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Comparative Study on Structural and Electronics Properties of Boron and Boron Nitride Nanodics

Piyush Gupta[1], Rahul Tripathi[2], C. K Dixit[3], Sanjeev Kumar Trivedi[4]
[1]*North East Frontier Technical University, Arunachal Pradesh-791001*
[2]*D.S.R.M.U Lucknow -226017*
[3, 4]*Mumtaz P.G College, Lucknow University, Lucknow-226020*

***Abstract:** We have employed first-principle calculations for investigating structural and electronics properties of Boron (B-nd) and Boron Nitride (BN-nd) nanodiscs by using density functional theory (DFT) implemented in SIESTA [1].*

Structural Analysis

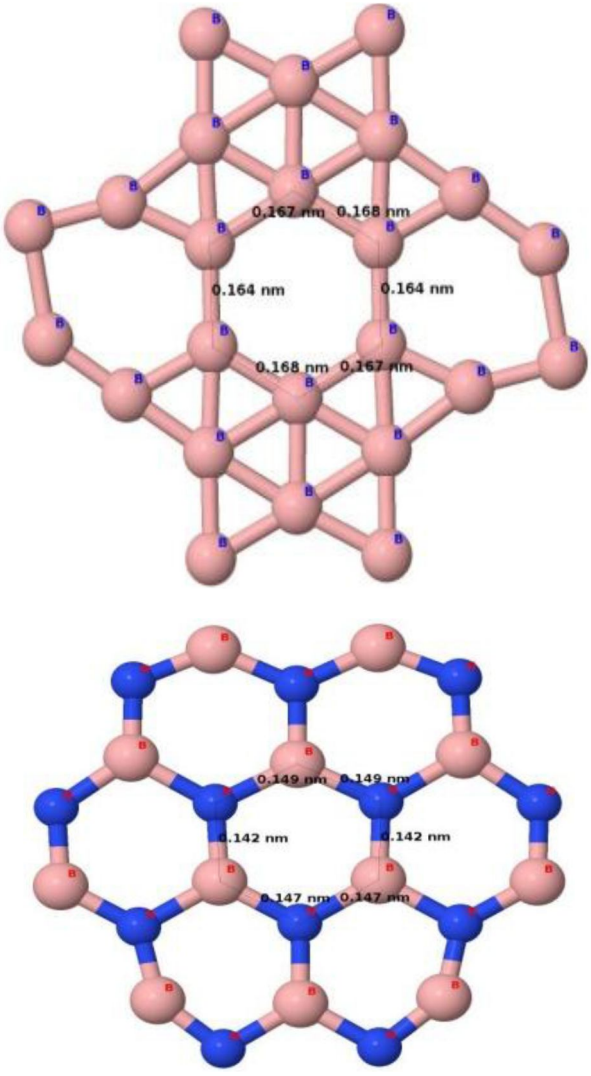

Fig 1: Equilibrium structures of B-nd and BN-nd

Total energy of B-nd and BN-nd of 24 atoms is calculated as -2117.0294 eV and -4332.4660 eV respectively. The calculated bond-length in range of 1.64 Å to 1.68 Å for B-nd and of 1.42 Å to 1.49 Å for BN-nd , which values are in close agreement with previously reported value [2].

