

On the Mn-In-Ni Diatoms: Electronic Properties Depending on Spin Multiplicity

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ABSTRACT

In this study, Ni, Mn and In atoms formed by different combinations of diatoms due to the spin multiplicity of electronic structure characteristics have been investigated. Calculations have been performed by Density Functional Theory within B3LYP functional and CEP-121G basis set. Diatoms with the first five spin multiplicity configurations have been investigated and the most stable state has been determined. The energetics, such as binding energy, frontier molecular orbital energies of six possible diatoms have been calculated in their ground state with their lowest five spin multiplicities.

Keywords: Mn-In-Ni diatoms, density functional theory, electronic properties, spin multiplicity.

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I. INTRODUCTION

Clusters are defined as atom groups formed by a few or millions of atoms. Some researchers approved the clusters as the fifth state of the matter since the general definition is of clusters are the finite structures combined from different disciplines [1]. For this reason, there has been a considerable amount of interest in the theoretical and experimental studies of the atomic clusters in recent years because of their electronic and magnetic properties and practical applications in many different fields. Scientist run across many difficulties in the calculation of thermodynamical properties because, when the cluster size decrease, the quantities like temperature, surface tension, surface area, volume are not clearly explained for the macroscopic system [2-3]. Even for very small size clusters ab initio calculations are still difficult so parametrised models are more probable in this regard [4]. In small cluster simulations one of the most incompleteness is the inaccessibility of realistic potential functions explaining the interactions between the atoms in the cluster and also results of the simulations are related to the functional form of the potential. The results derived from the simple pair potentials are not satisfy quantative informations for the conceptualisation of the microcluster structures, but three-body interactions used in the simulations are gained considerable results [5-6]. In the recent years, there is an increasing interest to understand the metallic structure properties in the border of nano scale because of the minimization of the electronic devices. Metal clusters are beginning with the diatomic molecule access to several

thousand atoms with a countable number of atoms [7]. In literature, there are different types of studies related the materials including Mn, Ni, In atoms [8-15]. Also there are alloys with various ratios of the Mn, Ni, In atoms and theoretical prediction of shape memory behavior [16-21]. In these studies structural, electronic and magnetic properties of the shape memory behaviour materials have been investigated. Small atomic clusters are known to display geometrical arrangements and electronic properties that are significantly different from their bulk properties [15]. There is no an encountered study with the heteroatomic microclusters containing Mn, Ni, In atoms. In the studies with the Mn clusters the magnetic properties of the clusters have been investigated [22-27]. Also, there are studies related with the Mn ions [28-30] and diatomic alloys like MnNi, MnIn NiIn in the literature [31-34].

This work reports the electronic properties and energetics of six different diatoms composed of from the atoms In, Ni, Mn have been investigated. The three homonuclear diatoms (In₂, Ni₂, Mn₂) and the three heteronuclear diatoms (NiMn, NiIn, MnIn) have been studied in their ground state and the lowest first five spin multiplicity states. In the literature in most of the electronic structure calculations usually the lowest spin multiplicity case is considered. There is no guarantee that the lowest multiplicity corresponds to the most stable state. It is essential to check higher spin states for the stability of atomic systems. Diatoms are the building blocks of the clusters and nanoparticles. Understanding diatoms

will give considerable information for the larger systems.

Method of Calculation

The energetics, frontier orbital energies, dipole moments, dissociation energies of the Mn, Ni, In diatoms with the various spin multiplicities are calculated by density functional theory (DFT) [35] with B3LYP exchange-correlation functional [36] and core effective potential (CEP) [37, 38] basis functions with ECP triple-split basis (CEP-121G). All the calculations have been performed by using Gaussian 09.C1 [39] program and GaussView 5.0.8 [40] was used for visualization of the calculation results.

The core effective potentials or pseudopotential methods have been derived from numerical Dirac-Fock atomic wavefunctions using shape-consistent valance pseudo-orbitals and widely used for the systems with many electrons. Because these functions are including relativistic effects also which take into account only the valance electrons and the core electrons are excluded from the calculations. This is another advantage of CEP basis functions, which reduces computation time considerably.

In CEP-121G basis set, the valance electrons have three sets of atomic orbitals composed of 1, 2 and 1 Gaussians, respectively. In quantum chemistry

studies, CEP basis sets have been widely used to investigate the equilibrium structures and to calculate the spectroscopic properties of systems with heavy atoms [37, 38, 41, 66].

