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Structural, electronic and optical properties of Zn_2VN_3 compound by density functional theory

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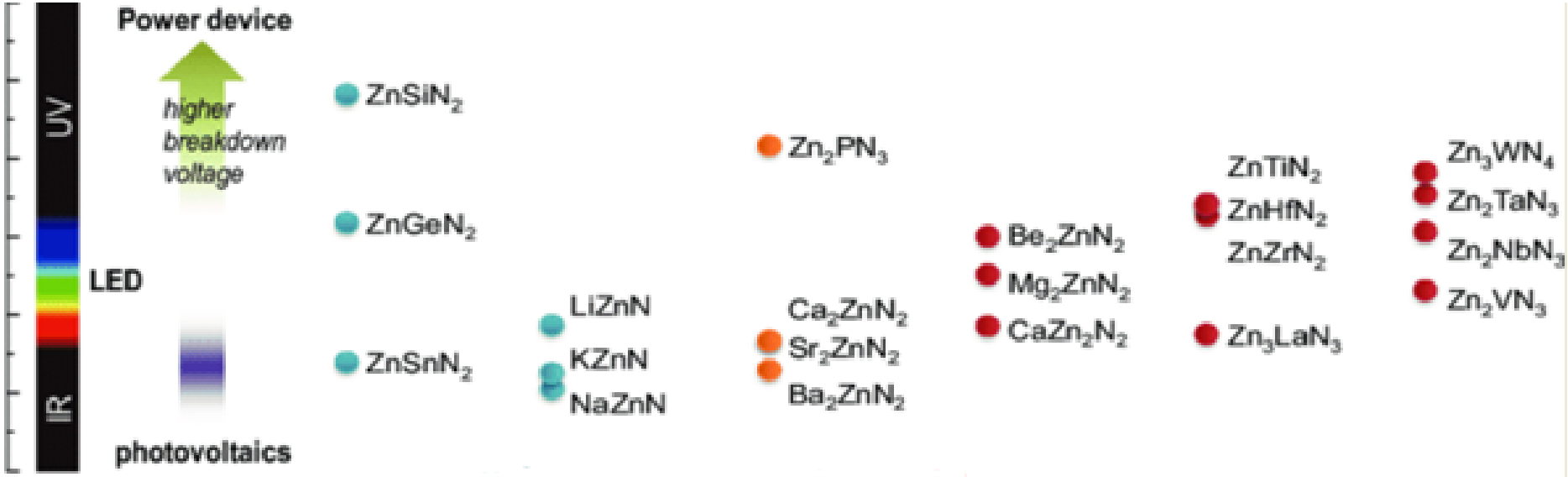
Plan

- Introduction
- Computational Methods
- Results and discussion
- Conclusion

Introduction



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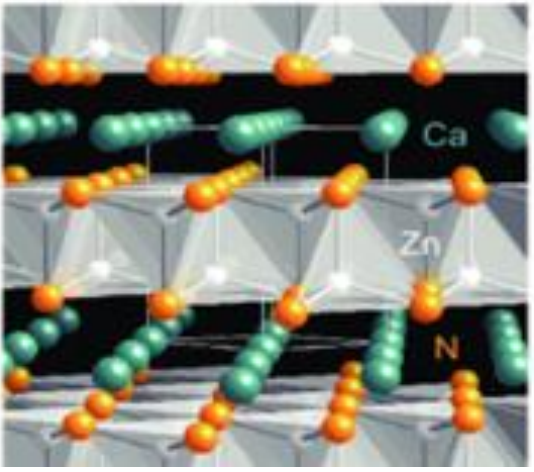
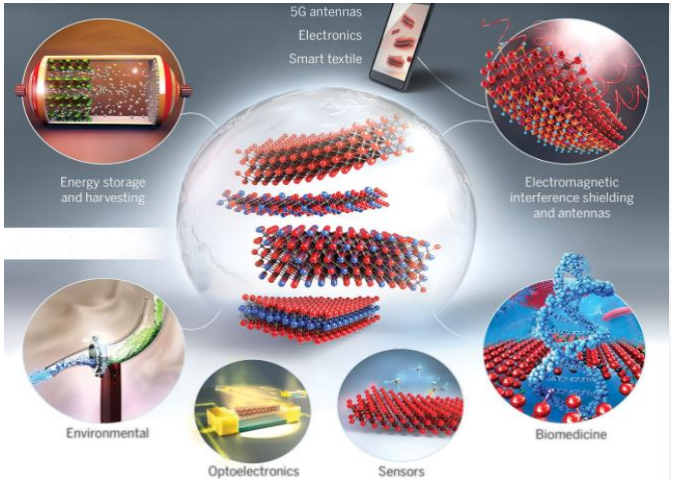
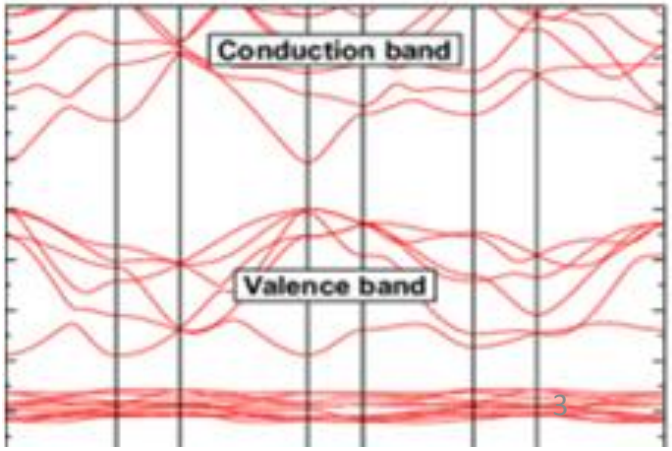






