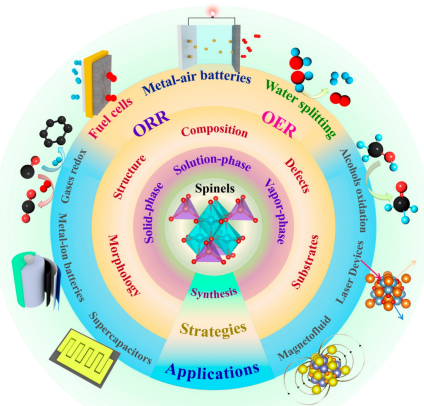




# Breakdown of the Small-Polaron Hopping Model in Higher Order Spinels FOCUSING ON THE FUTURE

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## Motivation: Integration of Spinels in Energy



Spinel oxides have exciting electronic, electrochemical, and magnetic properties

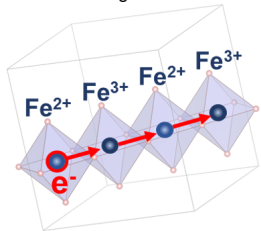
Useful for application in data storage, batteries, supercapacitors, catalysis

Integration of spinels in devices limited by low electronic conductivity

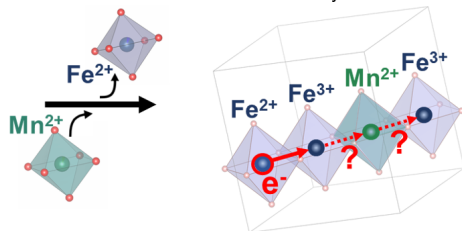
Zhao, Qing, et al., *Chemical reviews* 117 (2017)

## Problem statement: How does charge flow in spinels?

Charge transfer pathway along Fe atoms

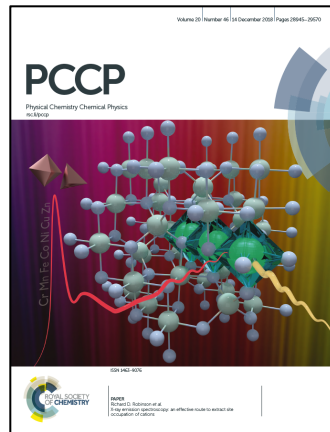
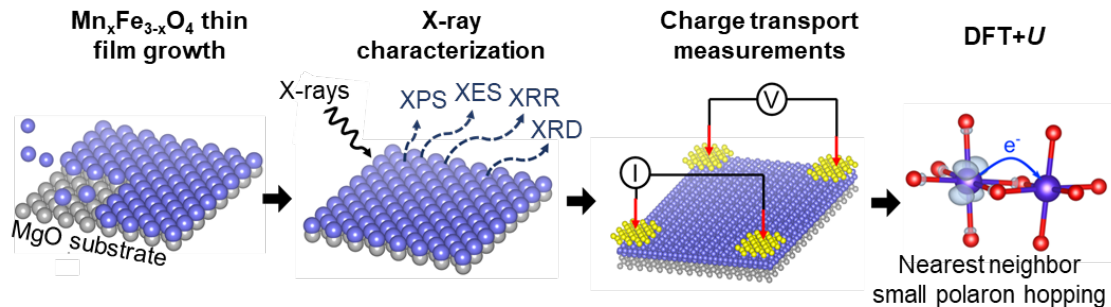


Charge transfer pathway affected by Mn atom



- Mechanism of charge transport: Nearest-neighbor small polaron hopping
- Original model does not consider presence of multiple active species at Oh sites!

## Our Approach to developing a new transport model



## New transport equation

$$\sigma = \chi \cdot \left[ \frac{\sigma_{0,mixed}}{T} \cdot \exp\left(-\frac{E_{A,mixed}}{KT}\right) \right] + (1 - \chi) \cdot \sum_M \gamma_M \frac{\sigma'_{0,M}}{T} \cdot \exp\left(-\frac{E_{A,M}}{KT}\right)$$

## Validation of our new polaron transport model

