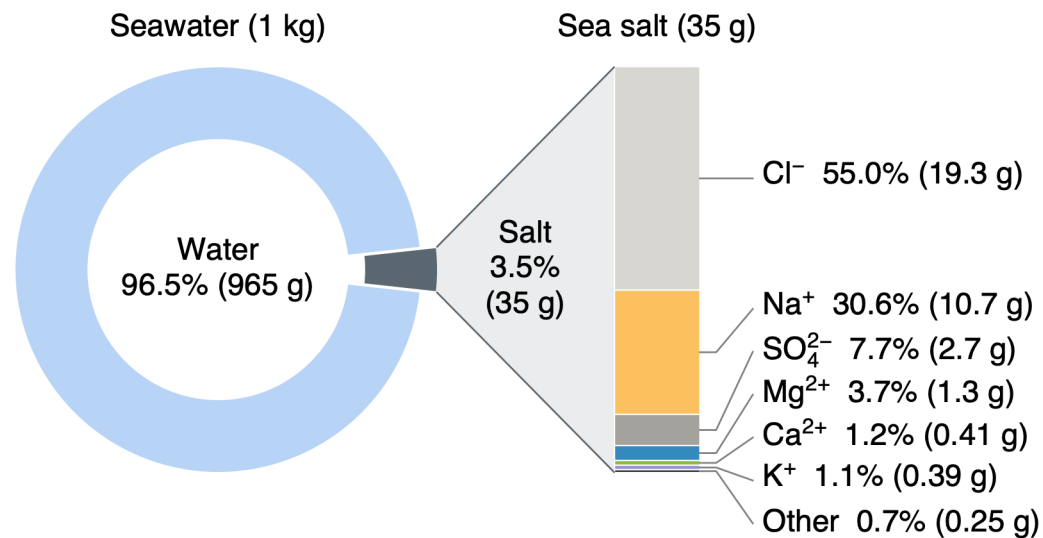
Solids may be
metastable!

[Li]=0.75 M
[Fe]=0.25 M
[P]=0.33 M



A solid's region of stability depends on the aqueous reservoir

Seawater Pourbaix diagrams and seawater stability window



Seawater: reservoir for electrochemical ion capture

- Myriad of salts present at non-dilute concentrations
- Similar to brines, recycling sources
- Each salt added is at least 2 chemical components

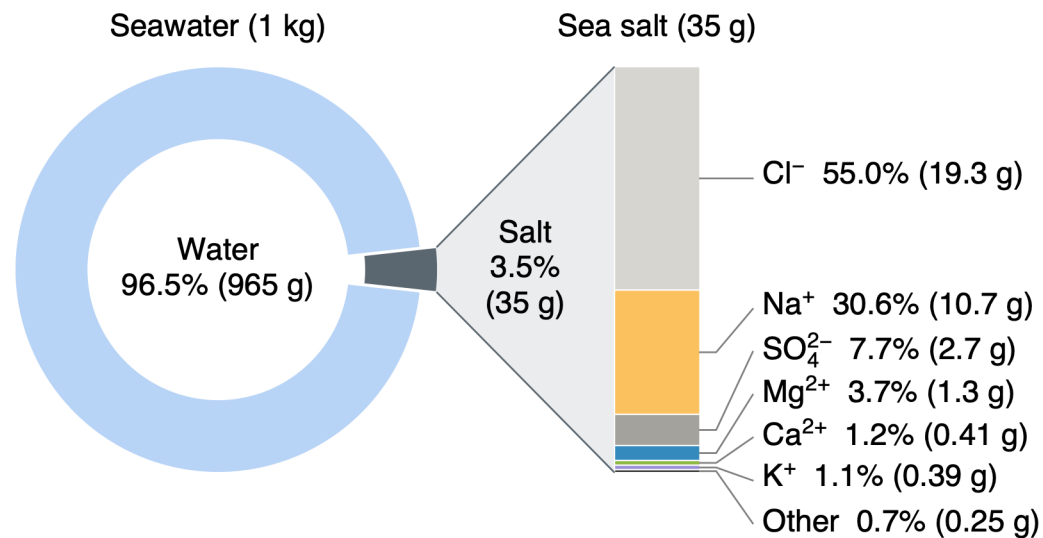
Also account for overpotentials with H₂ and O₂ evolution

- Seawater is slightly basic

Constructing high-throughput multi-component Pourbaix diagrams: non trivial!

- Compromise: consider top four elements in seawater (Cl, Na, Mg, S)
 - If not already present in the solid
- Include Ca +/- K in seawater if present in solid

Seawater Pourbaix diagrams and seawater stability window



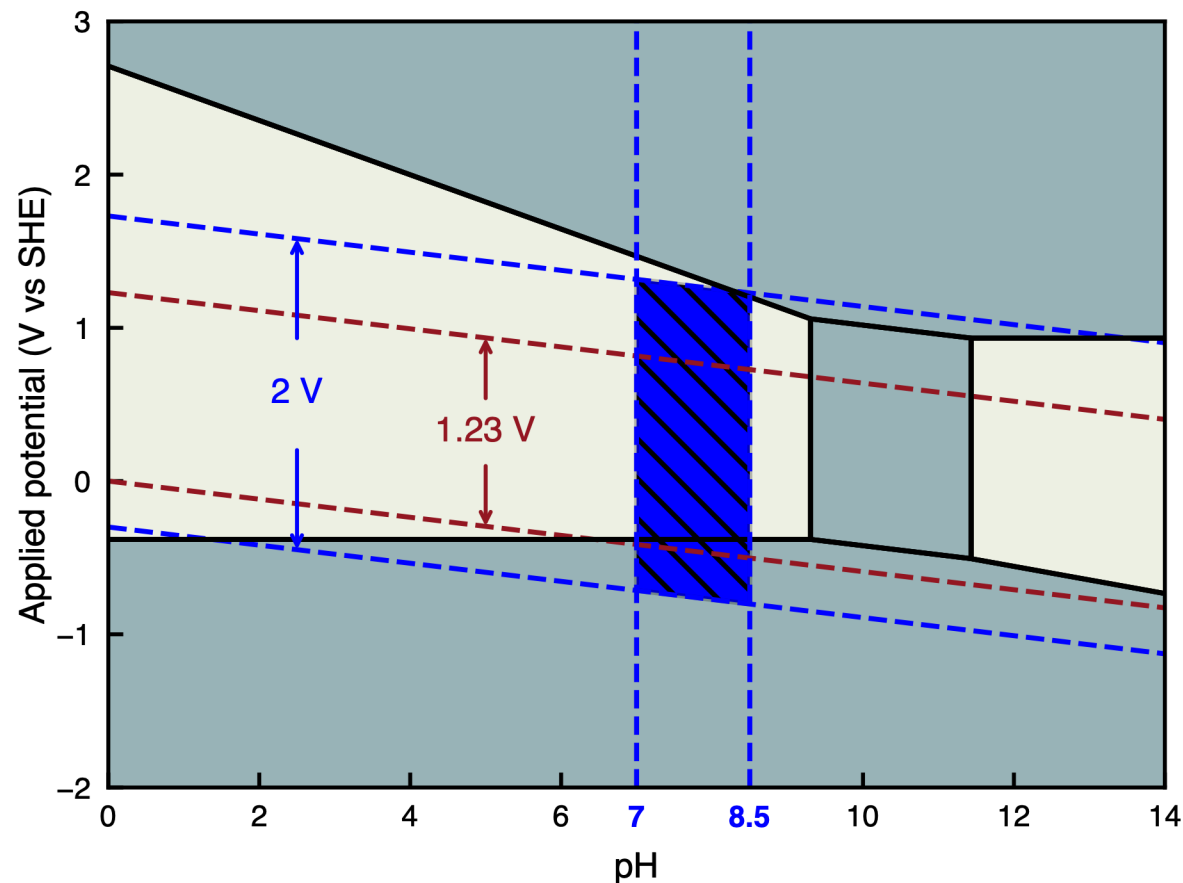
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Ion recovery screening

