First Principal Study of Magnesium Diboride (MnB2) Cluster

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Abstract

Using DFT theory, we have investigated various conformers of (MnF2)n (n=1,2,3) clusters and also these structure are compared with (B2)n(n=1,2,3) cluster. Their stabilities are discussed by ground state energy, vibrational frequency, NBO theory .The electronic properties are also explored for all the species. From charge density calculation it was found that larger electronic density in a specific plane increases the superconductivity behavior of this material, then it can be expected that these clusters should exhibit a similar super conducting behavior.

Keywords: *Density Functional Theory, conducting behavior, electronic density*

1. Introduction

2.

Diboride materials have Its superconductivity was first published in the journal Physical Review Letters in February 2001[1] Its critical temperature (Tc) of 39 K(−234 °C; −389 °F) is the highest amongst conventional superconductors. This material was first synthesized and its structure confirmed in 1953[2] but its superconducting properties were not discovered until 2001[3]. MgB2 is a type-II superconductor, i.e. increasing magnetic field gradually penetrates into it. Non-oxide ceramics, such as carbides, nitrides and borides represent one of the fastest growing classes of new advanced materials to be considered and pursued by today's industries. Transition metals diboride are having high conductivity high melting point high hardness and chemical inertness. So these type of materials are very useful for ultra high temperature ceramic where high temperature high thermal flux are needed. In our present study we choose a transition metal Mn diboride cluster. Using DFT/B3LYP method we see that how conductivity and structure are vary as number of atom increases from 1to 3.

2.Computational Methods

The DFT [4]theoretical calculations have been performed at B3LYP/LANL2DZ [5,6] level using Gaussian 03W program [7], involving gradient optimized geometry [8]. We deigned different structure of(B2)n(n=1-3)as well as(MnB2)n(n=1-3) on gauss view 5.0 program package[9]. For all systems, a full geometry optimization was performed and various initial geometries were used to guarantee the determination of the lowest energy equilibrium structure. Harmonic vibrational analysis was performed for each system not only to obtain the vibrational frequencies.

3. Result and Discussion

All most stable conformer of (B2)n{n=1to3} and(MnB2)n{n=1to3} are given in fig 1 &2 respectively. Optimized bond length as well as vibrational frequency are given in table 1&2.All frequency of (B2)n{n=1to3} and (MnB2)n {n=1to3} are real this show that given structure are real. In B2 isomer linear structure is stable however MnB2 triangular structure becomes stable .Both structure are planer shape. In this system both boron atoms are equal distance with Mn atom having same negative charge.Vibrational mode analysis show that vibration between B-B in MnB2 is more polarized than B2 atom. Vibration of B-B corresponding to MnB2 is larger than 15% vibration of B-B in B2 atom. Fig 1&2 show that 2D rhombus structure is more stable in B4 structure however in Mn2B4 hexagonal shape become stable in which both Mn atom goes out of plane to minimize surface area and gain stability. In this structure four B atoms are in plane and having negative charge .NBO analysis shows that Mn behave as electron donator and B atom acts as acceptor .Charge on boron atom distribute non symmetrical fashion such that Boron atom which are closer to Mn showed larger value of electronic density than other atom. However bond length of B-B in B2 is larger than Bond length of B-B in B4. In case of B6 none planer hexagonal structure are stable however (MnB2)3

unsymmetrical none planer structure are stable. From NBO analysis two B atom which are more closer to Mn atom having more negative charges(-0.487).Vibrational mode analysis shows that atom which are in plane are more characteristics frequency than other this shows that if we increase number of then more charge found in a plane which increase conducting properties.

4. Conclusion

In this study we see that planer as well as quasi-planer structure MnB2 as well as(rhombus) Mn2B4 are stable. Boron atom which are lying in a plane having negative charge however Mn are having positive charge act as electron donator. So if we increase number of Boron atom in a plane then number of charge increase in a plane .The larger electronic density in a specific plane increases the superconductivity behaviour of this material

Table-1
Average bond length of different structure (A0)

Cluster	$(C_{inf v})B_2$	$(D_{2h})B_4$	$(C_{2v})B_6$	$(C_{2v})MnB_2$	$(C_1)Mn_2B_4$	Mn_3B_6
B-B	1.68	1.56	1.60	1.55	1.76	1.73
Mn-B	-	-	-	2.10	2.03	1.90
Mn-Mn	-	-	-	-	2.85	3.08

Table- 2 Vibrational frequencies of stable structures (Cm-1)

MnB_2	Mn_2B_4	Mn_3B_6	B_2	B_4	B_6
478	80	91	913	234	123
598	107	123	-	315	134
1087	187	143	-	1015	336
-	207	185	-	1162	431
-	356	198	-	1182	475
-	526	220	-	1212	489
-	548	279	-	-	663
-	810	325	-	-	802
-	875	373	-	-	1009
-	987	413	-	-	1019
-	1023	432	-	-	1304
-	-	485	-	-	1353
-	-	502	-	-	-
-	-	532	-	-	-
-	-	545	-	-	-
-	-	603	-	-	-
-	-	713	-	-	-
-	-	823	-	-	-
-	-	976	-	-	-
-	-	1012	-	-	-
-	-	11034	-	-	-

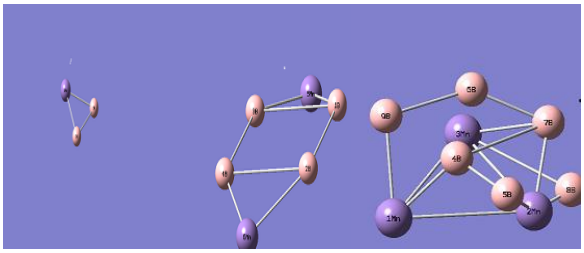

Fig-1 Stable structure of (MnB_2) n{n=1-3)

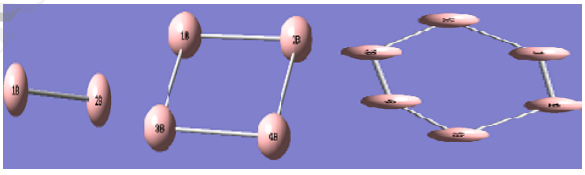

Fig-2 Stable Structure of (B2)n{n=1-3}

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