II. RESULTS AND DISCUSSIONS

The geometri optimization is the beginning point of the characteristics of the cluster properties so we optimized the equilibrium geometries of Ni₂, Mn₂, In₂, InNi, NiMn, MnIn. The binding energy (E_b), the equilibrium interatomic separations (r_e), fundamental frequencies (ω_e) and total energies (E_T) depending on spin multiplicities corresponding to the ground state and the most stable spin states of both homonuclear and heteronuclear diatoms Ni₂, Mn₂, In₂, InNi, NiMn, MnIn have been investigated by performing DFT method calculations with B3LYP/CEP-121G basis set. Some of the calculated values are presented in Tables 1-9.

Homonuclear diatoms

Ni₂ Diatom

For Ni₂, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated and the triplet spin state is found to be as the most stable state. Fig. 1 shows the variation of the total energy versus the spin multiplicity for Ni₂.

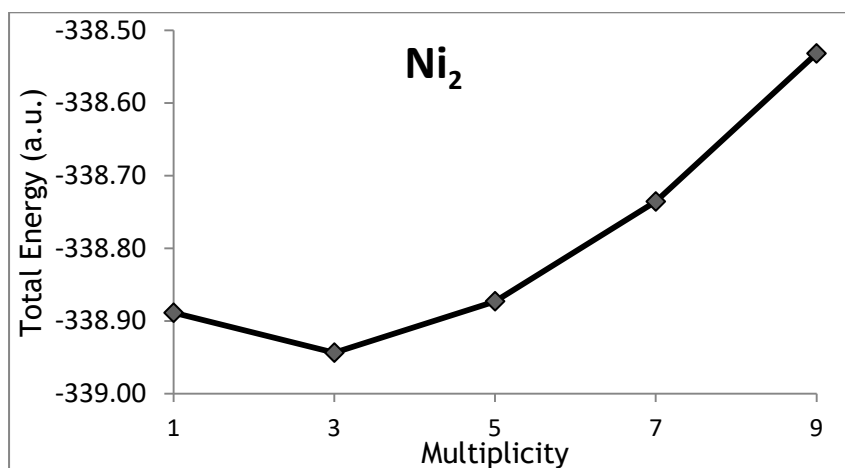


Figure1. The variation of the total energy versus the spin multiplicity for Ni₂.

For the Ni₂ homonuclear diatom the calculated quantities for the most stable structure and its ground state are given in Table 1. In the present study, bond length and vibrational frequency of Ni₂ diatom are calculated to be 2.0760 Å, 347.92 cm⁻¹ in the minimum multiplicity state (multiplicity = 1) and 2.0710 Å, 356.74 cm⁻¹ in the most stable spin state (multiplicity = 3) by B3LYP/CEP-121G level of theory. It is used singlet spin state of Ni atom which is the most stable state for the calculation of the

binding energy for the ground state of Ni₂. Conformably, for the calculation of the binding energy of Ni₂ in the triplet state it is considered triplet state is the most stable state of Ni atom. The calculated ground state binding energy is higher than the experimental value but on the other hand lower in the triplet state. The differences in the calculations are arised from the calculation processes and the different spin states.

Table 1. Spectroscopic constants of Ni₂ in ground state (with minimum multiplicity) and in the most stable state (with minimum total energy). Equilibrium interatomic separation r_e (Å), fundamental frequency ω_e (cm⁻¹), total energy E_T (a.u.).

Multiplicity (2S+1)	r _e	ω _e	E _T	Method	Reference
1	2.0760	347.92	-338.8888	DFT	This work
3	2.0710	356.74	-338.9437	DFT	This work
3	2.13			DFT	[42]
	2.06			DFT	[43]
	2.01			MD	[43]
	2.05			DFT	[49]
	2.155			Exp.	[43]
	2.05			MD	[46]
	2.01			MD	[47]
	1.99			Ab initio	[47]
	2.20	289		CI	[48]
	2.60	236		HF	[48]
	2.38	240		RHF	[50]
	2.00			DF	[51]
	2.04	344		ECP-GVB-CI	[52]
	2.18	320		DFT	[53]
	2.33	211		ECP-CI	[54]

Mn₂ Diatom

For Mn₂, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated and the nonet spin state is found to be as the most stable state as seen from Fig.2.