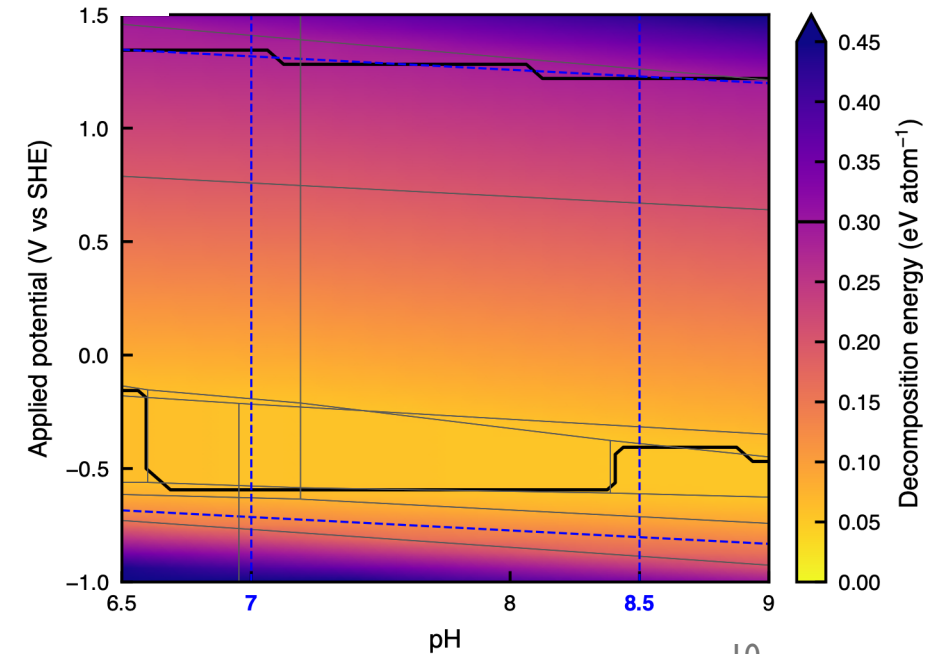
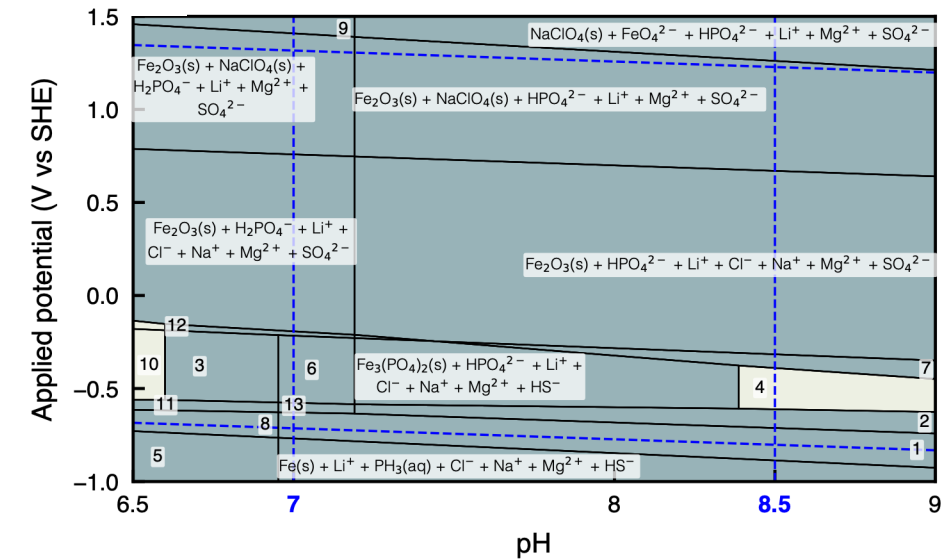


Seawater Pourbaix diagrams + seawater stability window

- Target region for solid (meta)stability

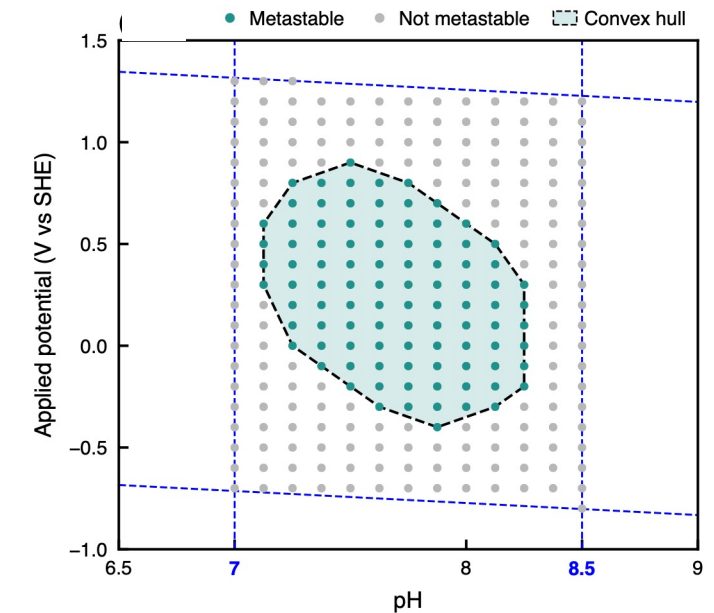
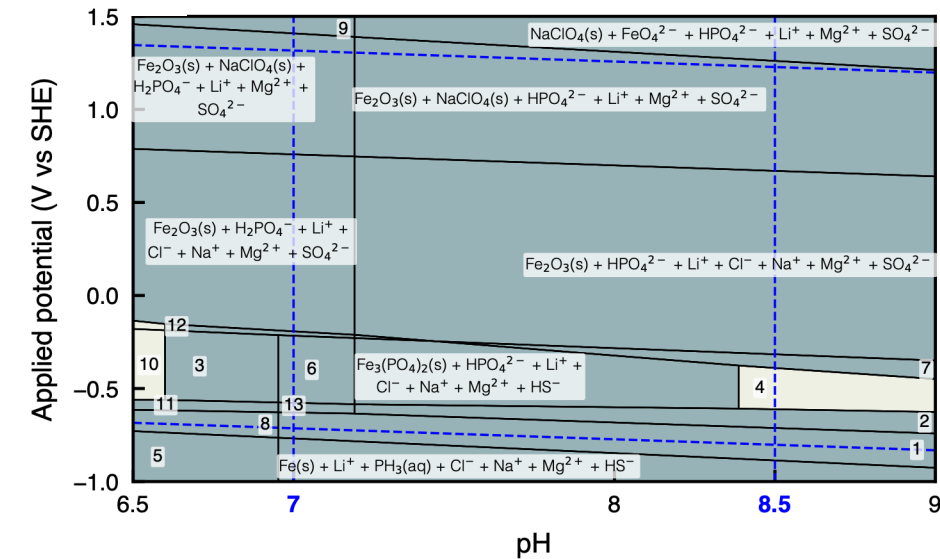
Metastability and overlap

