Electronic and vibrational properties of electron-doped transition-metal nitride halides RNX(R= Zr and X= Br, I) from first principles

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Abstract

- Using density functional theory (DFT), we study transition metal nitride halides *RNX* (*R*= Zr; *X*= Br, I).
- The metal nitride halides *RNX* form two different polymorphs (α and β) in their layered crystallized structures.
- The parent compounds are band insulators, that when electron-doped become superconductors.
- We used DFT calculations to calculate the energy as a function of electron density.
- We will discuss the electronic structure of *RNX* and the effects of electron doping on these materials in β-form.

Introduction

- *We* studied both α and β semiconducting structures and compared their electronic structures using DFT.
- Our interest was in knowing what would happen when using the halides bromide and iodide.
- α- form polymorph crystallizes in the orthorhombic space group *Pmmn* (#59).
- β -form polymorph crystallizes in the rhombohedral space group R3m*(#166)*.

Methodology

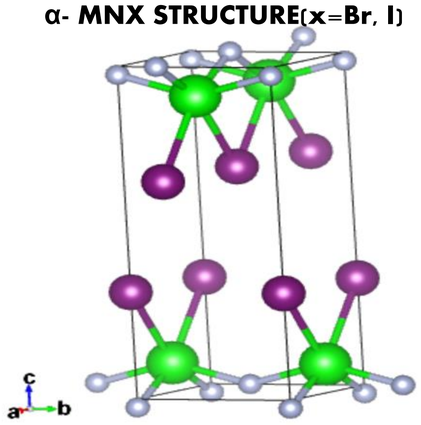
- Performed first-principles calculations by using the Quantum-ESPRESSO software package.
- Generated experimental cell parameters using previous research
- Converted the cell parameters for our electron-doped beta structures from hexagonal to rhombohedral cell.
- The different pseudopotentials were generated with a non-relativistic calculation
- The Exchange-Correlation potential has been defined utilizing the PBE functional.

Materials & Results

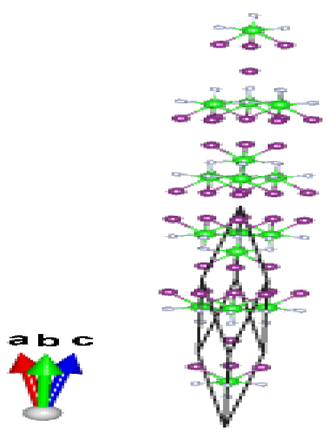
Orthorhombic space group *Pmmn* (#59)

Rhombohedral space group R3m*(#166)*

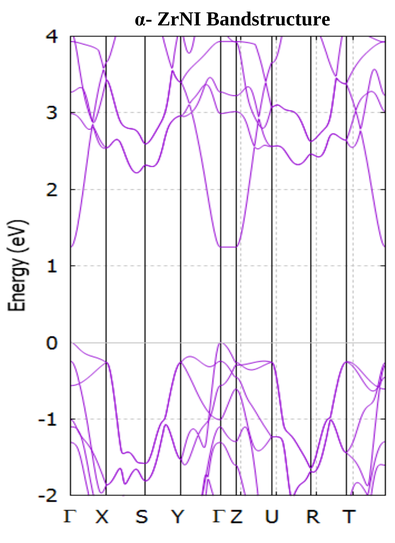
α- MNX STRUCTURE(x=Br, I)



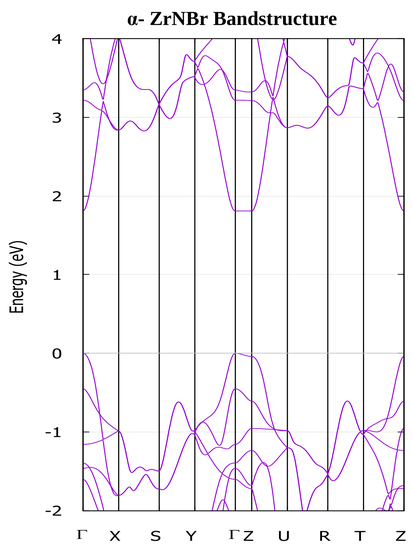
β-MNX STRUCTURE(X=Br)



