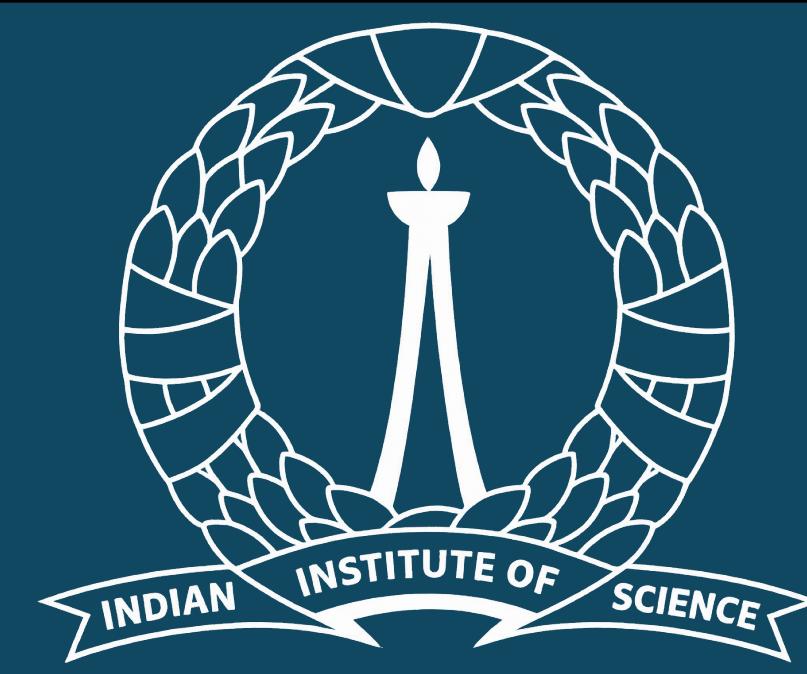


High-throughput screening of intercalation electrodes for electrochemical ion-capture and desalination



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भारतीय विज्ञान संस्थान

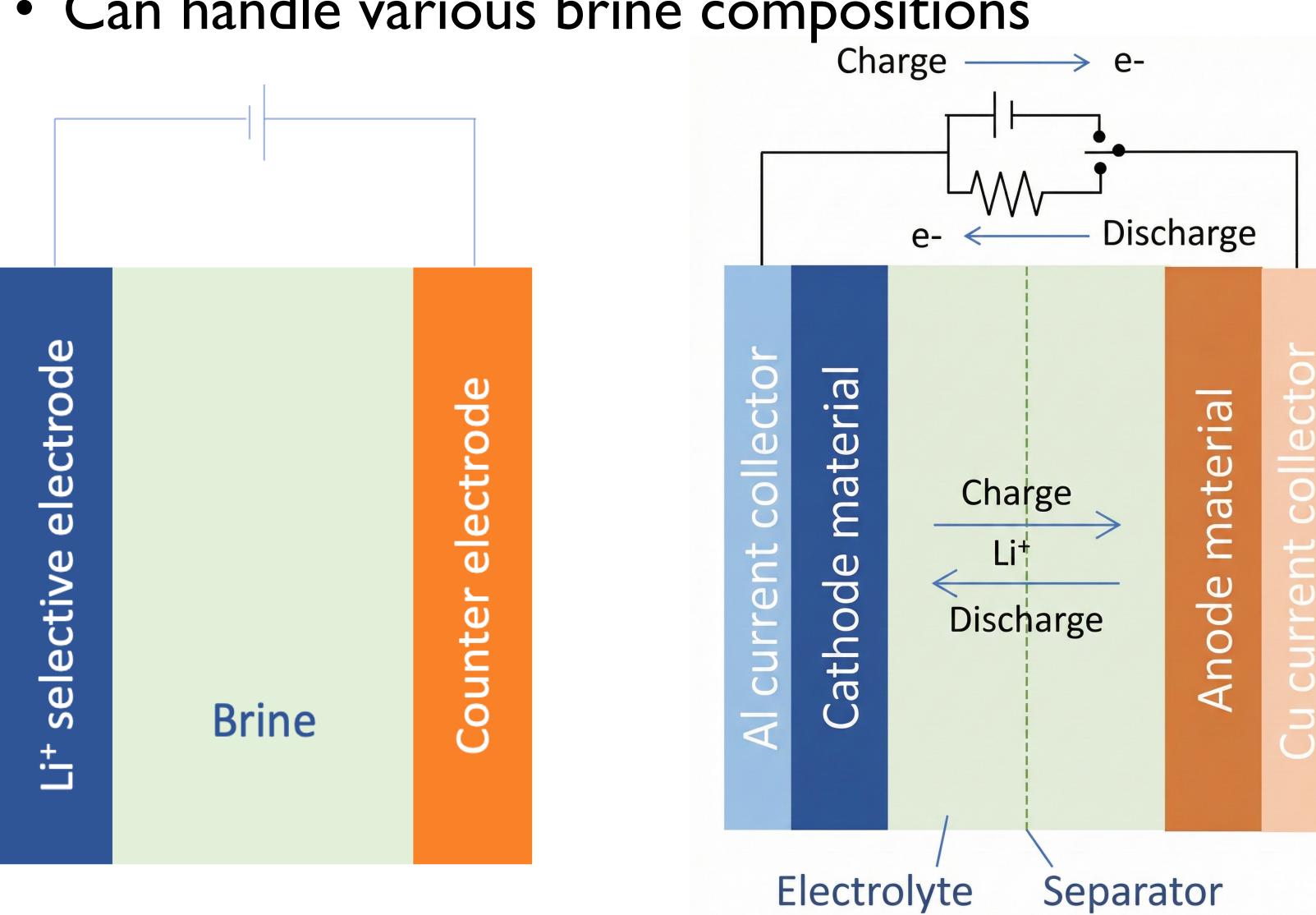
INTRODUCTION

- Li in brine sources > Li in rock sources
- Extraction cost from rocks $\approx 2 \times$ cost from brines¹
- Slow traditional extraction methods from brines