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I. ELECTRONIC PROPERTIES

Fig 2

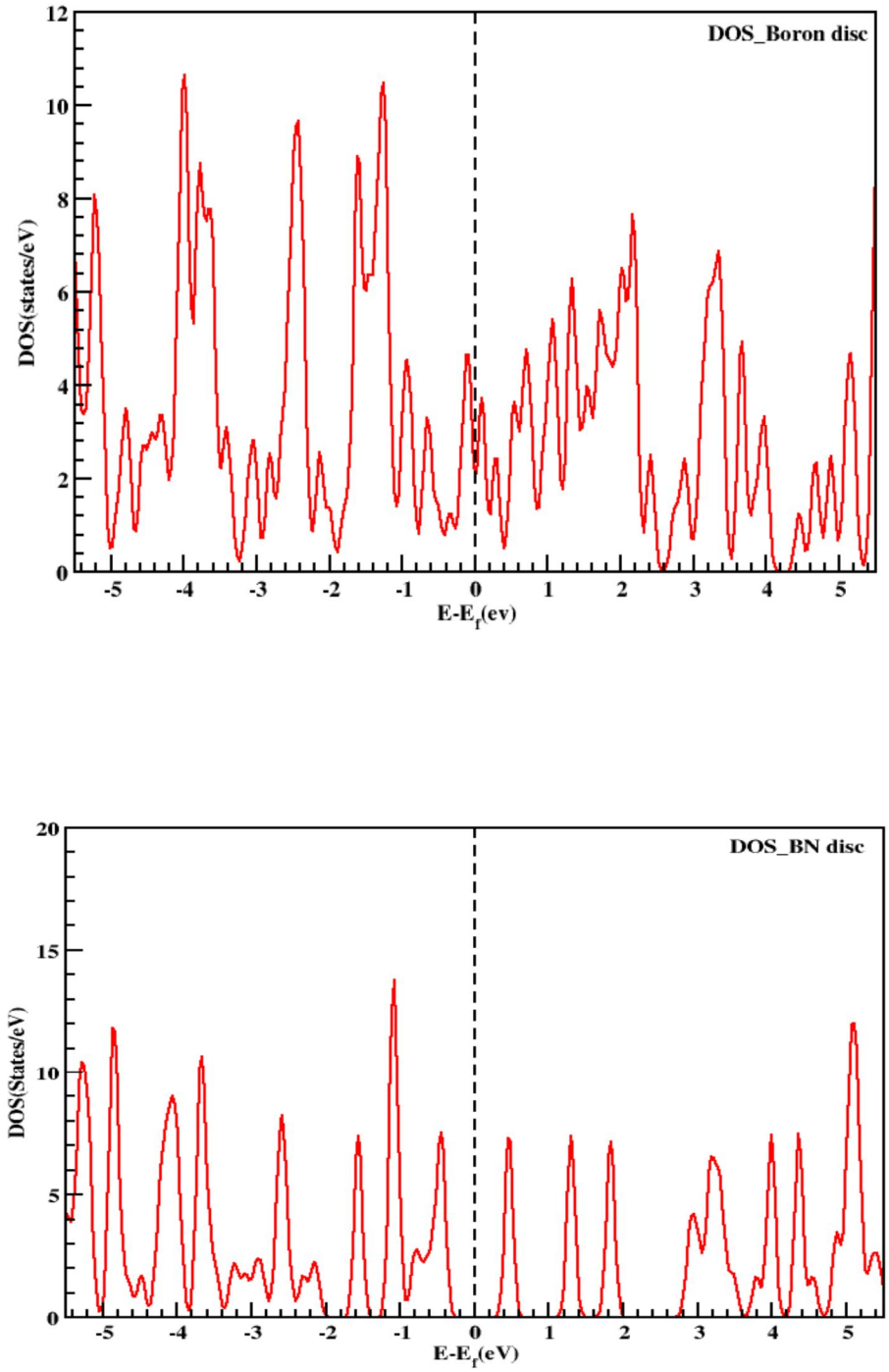

Fig 2: Total density of states of B-nd and BN-nd

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From fig 2, it is observed that for B-nd there is finite electrons in Fermi level but in case of BN-nd there is no electrons in Fermi level. Therefore high value of electronic states at Fer-mi level corresponds high conductivity, thus high value of DOS at Fermi level shows higher conductivity. From the study of DOS it can be concluded that B-nd is more conducting than BN-nd, while BN-nd is of semiconducting in nature with HOMO-LUMO gap of 0.80 eV.

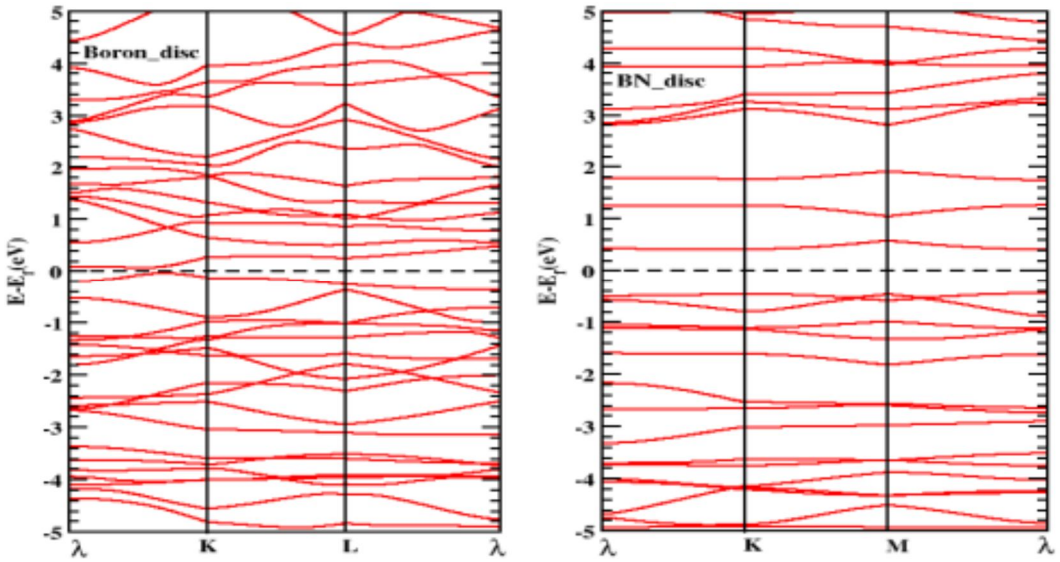

Fig 3: Energy bands of Boron and BN-nd

From Fig 3, we observed that in case of B-nd there is no band gap while for BN-nd there exists finite band gap (0.80eV) [3] which is well defined as a semiconducting nature but B-nd exhibits conducting nature.