- What defines metastability of a solid under seawater?
 - Should form a non-elemental, non-electroactive-ion containing solid as a decomposition product
- Within a certain threshold
 - Decomposition energy ≤ 0.3 eV/atom

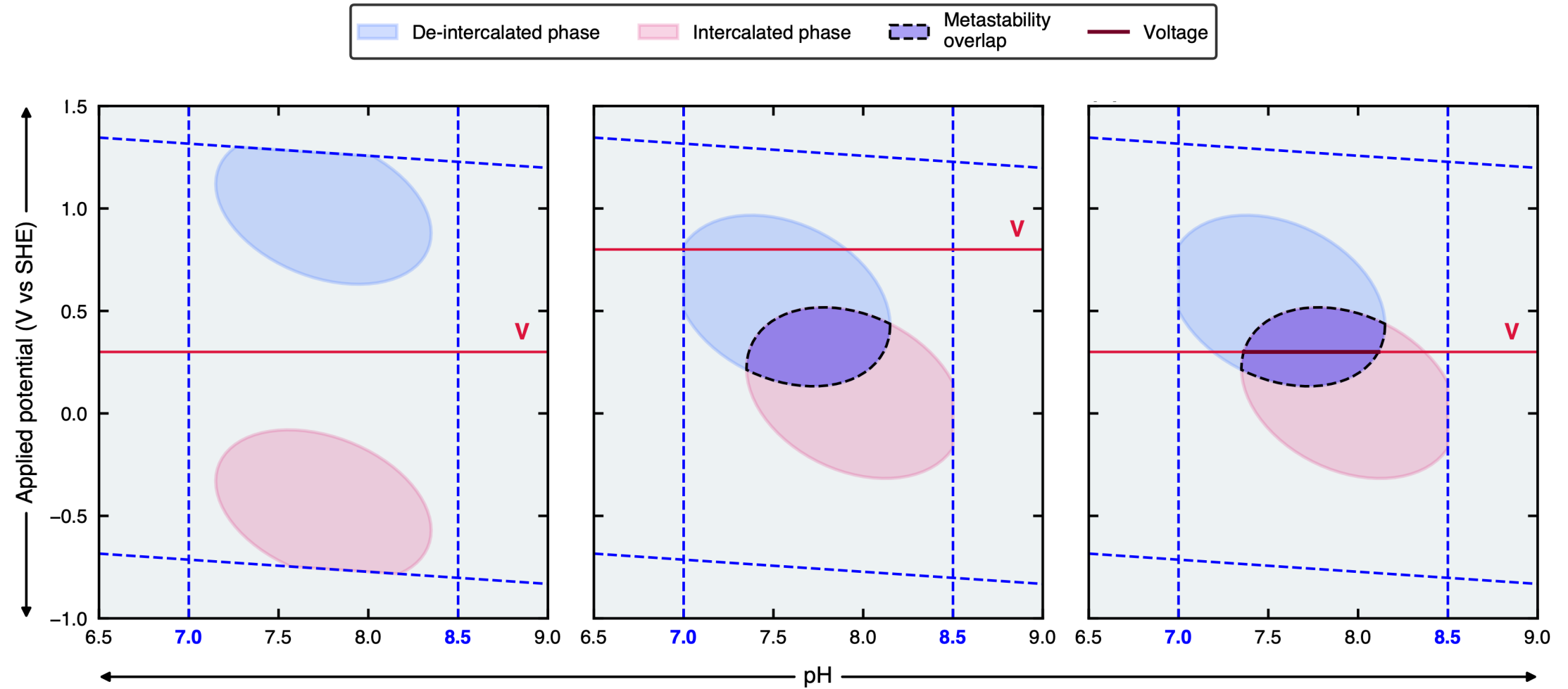


Metastability and overlap

- What defines metastability of a solid under seawater?
 - Should form a non-elemental, non-electroactive-ion containing solid as a decomposition product
- Within a certain threshold
 - Decomposition energy ≤ 0.3 eV/atom
- Should be metastable over a 'significant' region of the seawater stability window
 - 80% area (*vide sequentia*)