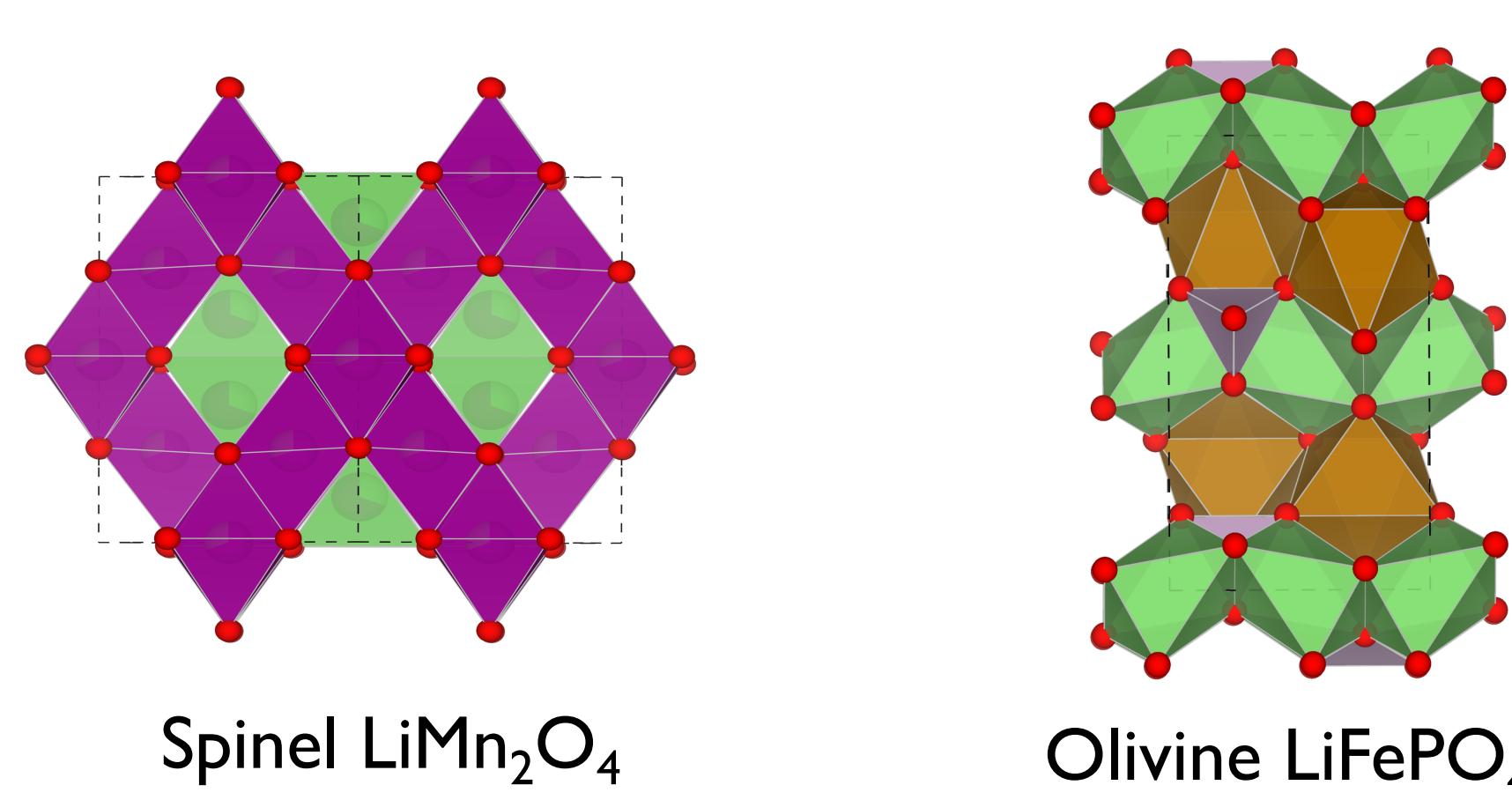
Electrochemical ion-recovery:

- Faster, low energy consumption
- Similar to Li-ion Battery (LIB)
- Can handle various brine compositions



Current state of the art electrodes:

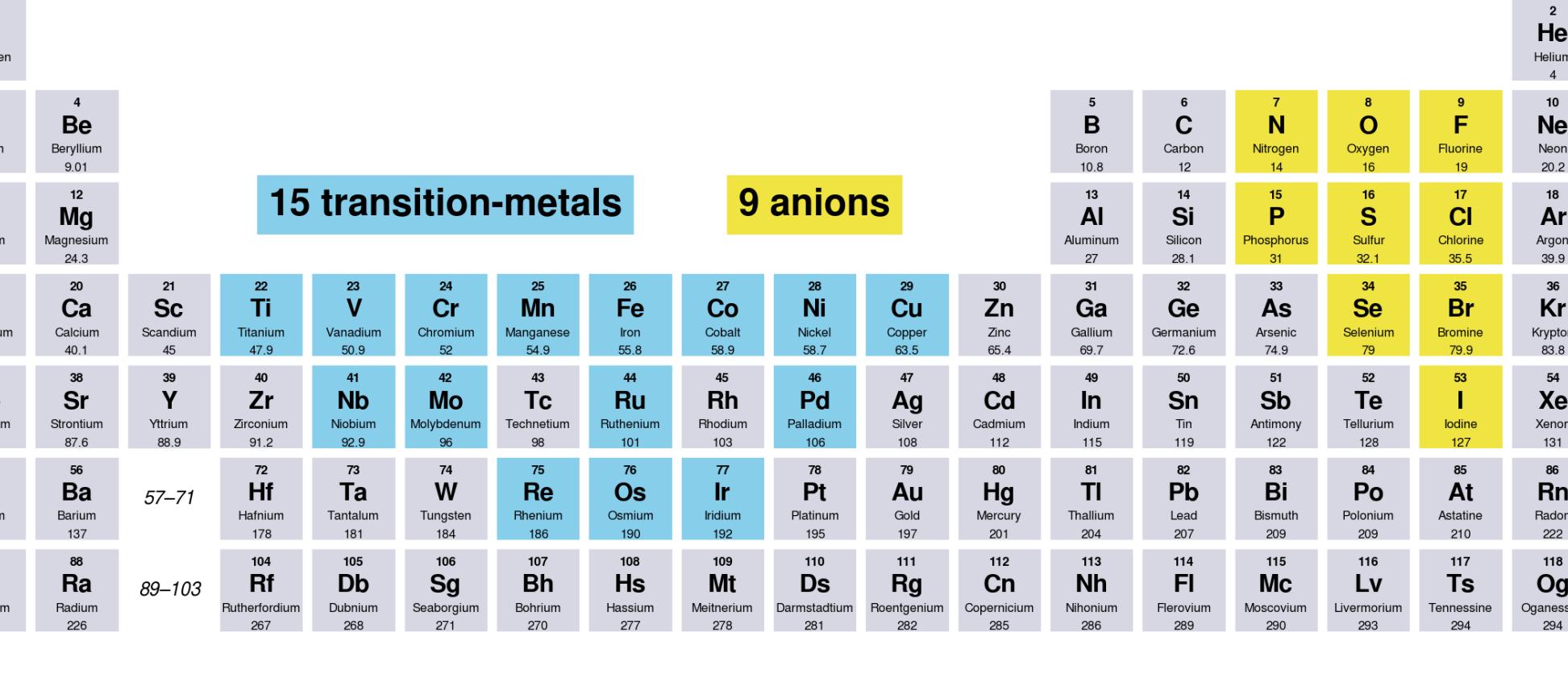
- Poor cycling stability of LiMn₂O₄
- Poor electronic conductivity of LiFePO₄
- Can better ion-capturing electrode be found from the pool of battery intercalation cathodes?