II. RESULT AND CONCLUSION

In this work, we have performed first principles calculations in order to study structural and electronics properties of Boron and BN-nd configurations. The finite value of DOS at Fermi level shows metallic nature of B-nd while BN-nd has semiconducting behaviour with band gap of 0.80 eV which could be useful for further theoretical investigation. This semi-conducting nature of Boron Nitride Nano disc will be also applicable to save nature and natural resources by using such materials instead of carbon materials. In addition, it is found that while doping of nitrogen in boron disc it creates energy gap and decreases the conductance also.

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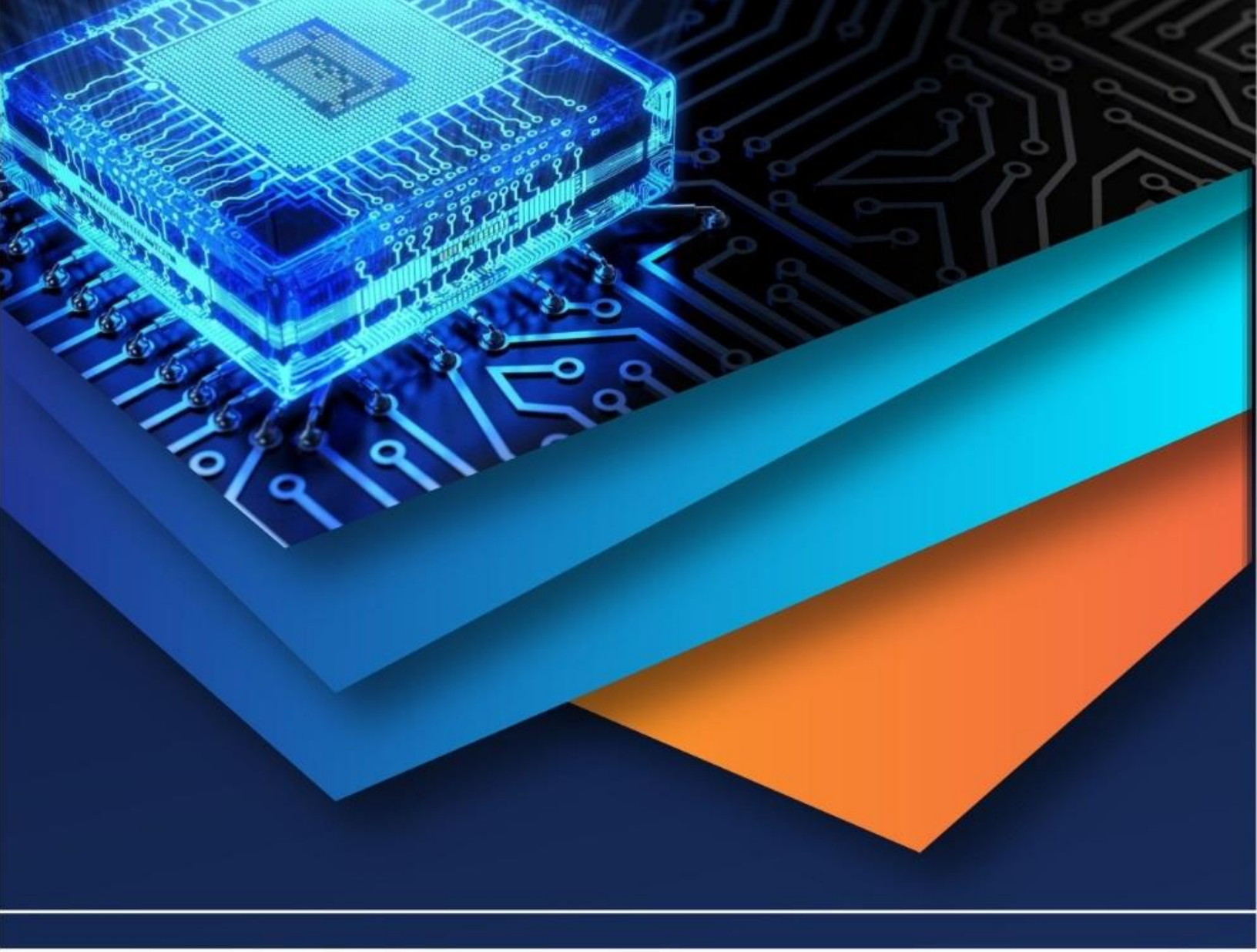

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