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AB Initio Study of $(ZrB_2)_n$, (n = 1-4)

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***Abstract:** In the present work we have studied various conformers of $(ZrB2)_n$,(n=1-4) as well as (B2)n(n=1-4) using combination of DFT/LanL2DZ method and basis set. On comparing the results obtained by the above method and basis it gave a better understanding about how a non metallic cluster changes it properties when they combine with a metallic complex. Vibrational mode analysis HOMO-LUMO as well as 3D potential energy plot, local charge density optimized geometry, binding energy etc use as a tool to determine stability, electronic reactivity symmetry of above complexes. If there is an increase in the number of atoms in ZrF2 complexes, the conductivity increases rapidly and complexes behave a super conductor.*
***Keywords:** Density Functional Theory, Conducting Behavior, Electronic Density*

I. INTRODUCTION

Material which have Diborides altercates attention of researches because of it's super conductive Nature[1,2]. Specially it is found that MgB_2behave as a super conductor at a Relatively high critical temperature. Perhaps it critical temperature is not high as other oxide, it preparation is very cost effective. Transition metals ceramics diborides such as Zirconium Diborides are Members of a family of materials with extremely high melting temperature. These compounds are known as ultra high temperature ceramics.

A. Computational Methods

The computational methods used in this study was based on Ab-initio methods with Density functional Theory Approximation using three Parameters hybrid function B3LYP/LANL2DZ[3,4] as the basis set.TheLANL2DZ[3,4]as the basis set are very use full basis set in conformer under case of two electron Integrals in case of two electron Integrals in case of heavy element. It is also more effective core basis set to provide information for geometrics stabilities and electronics properties for transition metal cluster for all system, geometrical optimization was performed under small level of theory, all the computational are performed with Gaussian09 program[5]&relevant graphics was created with the help of Gauss View 5.0 Package[6].

II. RESULTS & DISCUSSION

The bond lengths of all the optimized Structures are shown in Figure 1. It is Observe that all the frequencies are real &positive which shows that molecule belong to a global minima. The structure Zr_2B_4 and B_4 show a planner arrangement of atoms, with the boron atoms in two-Dimensional unsymmetrical rhombic arrangements for Zr2B4 and perfect square for B4.The structures of B6 do not show a planner structure. The arrangement of atoms is different to the one obtained in the molecular species. The vibration analysis Show all positive frequencies and similar to the previous system.

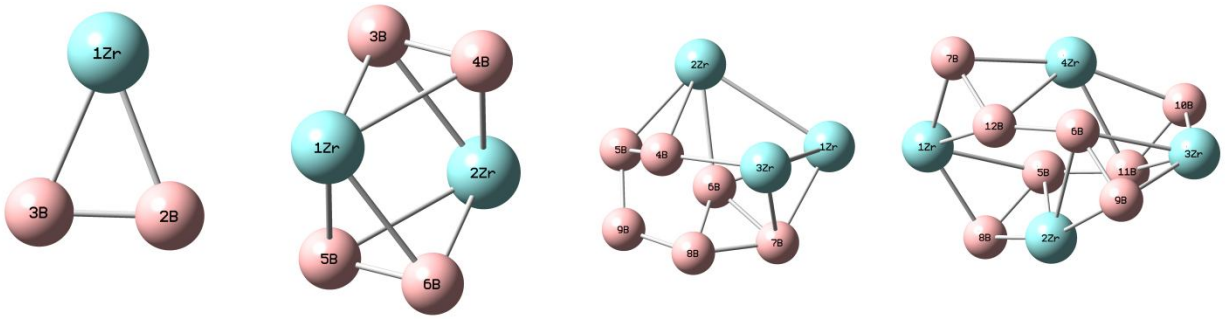

Figure 1. Optimized structures of ZrB_2, Zr_2B_4, Zr_3B_6 and Zr_4B_8

III. CONCLUSION

In all Cases, the lowest energy equilibrium structures for ZrB_2 Cluster showed an arrangement of Boron atoms and hence the Zr atoms are acting as electronic donating species. The larger electron densities in a specific plane induce the super conductive nature So it can Show a Similar Super Conducting.