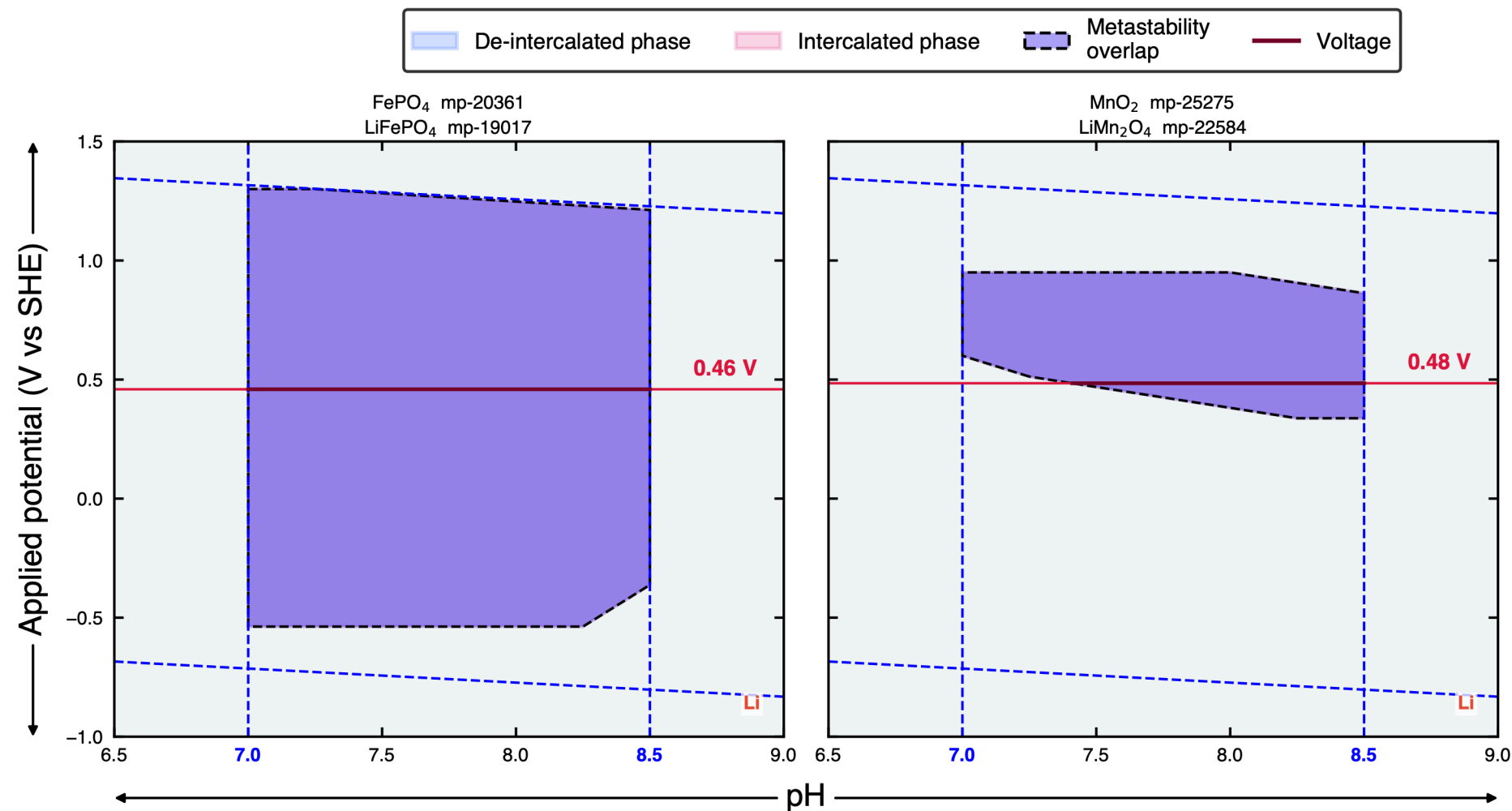


Intercalation voltages and metastability intersection



Intercalation voltage should pass through region of metastability overlap

Intercalation voltages and metastability intersection

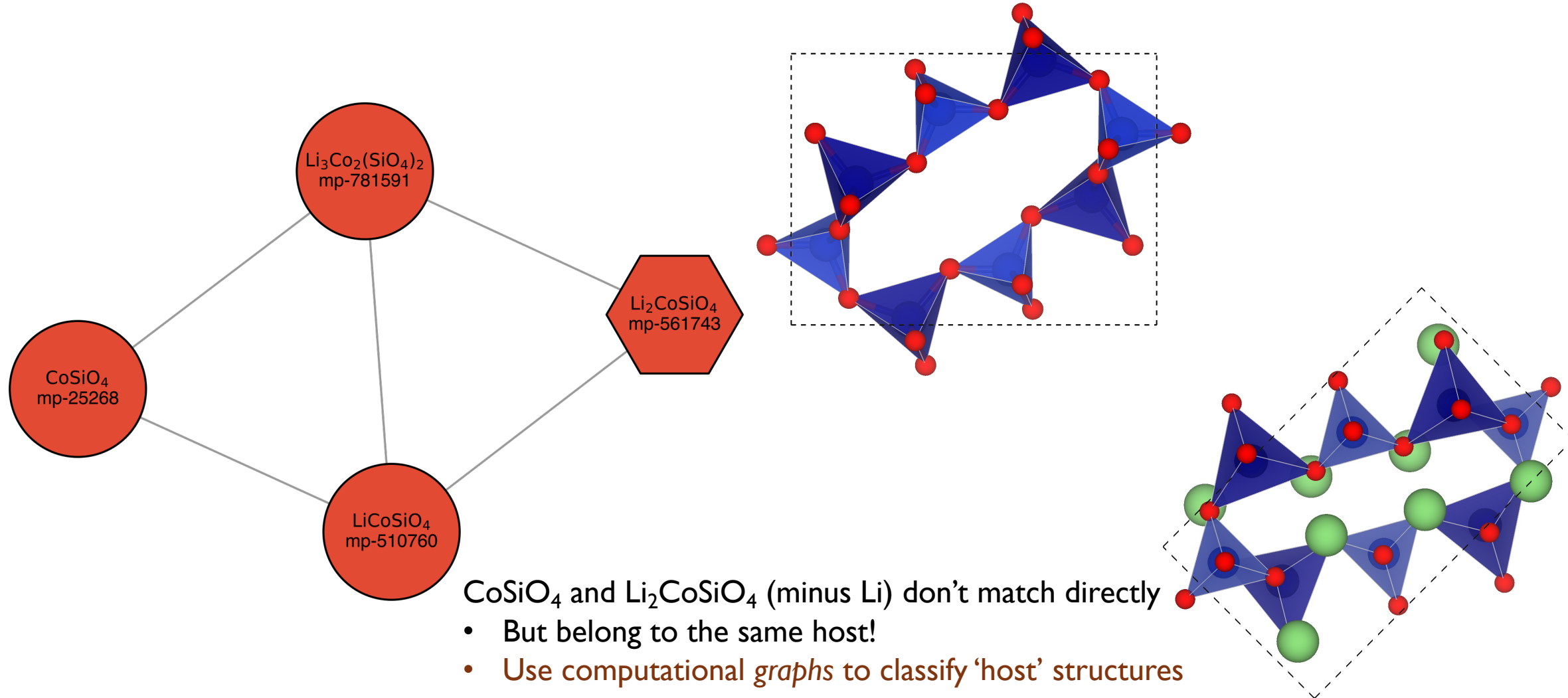


And voltage to be valid across entire seawater pH range

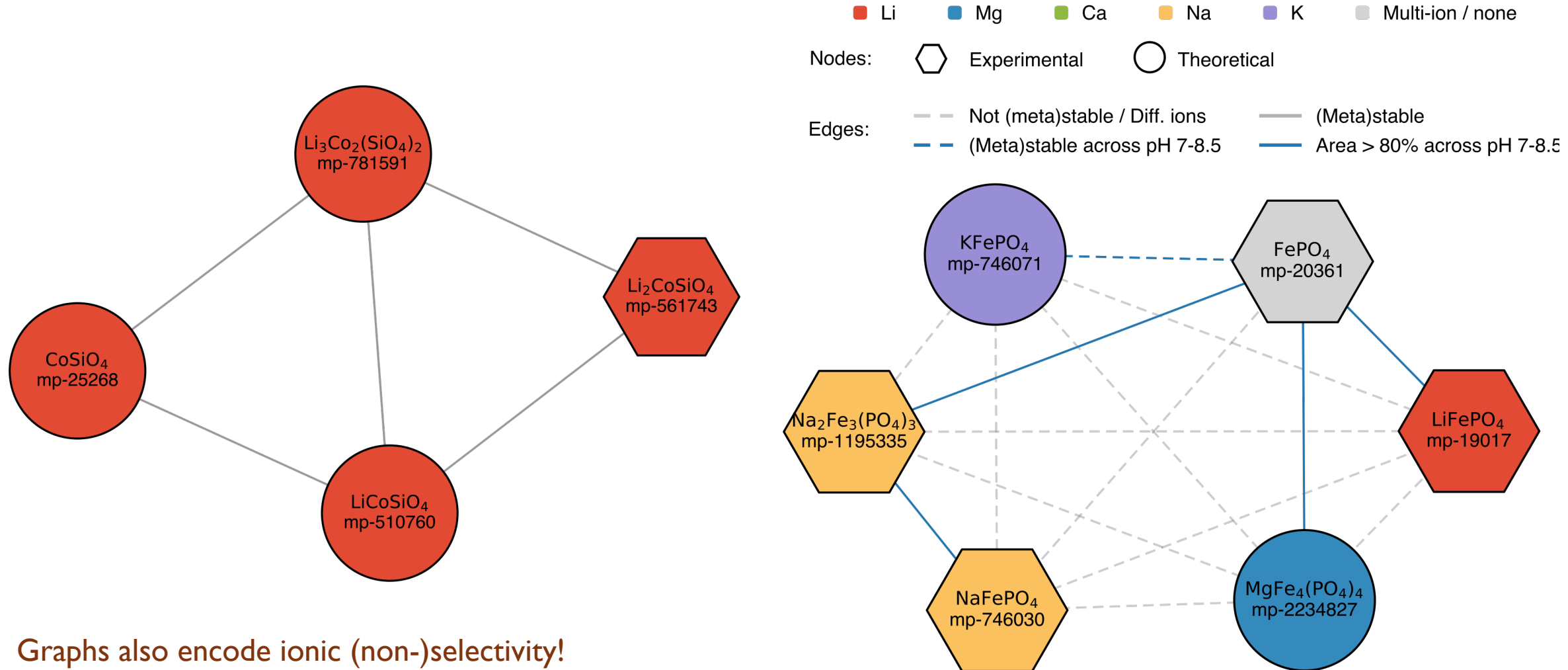
And intersecting metastability area should occupy $\geq 80\%$ of the seawater stability window