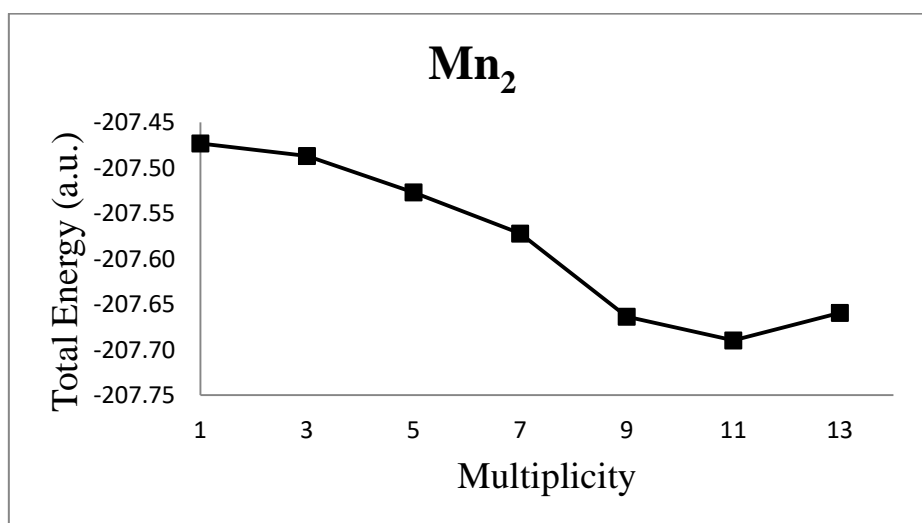


Figure 2. The variation of the total energy versus the spin multiplicity for Mn₂.

Mn₂ homo-nuclear diatom for the most stable structures and its energetically most favorable ground state are given in Table 2. In the present study, bond length and vibrational frequency of Mn₂ diatom are calculated to be, respectively, 1.6604 Å, 719.49 cm⁻¹ in the ground state and 2.5884 Å, 214.06 cm⁻¹ in the most stable spin state (multiplicity=11) by B3LYP/CEP-121G level of theory. The present results are not

compatible with the literature. The differences in the calculations are arised from the calculation processes and the different spin states. It is used doublet spin state of Mn atom which is the most stable state while the calculation of the binding energy for the energetically most favorable ground state of Mn₂. Conformably, for the calculation of the binding energy of Mn₂ in the nonet state it is considered sextet state is the most stable state of Mn atom.

Table 2. Spectroscopic constants of Mn₂ in ground state [with minimum multiplicity] and in the most stable state (with minimum total energy). Equilibrium interatomic separation r_e (Å), fundamental frequency ω_e (cm⁻¹), total energy E_T (a.u.).

Multiplicity (2S+1)	r _e	ω _e	E _T	Method	Reference
1	1.6604	719.49	-207.4869	DFT	This work
11	2.62613	207.50	-207.6897	DFT	This work
1	1.651			DFT	[57]
3	1.564			DFT	[57]
5	1.753			DFT	[57]
7	1.860			DFT	[57]
9	2.094			DFT	[57]
11	2.506			DFT	[57]
	3.29	53.46		MCQDPT2	[55]
	3.42	62.64		MCQDPT2	[55]
11	2.53	240.47		MCQDPT2	[55]
11	2.501	245.8		NEVPT2	[58]
1	3.4	68.1		Exp.	[59]
	1.62			LSDA	[47]
	2.50			BPW91	[60]
	3.562			BP86	[56]
	3.11	47.3		MCQDPT	[60]
	2.61			DFT	[61]

In₂ Diatom

For In₂, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated and

the triplet spin state is found to be as the most stable state as seen from Fig.3.