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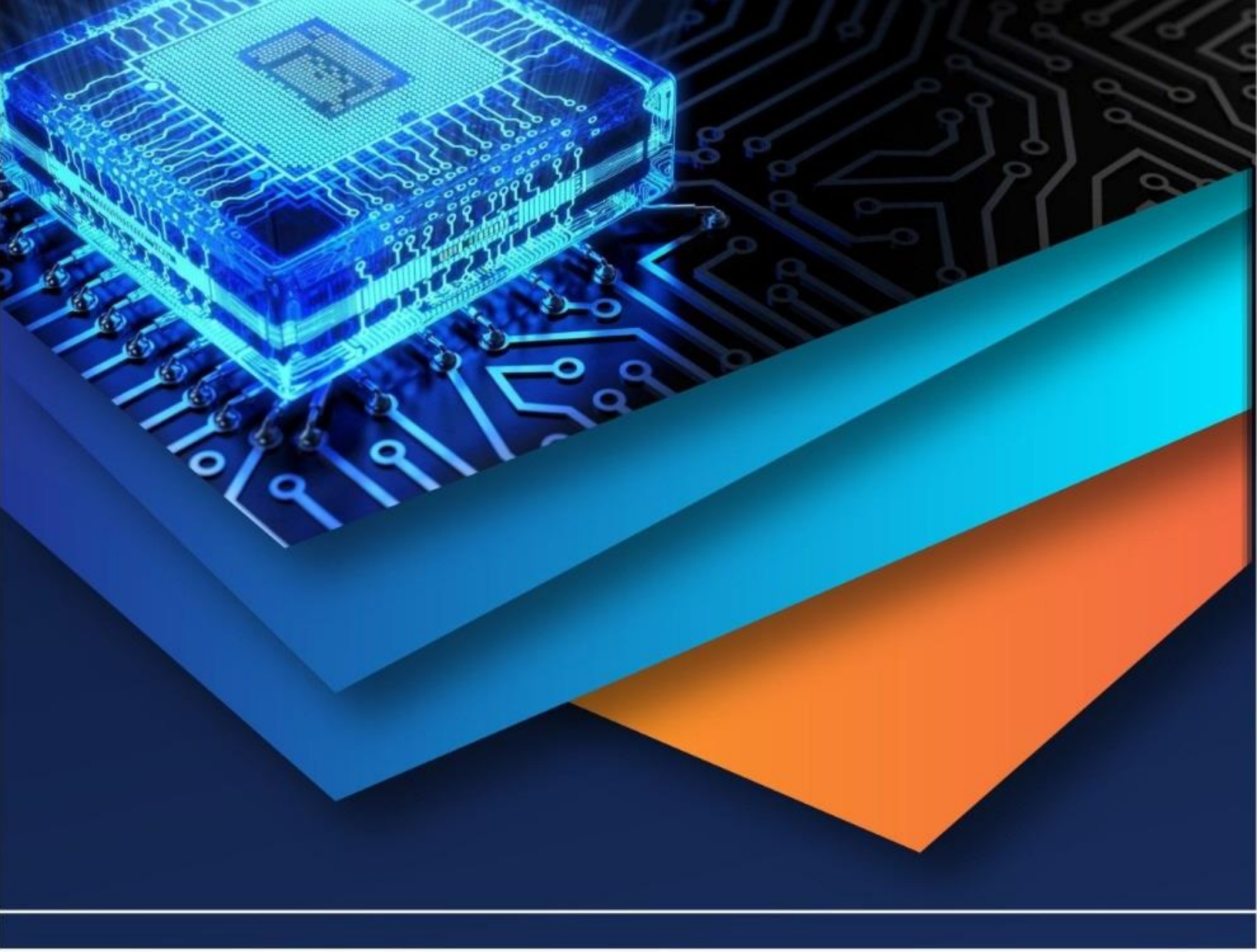

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