Introduction

Inorganic nitrides

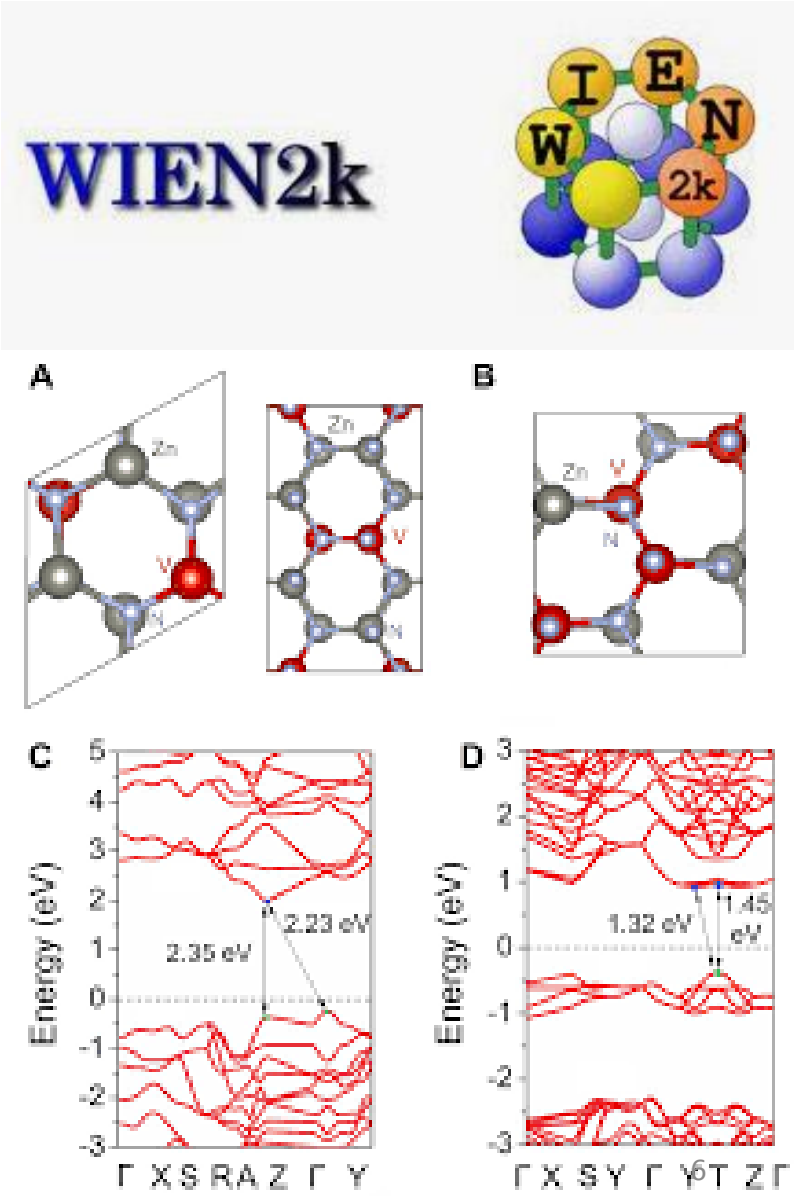
semiconductor wurtzite main group metal nitride	superconducting rocksalt transition metal (TM) nitride