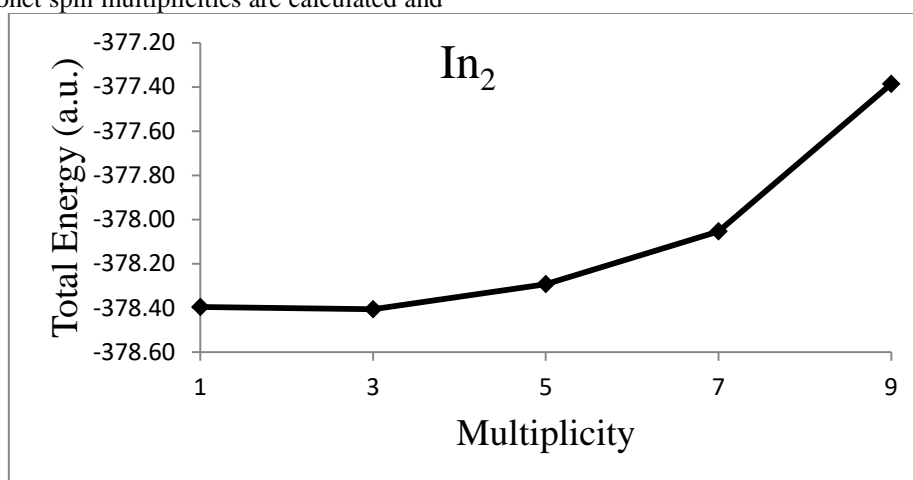


Figure 3. The variation of the total energy versus the spin multiplicity for In₂.

In₂ homo-nuclear diatom for the most stable structures and its ground state are given in Table 3. In the present study, bond length and vibrational frequency of In₂ diatom are calculated to be 3.3846 Å, 96.33 cm⁻¹ in the energetically most favorable ground state and 3.0894 Å, 106.58 cm⁻¹ in the most stable spin state [multiplicity = 3] by B3LYP/CEP-121G level of theory. The present results especially binding energy

agree very well with experimental result in the literature. It is used doublet spin state of In atom which is the most stable state while the calculation of the binding energy for the energetically most favorable ground state of In₂. Conformably, for the calculation of the binding energy of In₂ in the triplet state it is considered doublet state is the most stable state of In atom.

Table 3. Spectroscopic constants of In₂ in ground state (with minimum multiplicity) and in the most stable state (with minimum total energy). Equilibrium interatomic separation r_e (Å), fundamental frequency ω_e (cm⁻¹), total energy E_T (a.u.).

Multiplicity (2S+1)	r_e	ω_e	E_T	Method	Reference
1	3.3846	96.33	-378.3957	DFT	This work
3	3.0894	106.58	-378.4057	DFT	This work
	2.20	402		DFT	[62]
	2.80	111		Exp.	[63]

Heteronuclear diatoms

MnNi Diatom

For MnNi, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated and the octet spin state is found to be as the most stable state as seen from Fig.4.

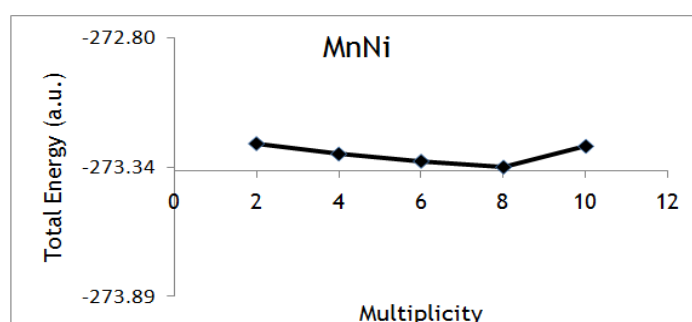


Figure 4. The variation of the total energy versus the spin multiplicity for MnNi.

Binding energy for MnNi calculated as 2.8249 eV in octet spin state. In the calculation regarding different spin state caused the difference between these two value.

Also, calculated equilibrium interatomic separation and fundamental frequencies both doublet and octet spin states for MnNi dimer are given in Table 4.

Table 4. Spectroscopic constants of heteronuclear diatoms in ground state (with minimum multiplicity) and in the most stable state (with minimum total energy). Binding energy E_b (eV), equilibrium interatomic separation r_e (Å), fundamental frequency ω_e (cm⁻¹), total energy E_T (a.u.).

Diatom	2S+1	r_e	ω_e	E_T	Method	Reference
MnNi	2	2.3903	212.19	-273.2429	DFT	This work
MnNi	8	2.4251	214.79	-273.3439	DFT	This work
MnIn	1	2.7065	179.89	-292.9247	DFT	This work
MnIn	5	2.5450	212.17	-293.0125	DFT	This work
NiIn	2	2.6500	168.55	-358.6996	DFT	This work

MnIn Diatom

For MnIn, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated

and the quintet spin state is found to be as the most stable state as seen from Fig.5.