Intercalation voltage should pass through region of metastability overlap

Computational graphs and ionic (non-)selectivity



Computational graphs and ionic (non-)selectivity

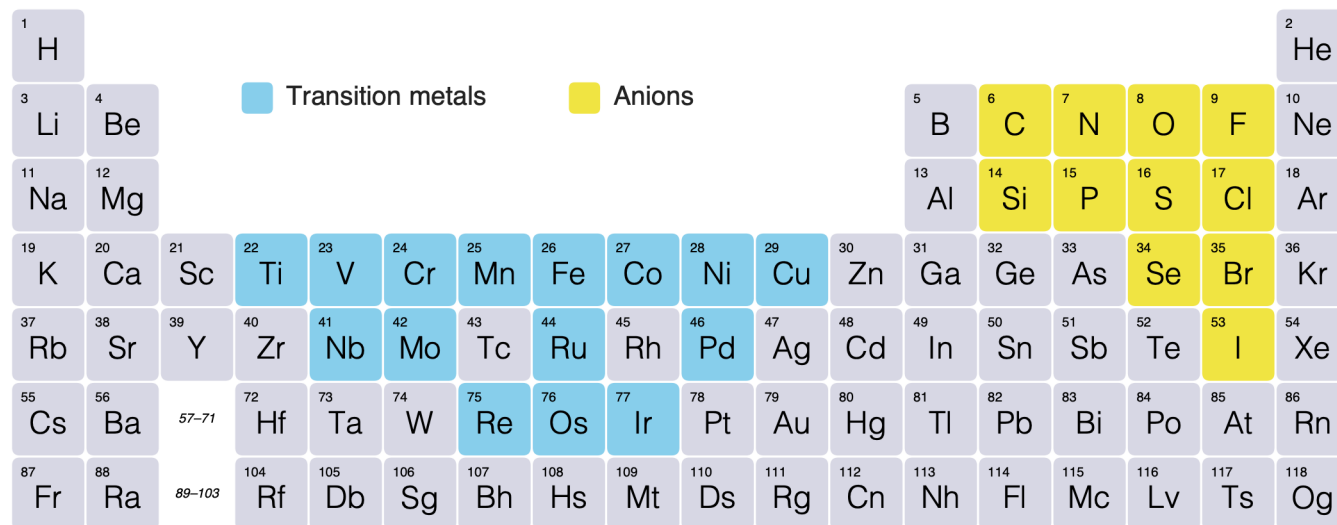


Graphs also encode ionic (non-)selectivity!

So, what do we get with this?

Need *seawater metastable* host structures with compatible (de)intercalation *voltage*, large intersecting *area of metastability*, and ionic *selectivity* (or non-selectivity)

Statistics (without selectivity)



Transition metals (blue) and Anions (yellow) are highlighted in the periodic table.

5 electroactive ions: **Li**, **Mg**, **Ca**, **Na**, or **K**

+

At most 3 out of 15 **transition metals**

+

At most 3 out of 11 **anions**

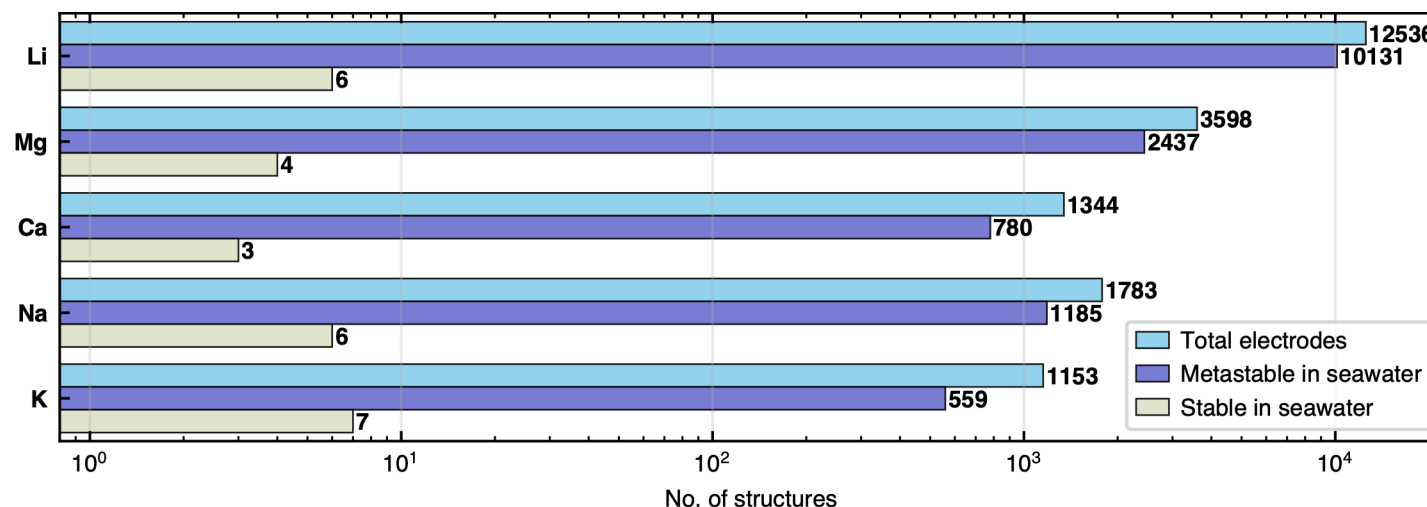
=

20,414 possible structures from Materials Project

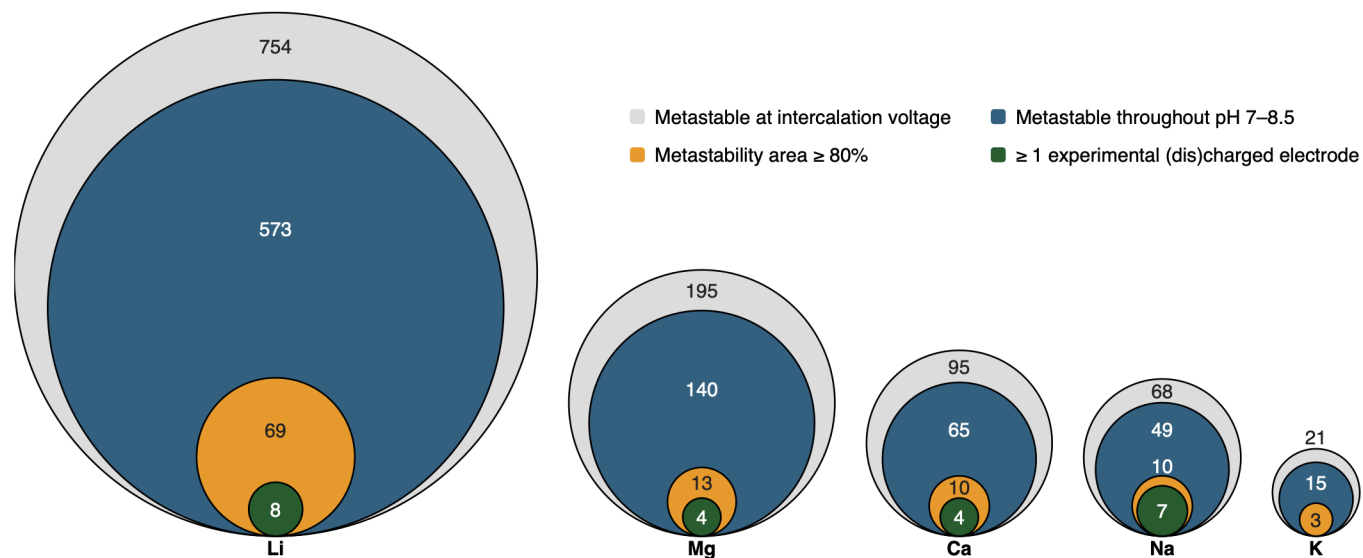
Total: queried electroactive-ion-containing structures