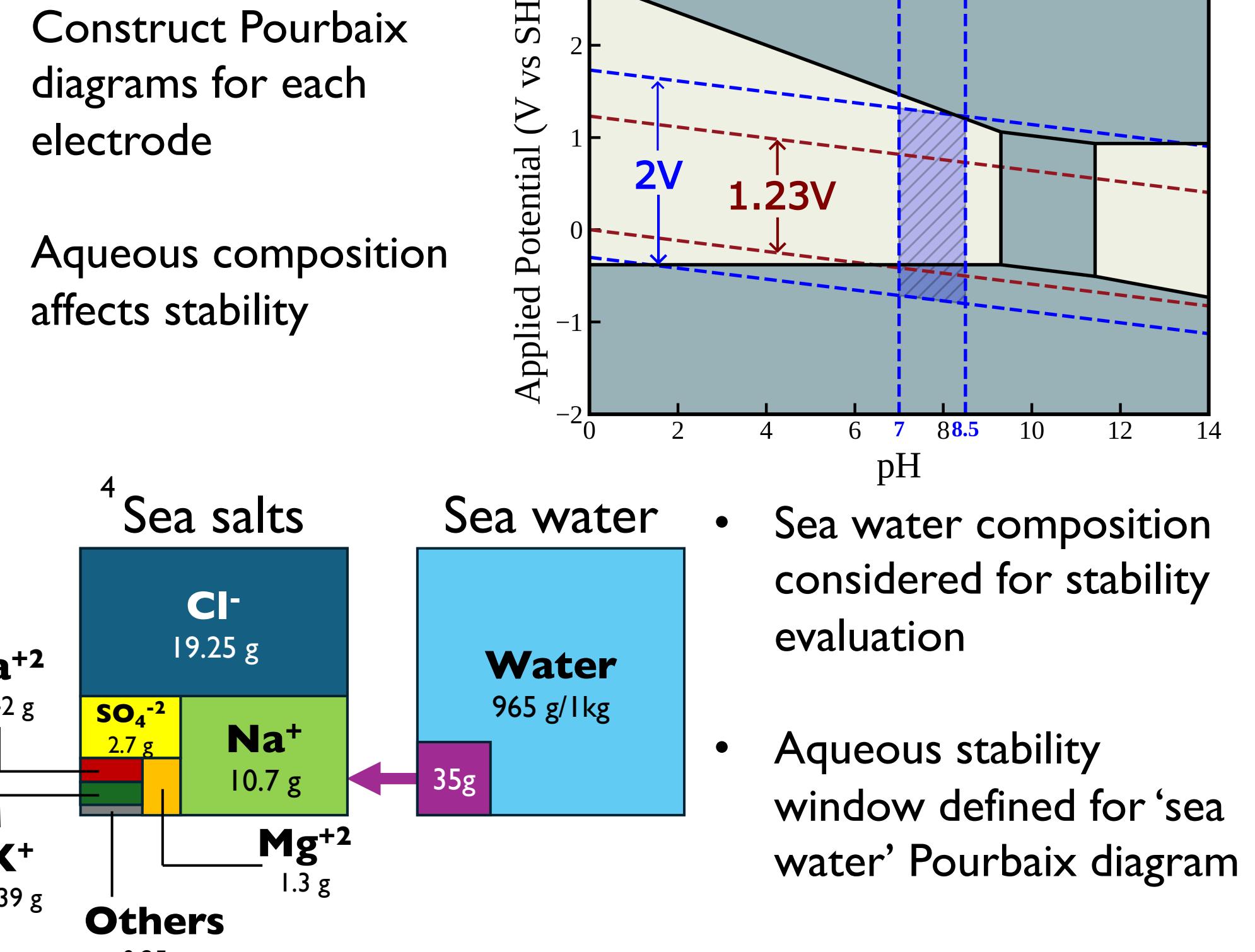
WORKFLOW

1 Query first-principles cathodes data across ions

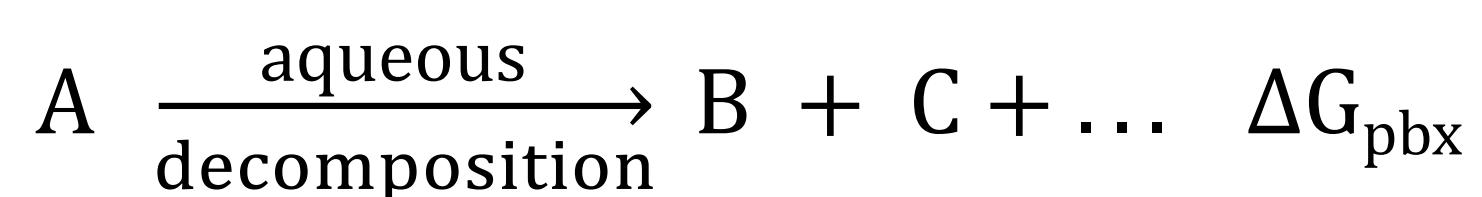
- All Li / Na / K / Mg / Ca electrodes with at most 3 transition metals and 3 anions from the Materials Project database



