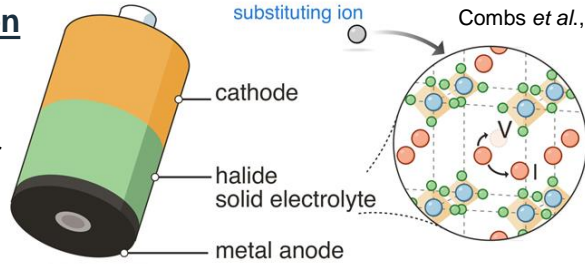


# Defect Studies in Halide Solid Electrolytes for High-Voltage Battery Applications

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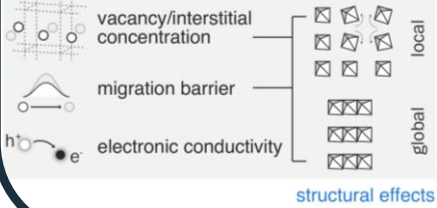
## Introduction

Solid electrolytes demonstrate improved stability and safety, but their ionic conductivity falls behind liquid counterparts



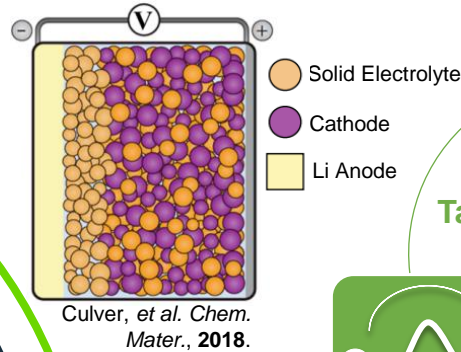
Combs et al., *J. Electrochem. Soc.*, 2022.

### aliovalent and isovalent substitutions



Chemical substitution enables physical changes beneficial to ion migration. Understanding these structure-property-dynamics relationships provides insight into targeted materials design.

## Graphs / Diagrams



Culver, et al. *Chem. Mater.*, 2018.

## Targeted Synthesis Approach



Using computational predictions to inform experimental targets – increased efficiency, decreased cost

**Challenge:** Poor ionic conductivity limits battery transport mechanisms

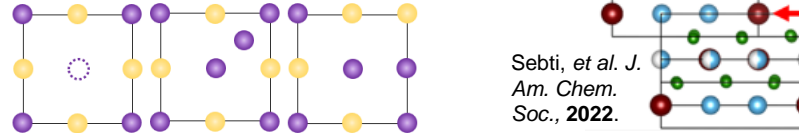
## Research Highlights

**Increased disorder in lattice structure increases ionic conductivity**

Thermal disorder → atoms move around in their sites

Site disorder → interrupting crystal periodicity

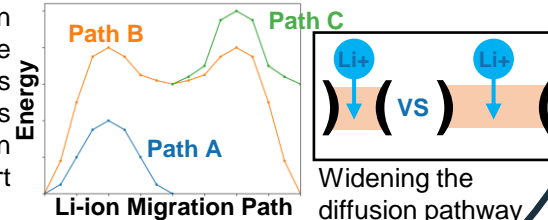
Stacking faults → interrupting plane periodicity



Sebti, et al. *J. Am. Chem. Soc.*, 2022.

**Increased ion migration is an artifact of lattice frustration**

Different migration pathways require different energies – lowest E path is best for fast ion transport



Widening the diffusion pathway allows ions to move more freely

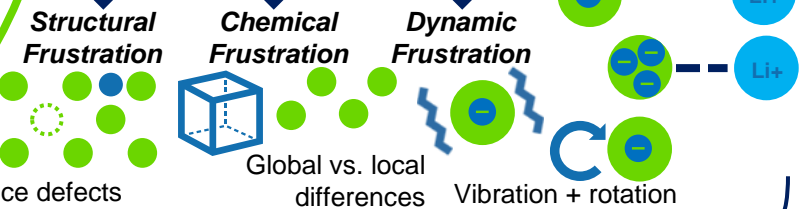
Atomic packing density dictates migration mechanism



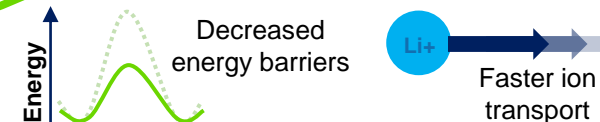
Induced disorder and lattice frustration will increase conductivity – *but how do we systematically introduce disorder?*

## Discussion

**Inductive Effects/ Bond Strength**



Lattice defects, Global vs. local differences, Vibration + rotation



**Better batteries!**

## Materials And Methods

- Solid state synthesis of  $\text{Li}_3\text{InCl}_6$  and  $\text{Li}_3\text{ScCl}_6$
- Substitution of 4+ metal at the 3+ metal site



- X-ray diffraction → Structural information
- Impedance spectroscopy → Electrochemical properties