Metastable: individual intercalated structures (not pairs)

Stable: too few, only over a small seawater region



Statistics (without selectivity)



Yellow: satisfies metastability (overlap and area), and voltage criteria

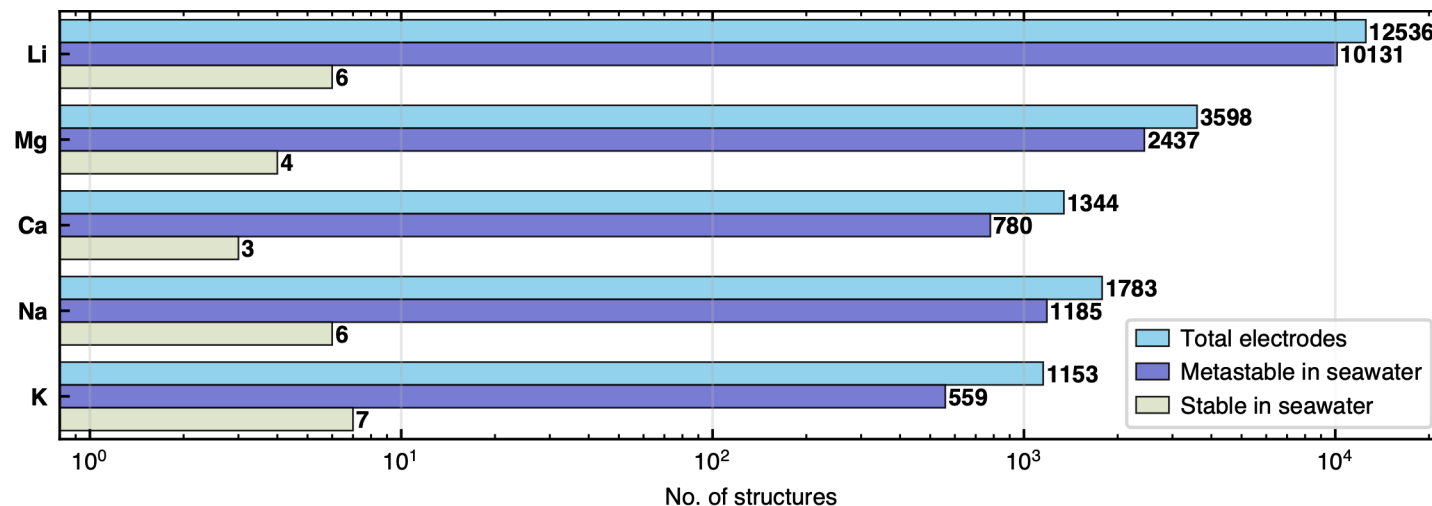
Green: at least one structure in the computational graph is experimental

No selectivity data included

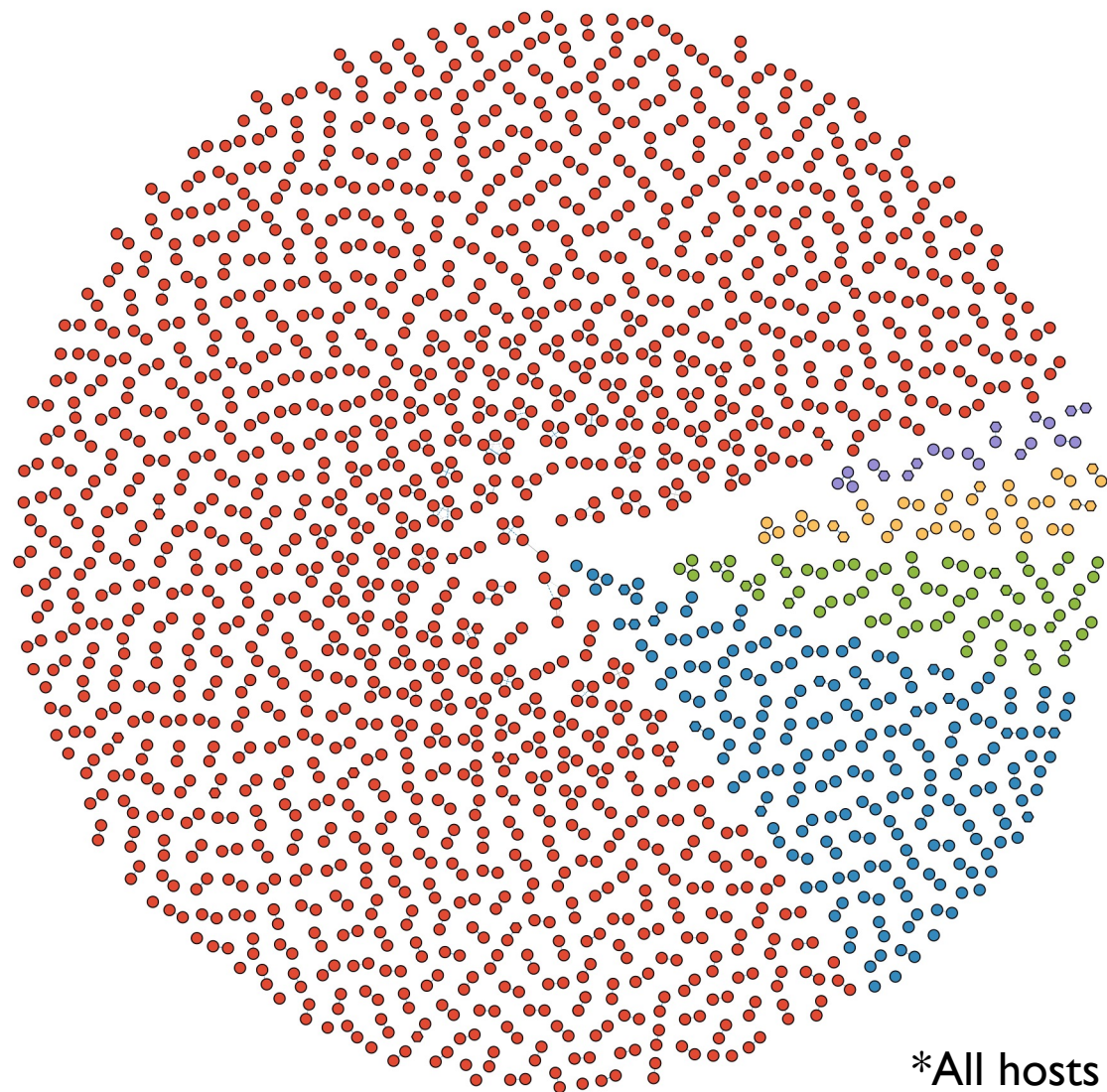
Total: queried electroactive-ion-containing structures

Metastable: individual intercalated structures (not pairs)