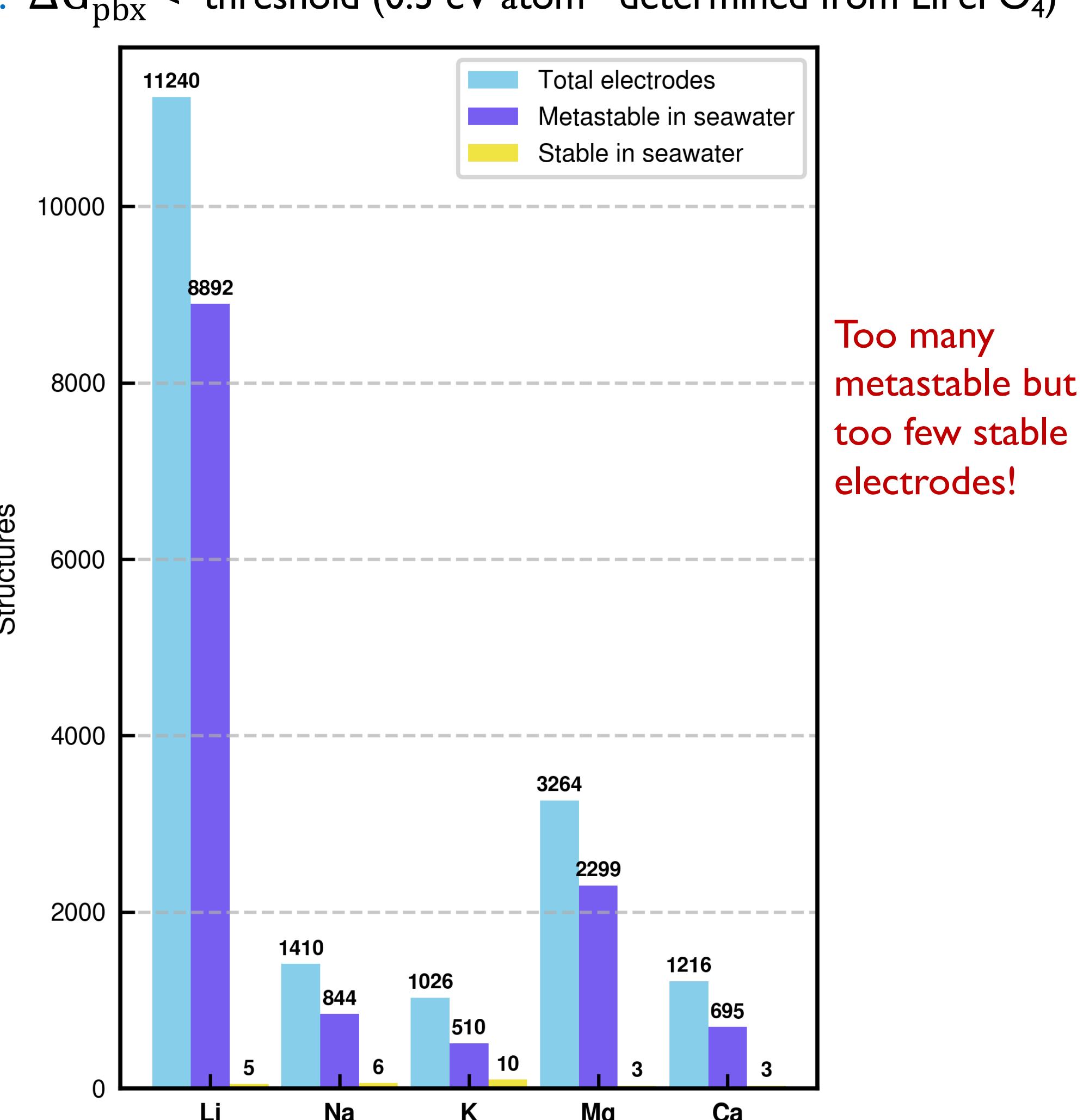
2 Determine aqueous stability of the cathodes