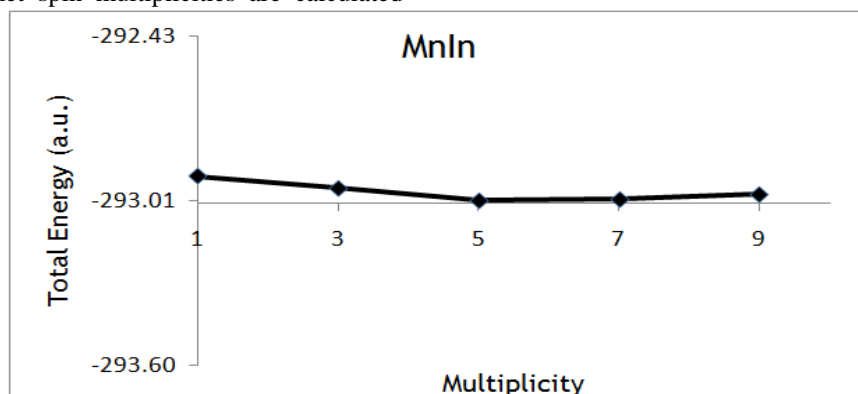


Fig. 5. The variation of the total energy versus the spin multiplicity for MnIn.

Binding energy for MnIn calculated as 1.1544 eV in quintet spin state. In the calculation regarding different spin state caused the difference between these two value. Also, calculated equilibrium interatomic separation and fundamental frequencies both doublet and octet spin states for MnIn dimer are given in Table 4.

InNi Diatom

For InNi, the energy of the singlet, triplet, quintet, septet and nonet spin multiplicities are calculated and the doublet spin state is found to be as the most stable state as seen from Figure 6.

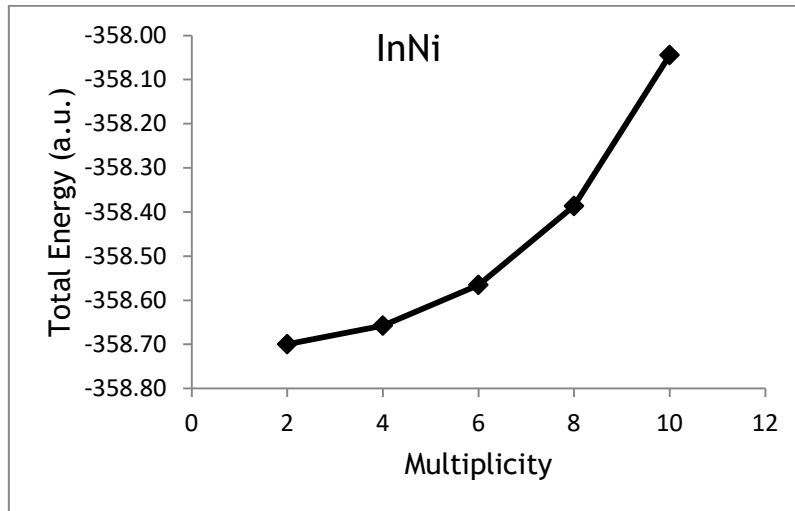


Figure 6. The variation of the total energy versus the spin multiplicity for InNi.

The most stable state and the ground state is the same so binding energy for InNi calculated as 1.9172 eV in doublet spin state. Also, calculated

equilibrium interatomic separation and fundamental frequencies both doublet and octet spin states for MnIn diatom are given in Table 4.

Table 5. The variation of the dipole moment according to the spin multiplicities.

Dimer	Multiplicity (2s+1)	E _T (Total Energy) (a. u.)	Dipol Moment (Debye)
InNi	2	-358.69961115	1.7122
	4	-358.65761688	0.0052
	6	-358.56533281	0.3042
	8	-358.38647785	0.5610
	10	-358.04435666	0.8973
MnIn	1	-292.92474121	1.1005
	3	-292.96760611	0.8127
	5	-293.01253643	1.1210
	7	-293.00707322	0.5548
	9	-292.99069811	0.6397
MnNi	2	-273.24293270	0.9890
	4	-273.28746312	1.1276
	6	-273.31883006	0.8916
	8	-273.34396817	0.9991
	10	-273.25429041	0.1481

Table 5 tabulates the total energy and dipole moment values of the diatoms according to the spin multiplicities. For the InNi (at spin state 2) and MnIn (at spin state 5) diatoms the dipole moments are the highest values while the total energies are minimum (stable state). However, for MnNi diatom the largest

dipole moment value does not correspond to the lowest energy value.

