# Boron Nitride Modulates Crystallinity and Charge Mobility in PEO Electrolytes

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## Introduction

**Why Polymer Electrolytes?**

- Sustainable battery technology is needed to store energy from intermittent renewable sources.
- Na is more abundant and less expensive than Li.[1]
- Polymer electrolytes improve Na-ion battery safety.
- We study how adding boron nitride (BN) nanoflakes to poly(ethylene oxide) (PEO) electrolytes with sodium nitrate. ($NaNO_3$) can modulate polymer crystallinity and ion transport properties.

**Why Boron Nitride?**

- Boron is Lewis acidic, while nitrogen is Lewis basic.
- Boron nitride (BN) is an **active filler**: its dual Lewis acidity and basicity allows it to bind with ions.

## Experimental Procedure

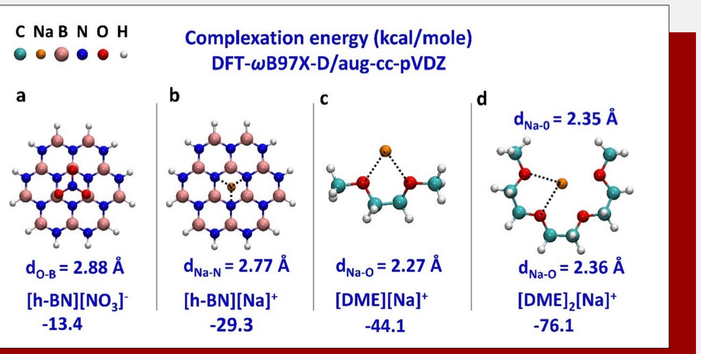
*Suspensions of PEO, $NaNO_3$, and BN in $H_2O$ cast on glass slides. Percolation threshold of BN is 3.48 wt%*

*Electrolytes vacuum dried at 120°C for 16 hours*

*Samples analyzed using microscopy, IR spectroscopy, X-ray diffraction, differential scanning calorimetry, and electrochemical impedance spectroscopy*

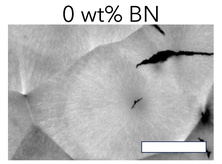
*Results compared with Density Functional Theory (DFT) calculations*

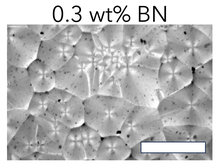
## DFT Calculations Show BN–Ion and BN–PEO Interactions

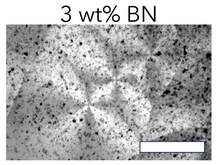



*Optimized geometries and corresponding binding energies for BN, $Na^+$ and $NO_3^-$, and PEO. BN interacts strongly with both ions, especially $Na^+$, which could hinder ion mobility in PEO.*

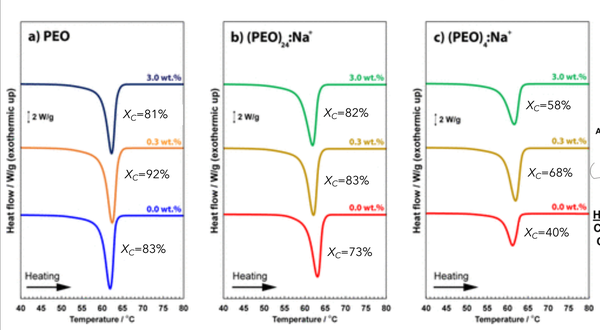
## Adding BN Increases Polymer Electrolyte Crystallinity

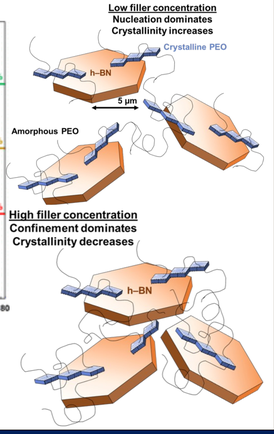


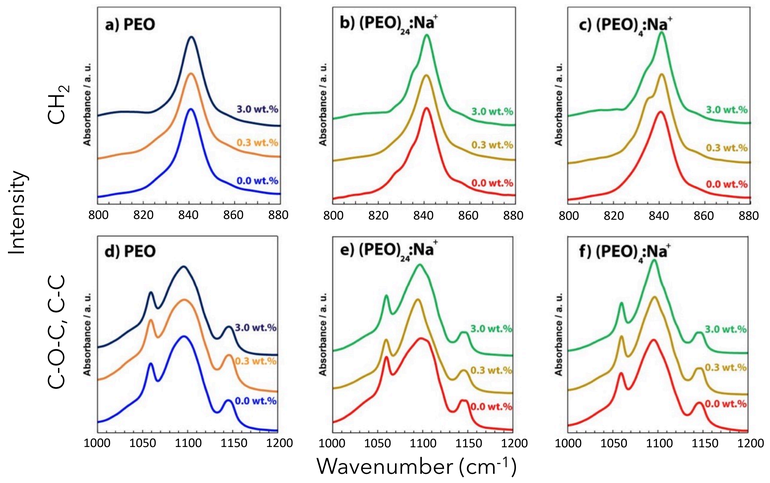

*Optical microscope images show PEO spherulites at each BN fraction. BN flakes are visible in the 0.3% and 3% images. Scale bars are 500 μm.*



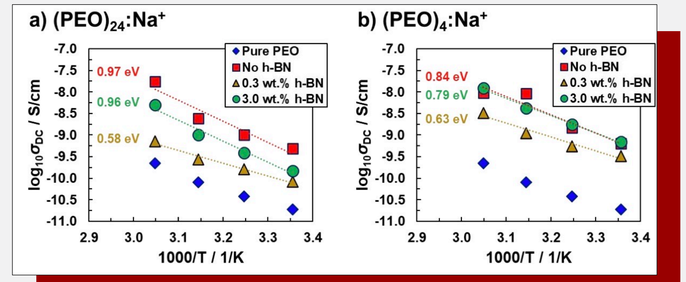

*Heats of fusion from DSC experiments show BN has a non-monotonic effect on polymer crystallinity.*

## Vibrational Spectroscopy




*FTIR spectra show the 840 $cm^{-1}$ (top) and 1100 $cm^{-1}$ (bottom) vibrational modes of PEO. Peak broadening indicates complex formation, which is influenced by BN flakes.*

## BN Has a Non-Monotonic Effect On Ionic Conductivity




*Arrhenius plots of ionic conductivity for low (left) and high (right) salt concentration PEO-$NaNO_3$ samples from 25°C to 55°C. The highest ionic conductivity is observed in the BN-free electrolytes, and the lowest values are observed for the 0.3% BN electrolytes. The inlaid text indicates the calculated activation energies for ion transport.*

## Conclusions

- Adding BN can increase polymer crystallinity.
- Crystallinity is suppressed above 0.3% BN.
- BN binds with both Na+ and NO3- ions.
- Total ionic conductivity decreases relative to controls when BN is added.

## Next Steps

Analyze PEO-NaFSI system → Measure Transference Number → Select New Fillers

## References

1. R. Usiskin et al., Nat. Rev. Mater. 6 (2021)
2. S. S. Pathreeker, C. A. Snyder, G. V. Papamokos, and R. J. Composto, J. Phys. Chem. C 128, 1 (2024)

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