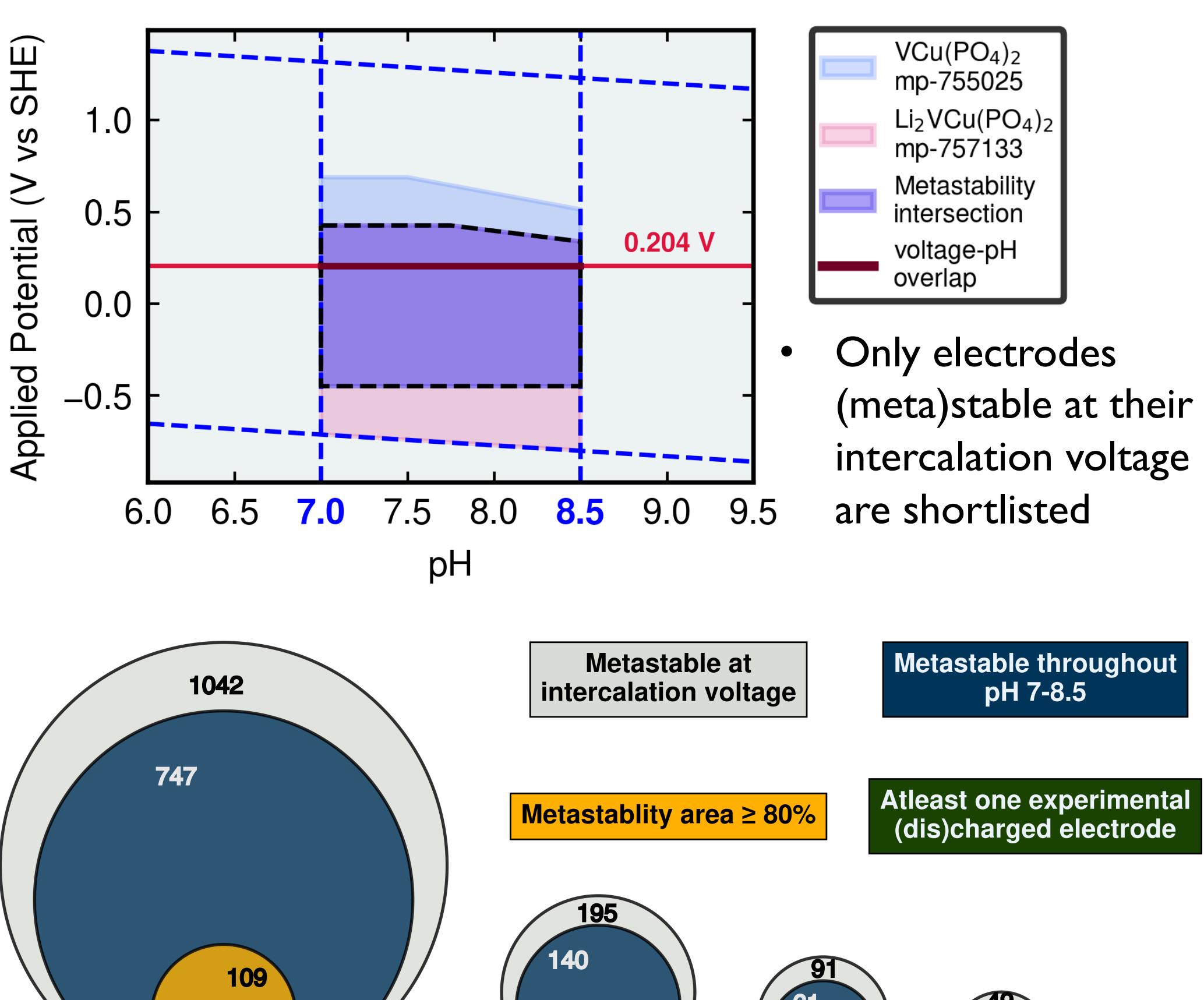
Sea water metastability criteria of electrode 'A':⁵



- At least one of B, C ... is a solid
- The solid is non-elemental and doesn't contain the working ion
- $\Delta G_{\text{pbx}} <$ threshold (0.3 eV atom⁻¹ determined from LiFePO₄)