Electronic Properties

For understanding many molecular properties of a molecule like chemical reactivity, UV-Vis spectra and the stability of the molecule along with optical and electrical properties, analysis of the molecular orbitals gap gives us some informations. Also, the structure properties of the

clusters can be examined by investigating highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) [64]. The frontier molecular orbitals of the most stable states of the diatoms considered are presented in Fig.7.

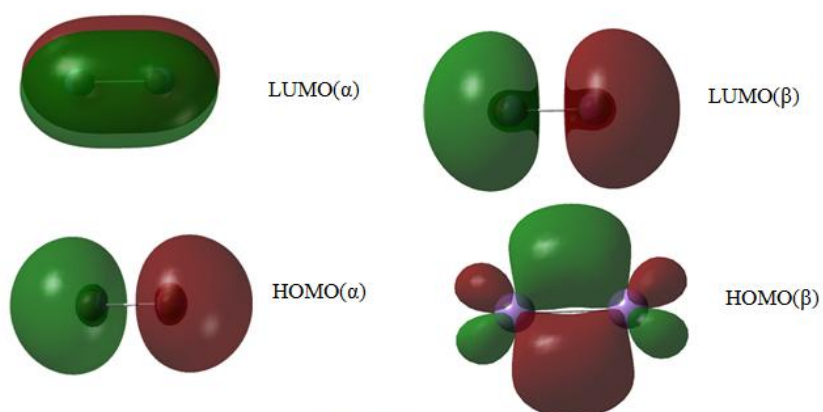


Figure 7 (a)

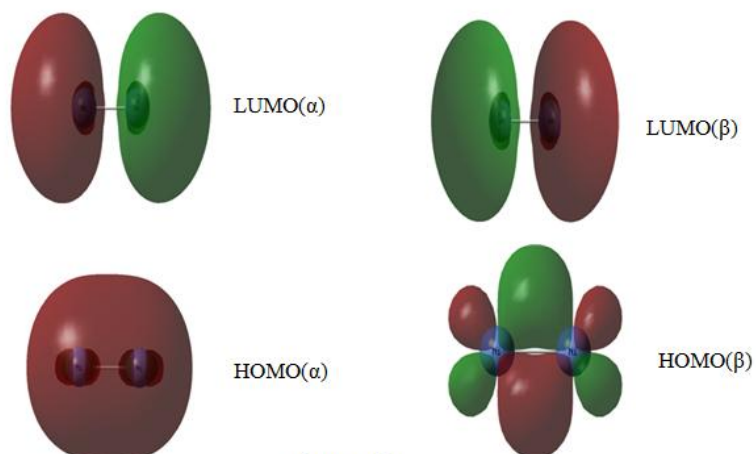


Figure 7 (b)

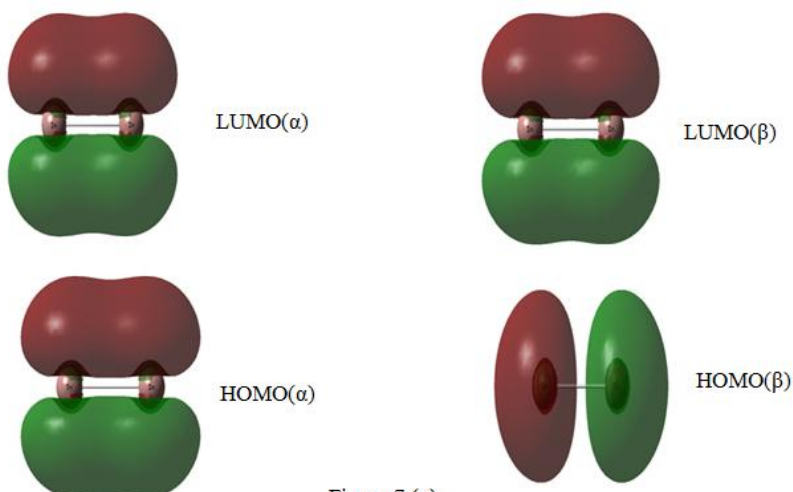


Figure 7 (c)