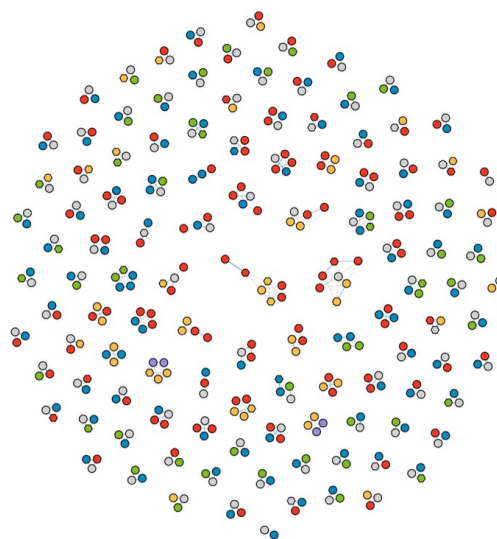
Stable: too few, only over a small seawater region



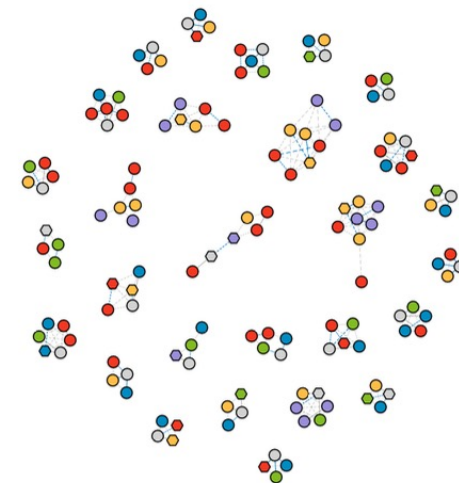
Statistics (with selectivity, ignoring area*)



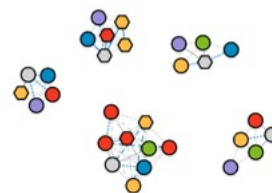
859 ion-selective hosts (690 **Li**, 108 **Mg**, 33 **Ca**, 18 **Na**, 10 **K**)



115 2-ion hosts

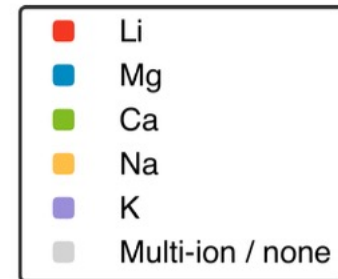


28 3-ion hosts



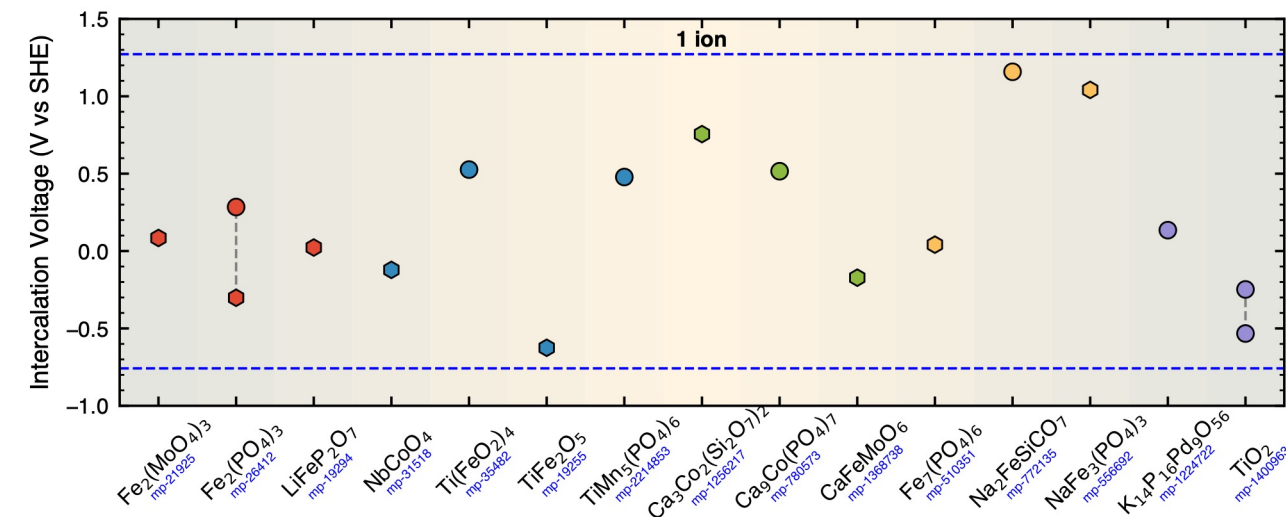
5 4-ion hosts

0 5-ion hosts



*All hosts have voltage within their metastability overlap

Combining all criteria: 1 ion-selective, 8 non-selective hosts are promising



Include ionic selectivity + progressive filters on metastability and voltage

Li: focus on experimentally known hosts (3)

2 experimentally known hosts each for **Mg**, **Ca**, and **Na**

Hollandite-TiO₂: theoretical, promising **K**-selective host

Similarity in intercalation voltages: also needed for non-selective intercalation

Fe-containing non-olivine FePO₄ polymorphs, Fe₂(MoO₄)₃, Fe(PO₃)₃, and FePCO₇: for 2-ion intercalation

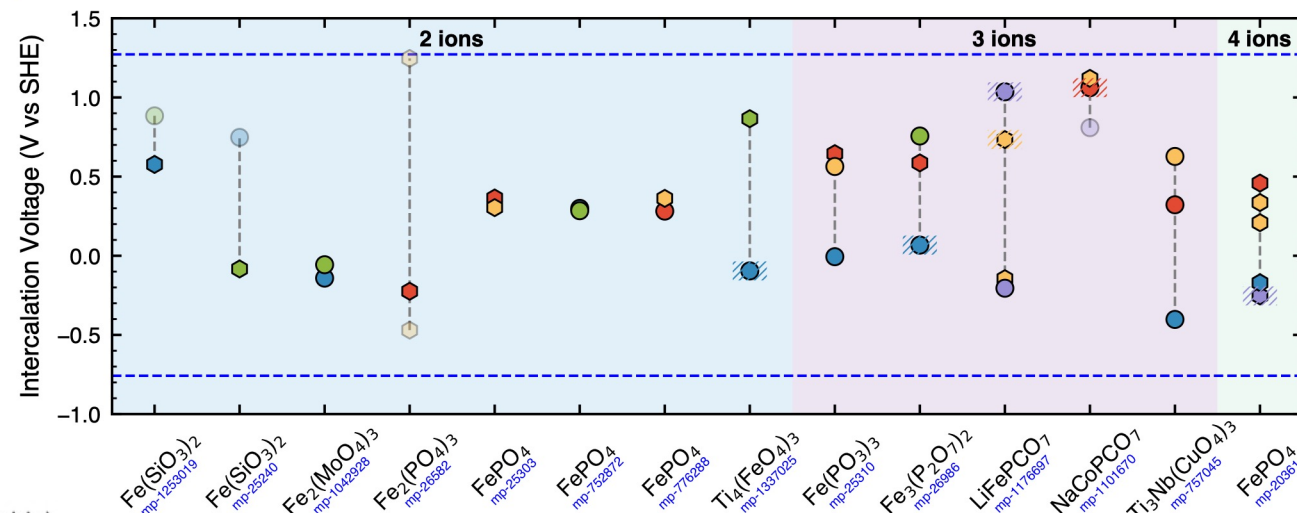
Olivine-FePO₄: best possible desalination electrode

 Experimental
  Theoretical
  70% < area < 80%
  Other ion (not seawater stable)