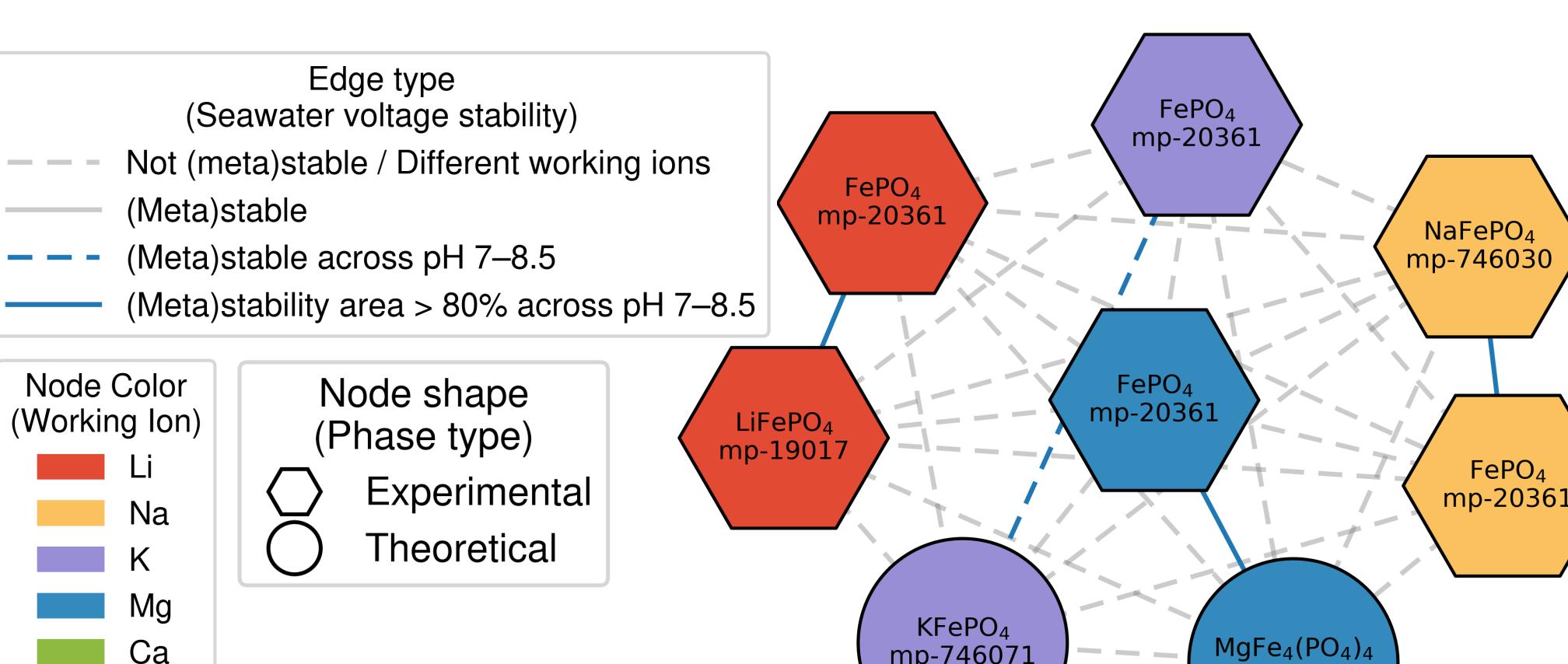
3 Calculate the intercalation voltage



- Only electrodes (meta)stable at their intercalation voltage are shortlisted

4 Compare frameworks across ions

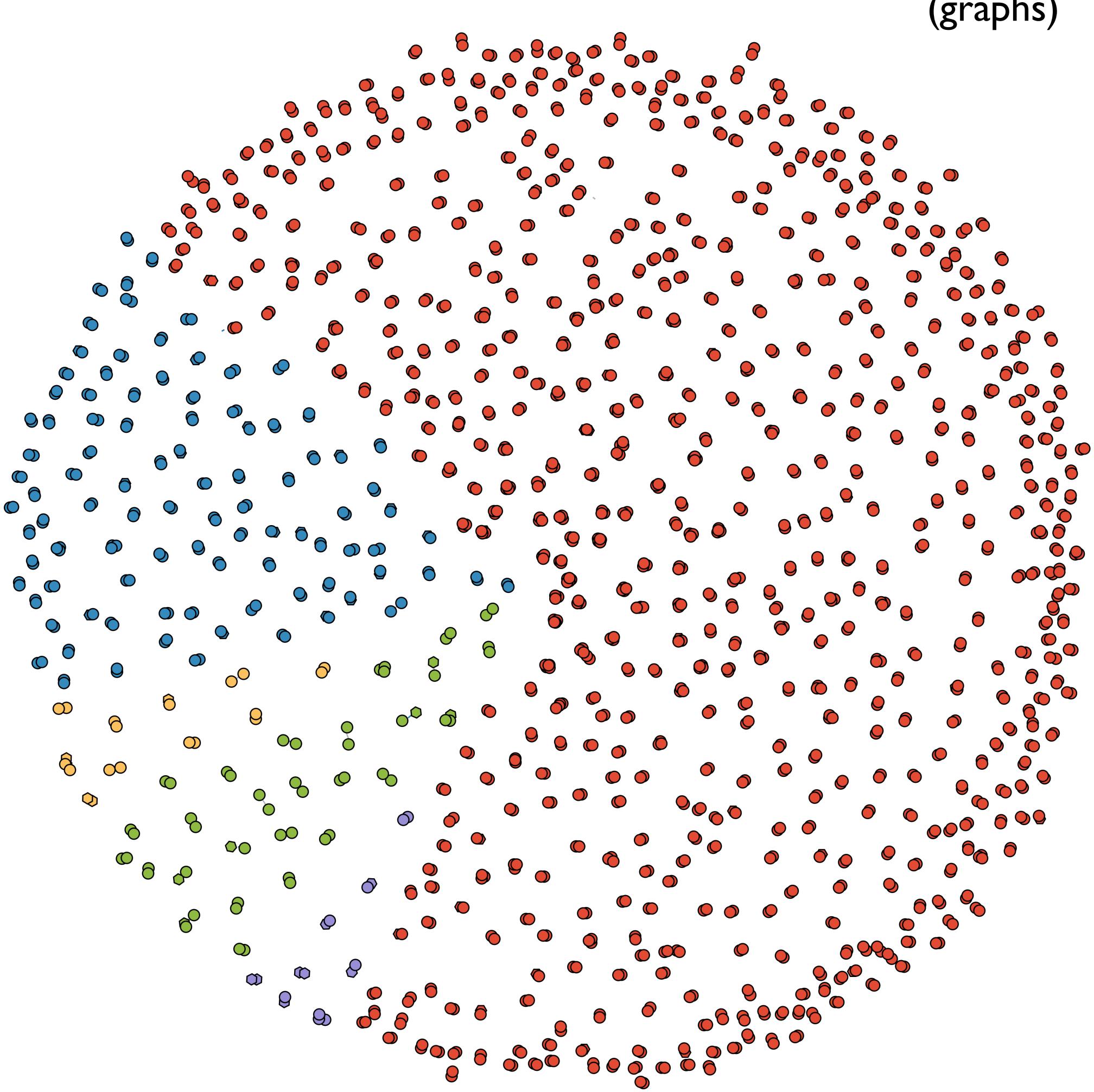
- Computational graphs are created to identify Li-selective and multi-ion selective (desalination) electrodes