- **What is about Zn_2VN_3 ?**

- **what are the structural, electronic and optical properties of this material ?**

computational methods

- **Density functional theory**
- **First principles full potential linearized augmented plane-wave (FP-LAPW)**
- **The generalized gradient approximation (GGA) in the form of Perdew–Burke–Ernzerhof (PBE)**



Structural properties

- Orthorhombic structure
- 36 Cmc21 space groupe

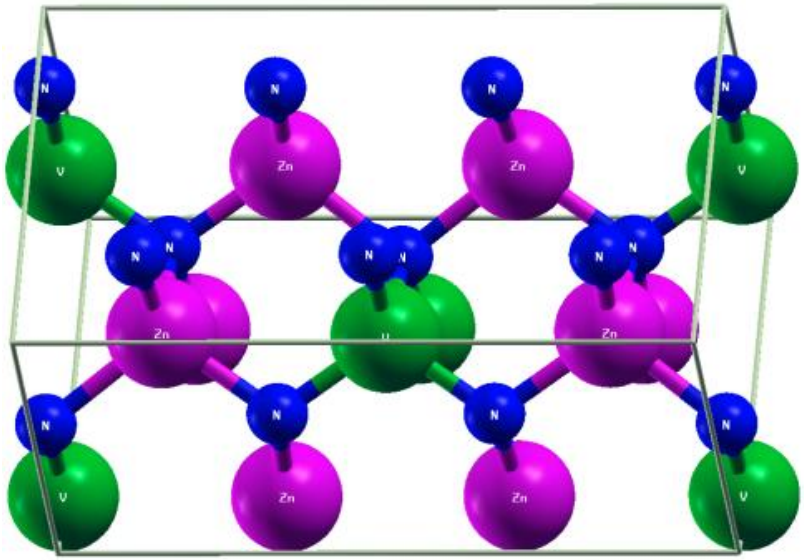


Figure 1: Zn_2VN_3 optimized structure

Electronic properties of Zn_2VN_3

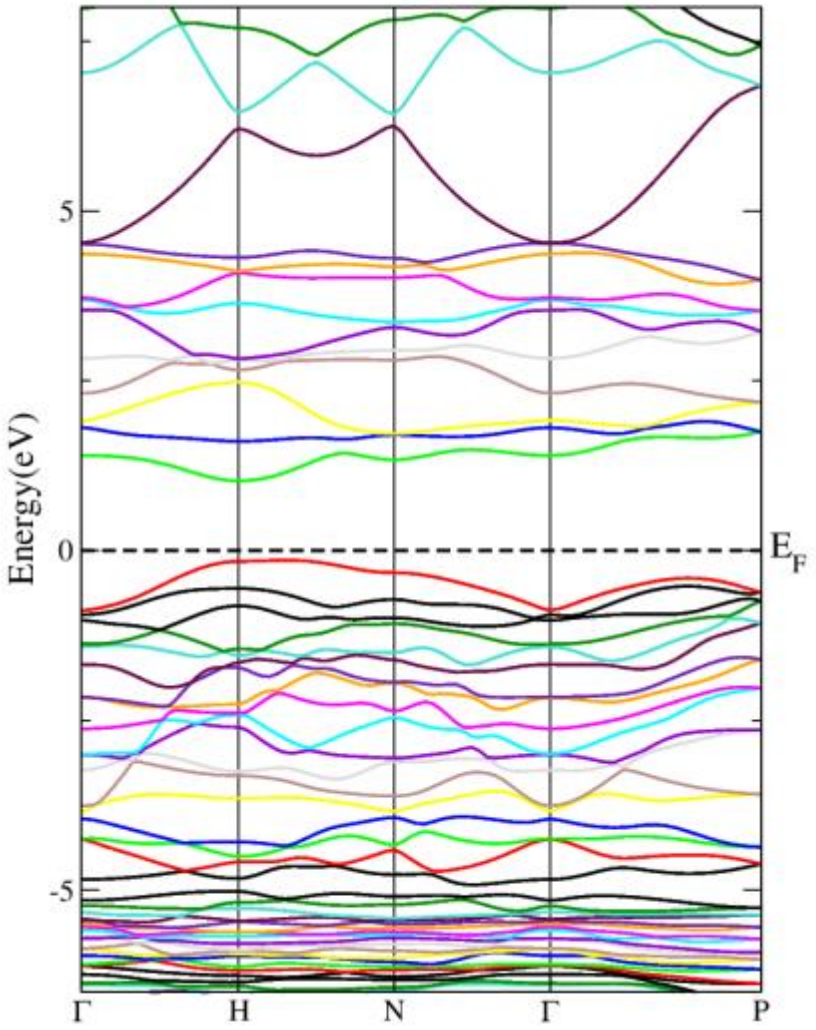