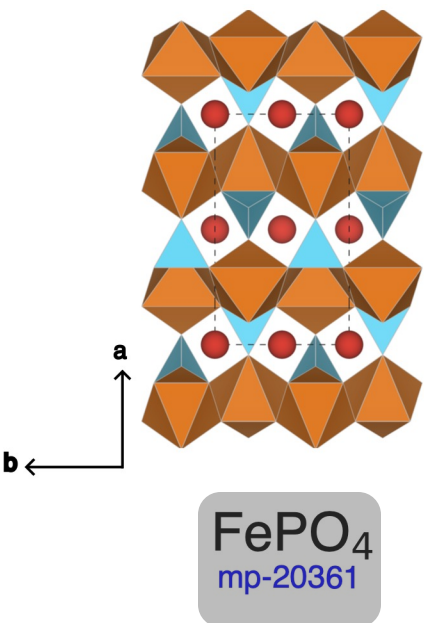
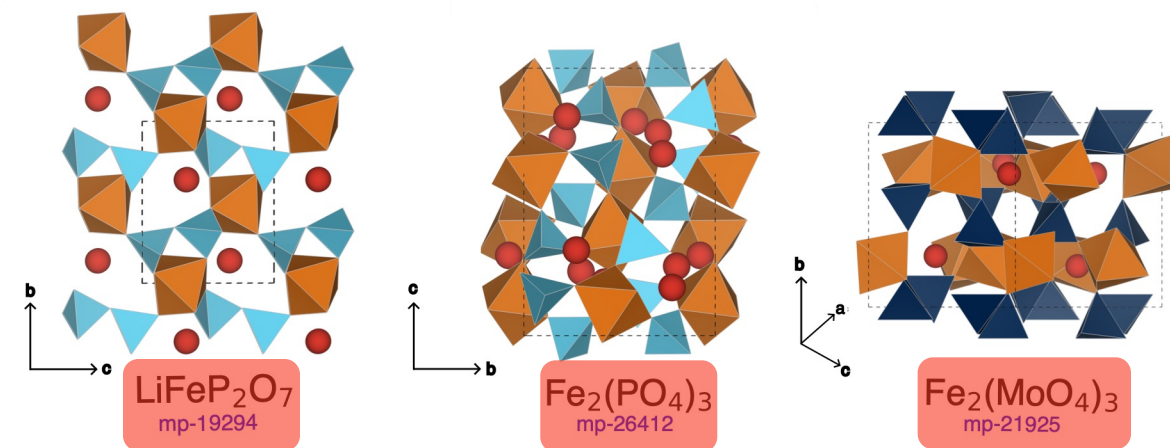
Ion recovery screening

Li, **Mg**, **Ca**, **Na**, **K**

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Candidate ion-selective and desalination electrodes



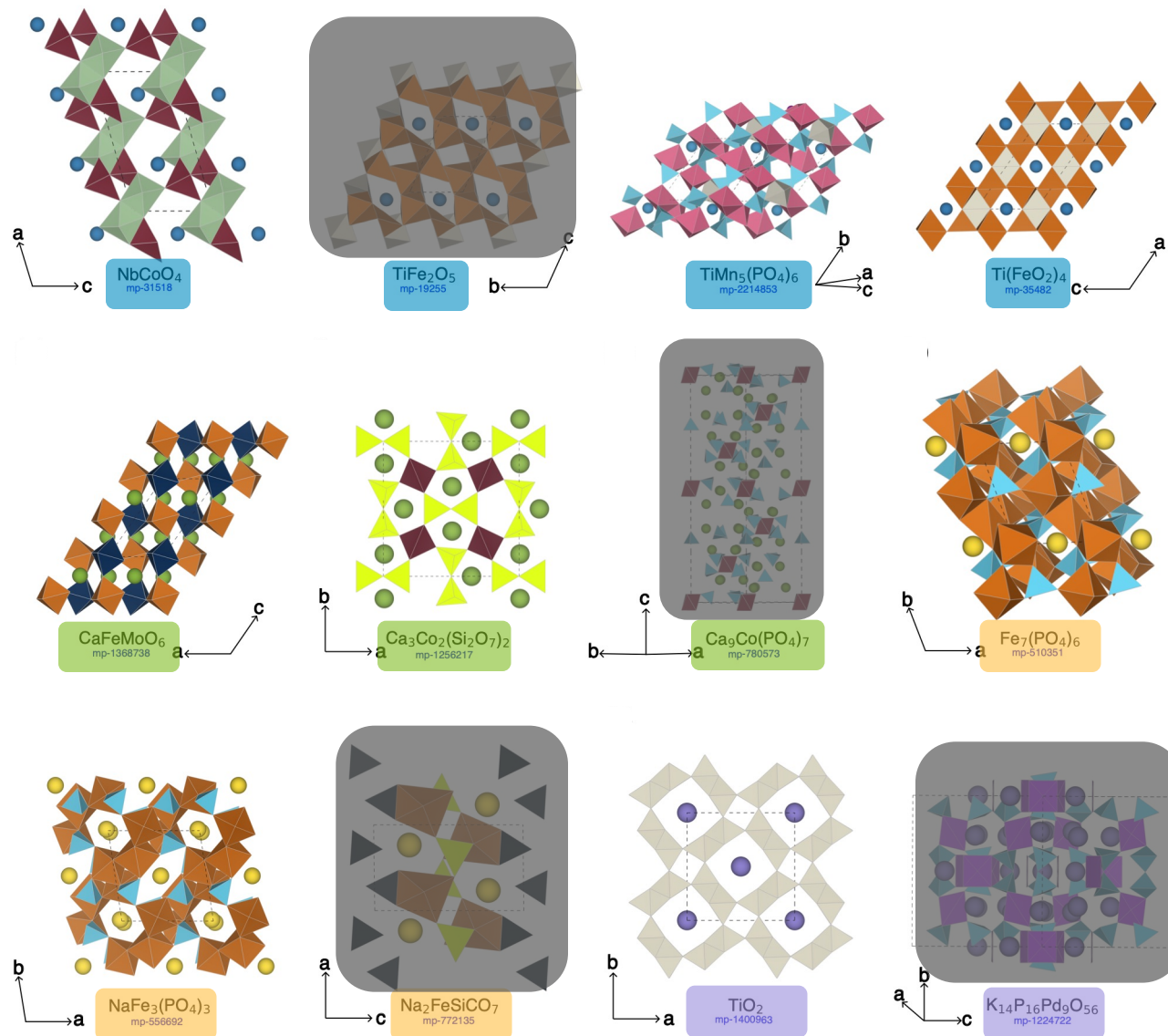
Ion recovery screening

No ideal desalination electrode

Possible kinetic, capacity, synthesis,
and cost limitations: **II** ion-selective

Several candidates with Fe and P:
solid decomposition product(s)

Li, Mg, Ca, Na, K



Take-aways

- Intercalation electrode discovery can improve electrochemical ion capture, for ion-recovery and desalination
- *Seawater* Pourbaix diagrams + stability windows, re-defining *metastability*, requirement of *overlap* and maximizing intersection area, optimal intercalation *voltage*, computational *graphs* for ionic (non-)selectivity
- **20,414** structures in Materials Project → **11** promising ion-selective, **8** non-selective (**1** desalination) hosts

“Identifying intercalation electrodes for electrochemical ion recovery and desalination”, S. Purohit, A. Kuhlmann, M. Huck, H-G. Steinrück, and G. Sai Gautam, under review [[arXiv 2610.20834](https://arxiv.org/abs/2610.20834) (2026)].

saigautamg@iisc.ac.in; <https://sai-mat-group.github.io>; <https://github.com/sai-mat-group>