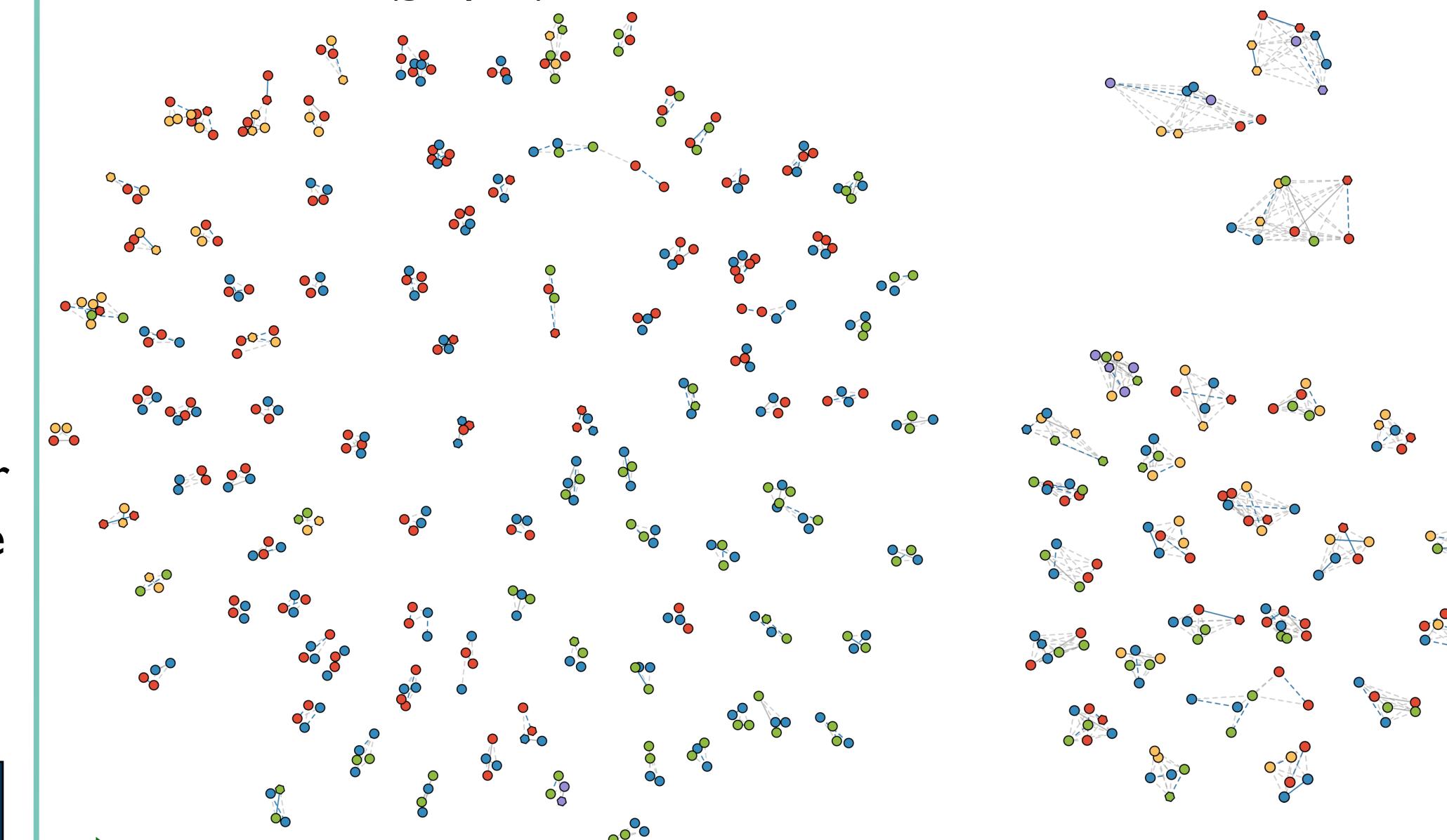
- Strongest candidates are graphs with solid blue edges connecting at least one hexagonal node

RESULTS

- 587 Li, 11 Na, 8 K, 94 Mg, and 27 Ca selective frameworks (graphs)

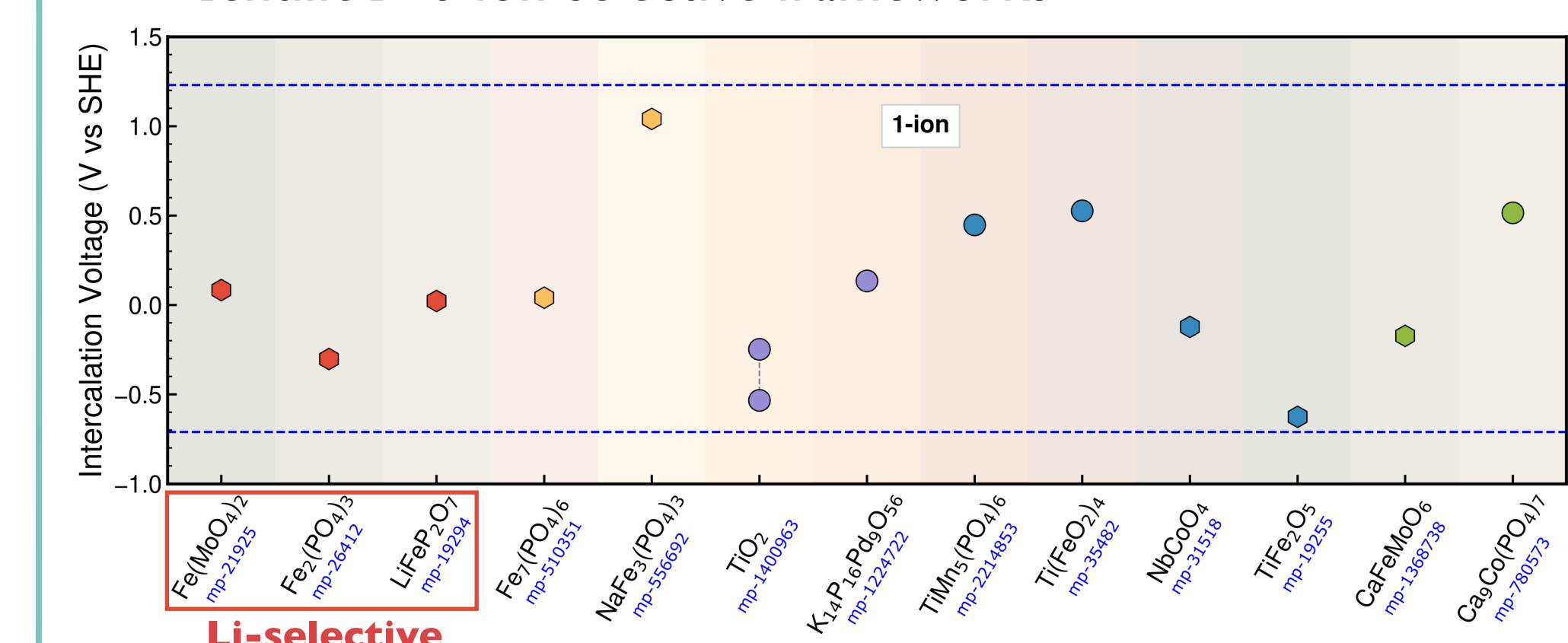


- 92 2-ions, 22 3-ions, 3 4-ions and 0 5-ions intercalating frameworks (graphs)