Figure 2: Band structure of Zn_2VN_3

- ❖ Direct band gap
- ❖ band gap of 1.7eV
- ❖ Semiconductor behavior

Electronic properties of Zn_2VN_3

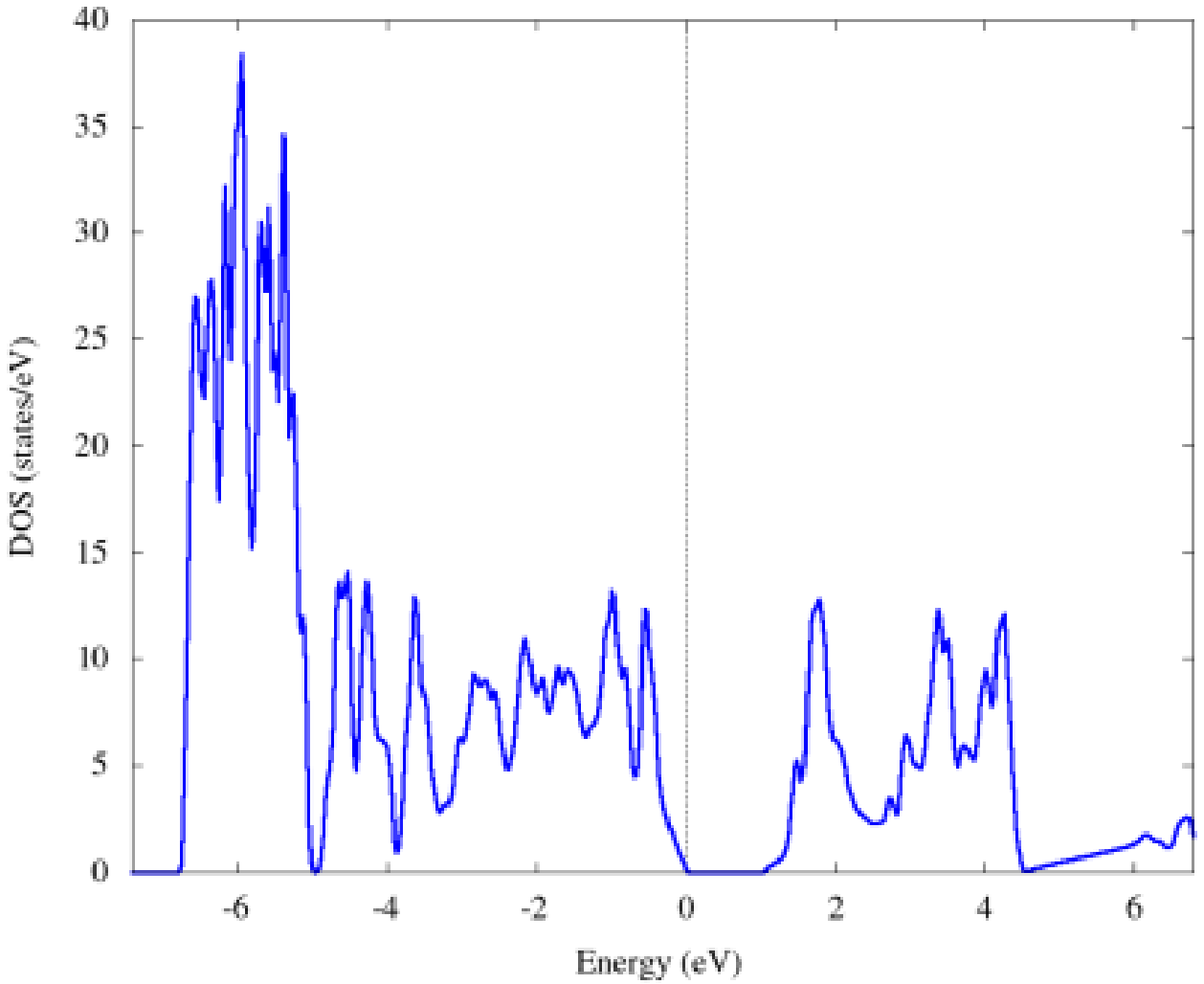
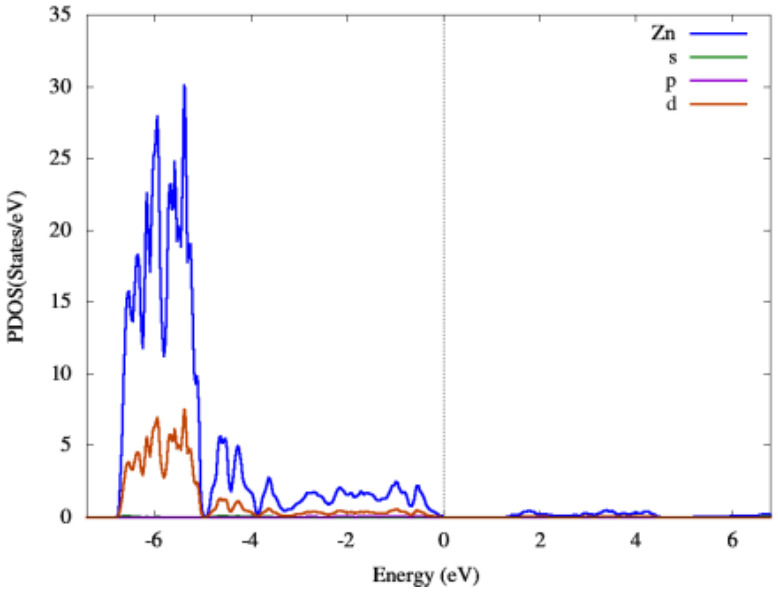
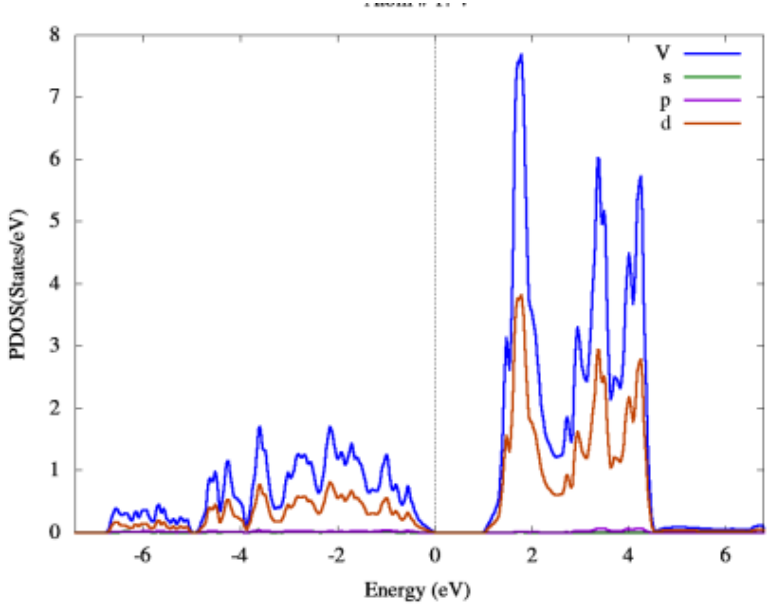


