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# AB Initio Study of $(\text{ZrB}_2)_n$ , $(n = 1-4)$

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**Abstract:** In the present work we have studied various conformers of  $(\text{ZrB}_2)_n$  ( $n=1-4$ ) as well as  $(\text{B}_2)_n$  ( $n=1-4$ ) 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 its 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  $\text{ZrF}_2$  complexes, the conductivity increases rapidly and complexes behave as a super conductor.

**Keywords:** Density Functional Theory, Conducting Behavior, Electronic Density

## I. INTRODUCTION

Material which have Diborides attracts attention of researchers because of its super conductive Nature[1,2]. Specially it is found that  $\text{MgB}_2$  behave as a super conductor at a Relatively high critical temperature. Perhaps its critical temperature is not high as other oxide, its 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 were based on Ab-initio methods with Density functional Theory Approximation using three Parameters hybrid function B3LYP/LANL2DZ[3,4] as the basis set. The LANL2DZ[3,4] as the basis set are very useful 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 geometrical 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 observed that all the frequencies are real & positive which shows that molecule belongs to a global minima. The structure  $\text{Zr}_2\text{B}_4$  and  $\text{B}_4$  show a planar arrangement of atoms, with the boron atoms in two-Dimensional unsymmetrical rhombic arrangements for  $\text{Zr}_2\text{B}_4$  and perfect square for  $\text{B}_4$ . The structures of  $\text{B}_6$  do not show a planar structure. The arrangement of atoms is different to the one obtained in the molecular species. The vibration analysis shows all positive frequencies and similar to the previous system.

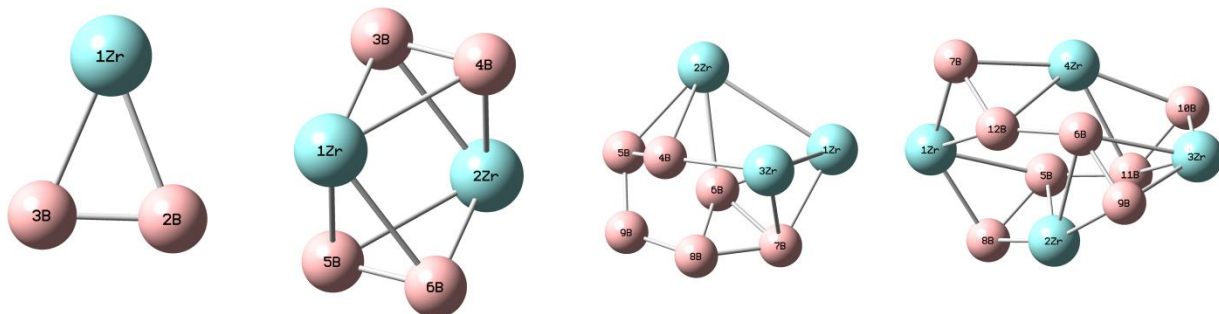


Figure 1. Optimized structures of  $\text{ZrB}_2$ ,  $\text{Zr}_2\text{B}_4$ ,  $\text{Zr}_3\text{B}_6$  and  $\text{Zr}_4\text{B}_8$

## III. CONCLUSION

In all Cases, the lowest energy equilibrium structures for  $\text{ZrB}_2$  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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