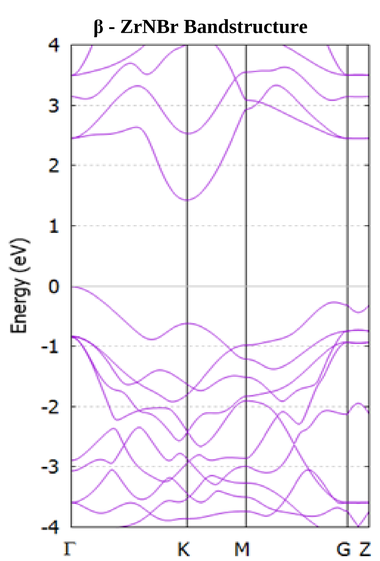
Undoped Bandstructures



α-ZrNI has a direct band gap of 1.247 eV at the Γ point.

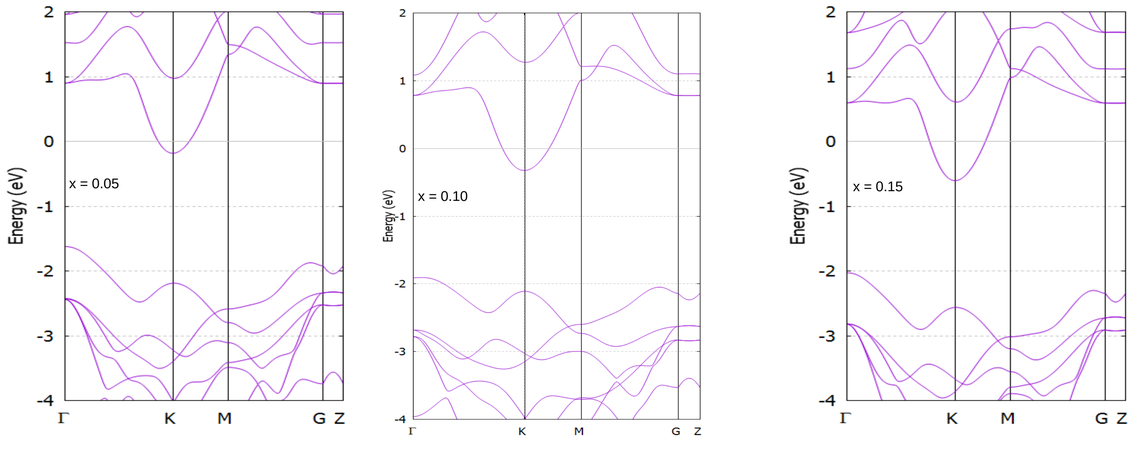


α-ZrNBr has a direct band gap of 1.810 eV at the Γ point



β-ZrNBr has a band gap of 1.441 eV.

Doped Li_xZrNBr Bandstructures



β-ZrNBr Fermi level increases as e- doping increases.

Applications used to Analyze & Perform DFT Calculations

QUANTUMESPRESSO

MATERIALSCLOUD

Conclusion

- Both α-ZrNBr and α-ZrNI are semiconductors with parabolic bands between Γ - X and Γ - Y.
- ZrNBr exists in the β-phase similar to β-ZrNCl in previous research.
- β-ZrNBr is a semiconductor with a single parabolic conduction band centered around the K-point.
- As β-ZrNBr is doped, the Fermi level shifts upward.

Future Work

For future work, we would like to calculate the vibrational properties better known as the phonons. We also would like to calculate the superconducting temperature.

Acknowledgements

- NSF Cooperative Agreement No. DMR2039380
- NSF Cooperative Agreement No. DMR2150446
- Betül Pamuk
- Darrell Schlom
- Jim Overhiser