Figure 3: total DOS of Zn_2VN_3

Electronic properties of Zn_2VN_3





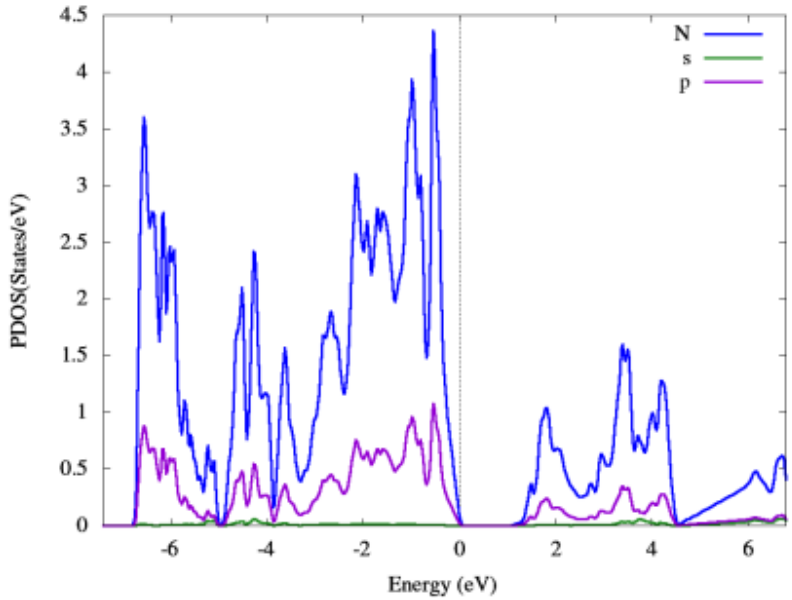


Figure 4 : Combined tot and partial DOS of Zn, V and N atoms

Optical properties of Zn_2VN_3

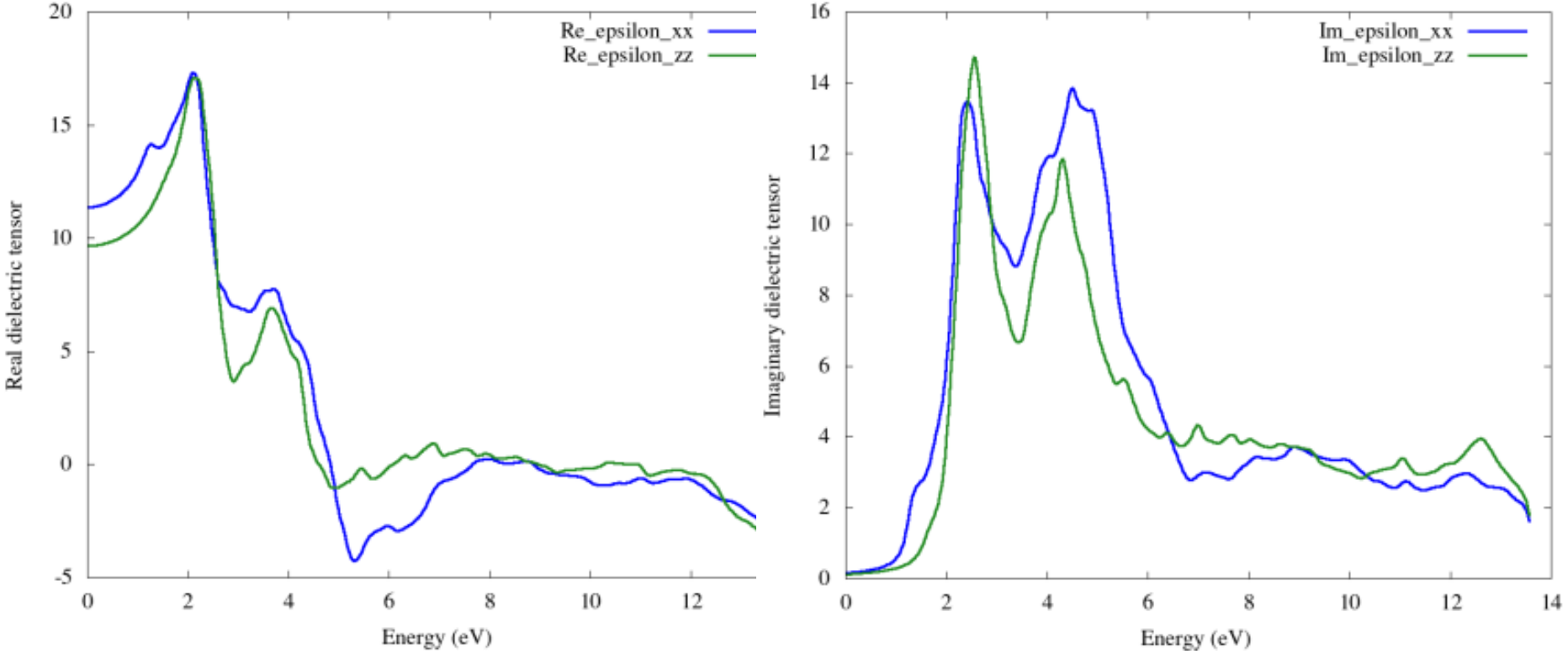


Figure 5: real and imaginary part of dielectric function of Zn_2VN_3

Conclusion

- **Direct band gap (1.7 eV)and semiconductor behavior .**
- **Main contributions are from V-d and N-p orbitals in good agreement with imaginary part of dielectric function.**
- **DFT calculation predect a helpful results benificial for avoiding high cost and error in experimental process especialy for novel materials.**
- **Doping ternary nitrides is a great opportunity for obtaining novel material with adjustable properties.**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FOR YOUR
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