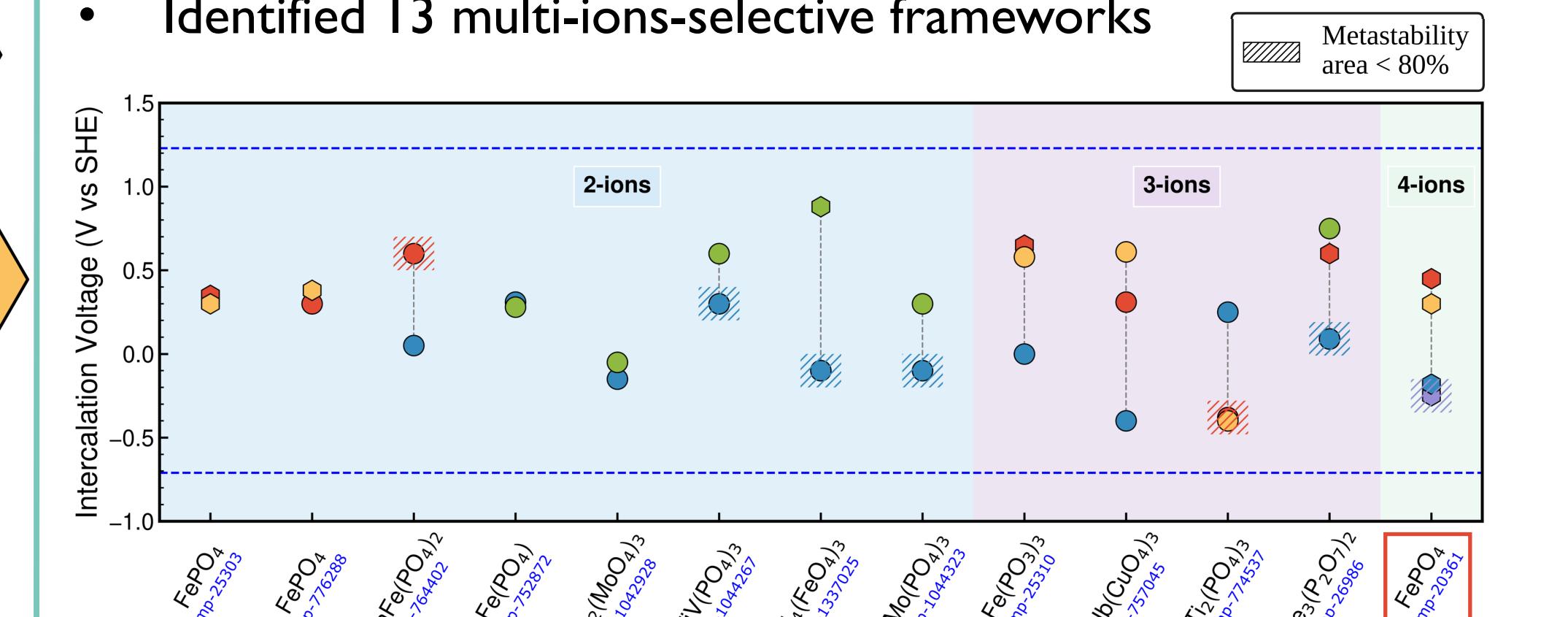
Ion-selective electrodes

- Identified 13 ion-selective frameworks



Multi-ion-selective electrodes

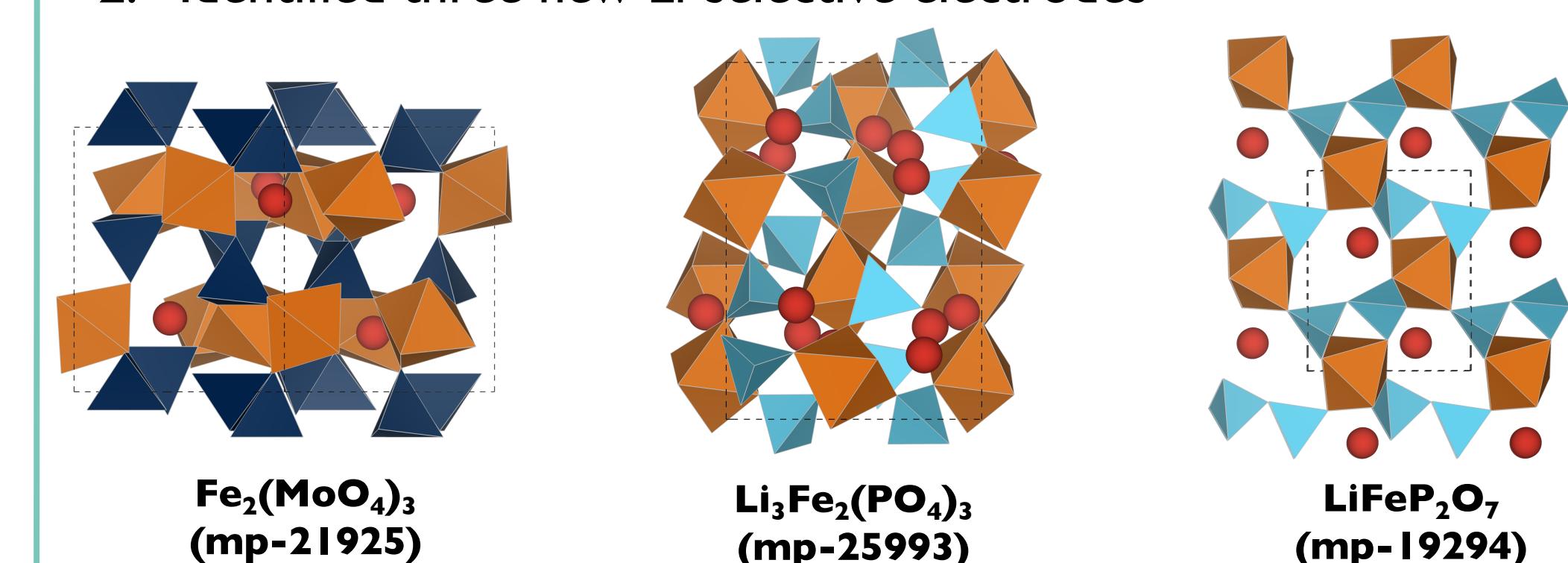
- Identified 13 multi-ions-selective frameworks



CONCLUSION

- Developed a framework to evaluate sea water (meta)stability of battery electrodes under operating conditions

- Identified three new Li-selective electrodes



- Identified olivine LiFePO₄ as a candidate desalination electrode

ACKNOWLEDGEMENTS

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