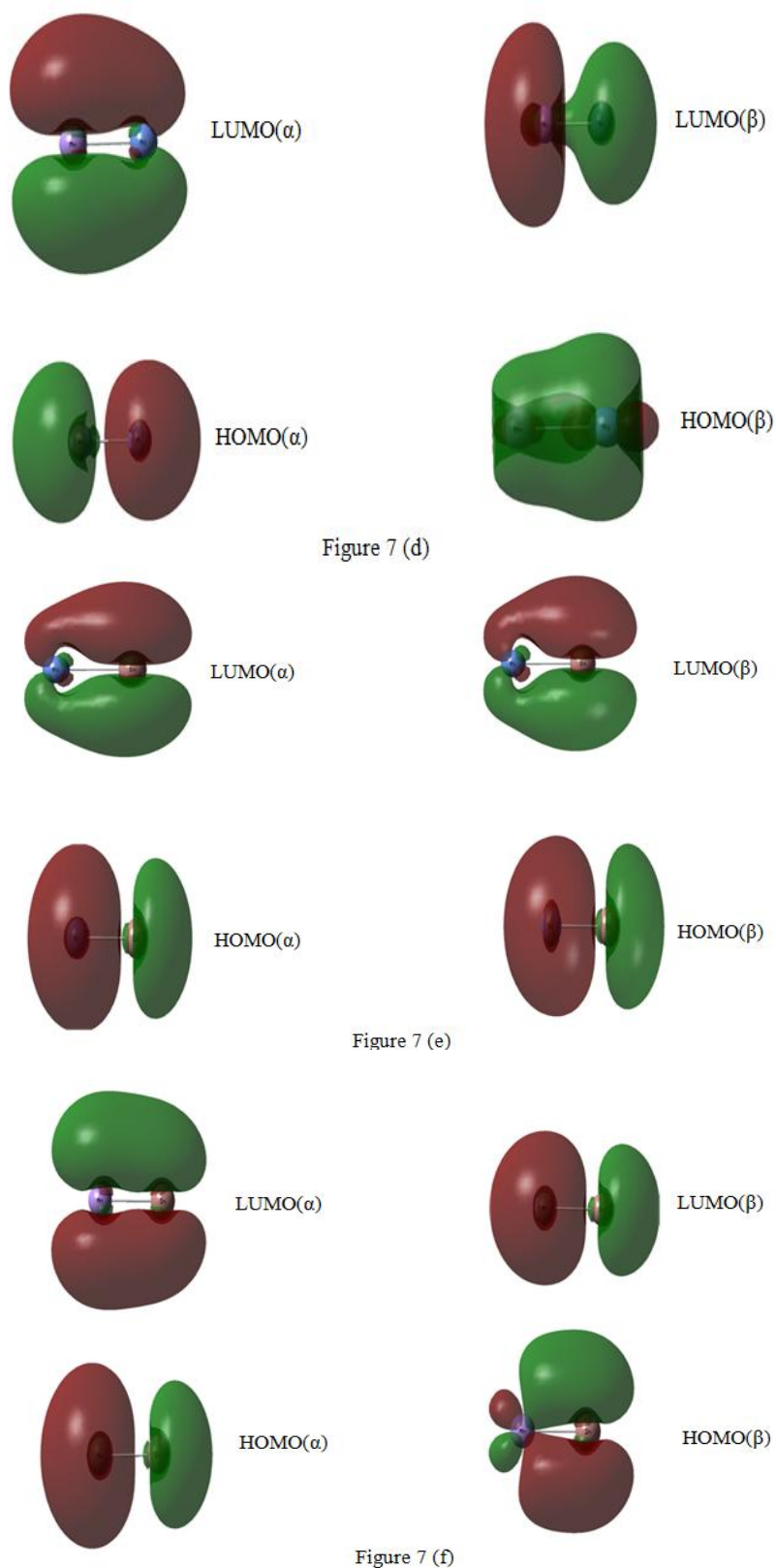


Figure 7. Figure 7 (a) Mn₂ 11-et, Figure 7 (b) Ni₂ triplet, Figure 7 (c) In₂ triplet, Figure 7 (d) MnNi octet, Figure (e) NiIn, Figure (f) MnIn quintet; 3D plots of HOMO and LUMO of the Mn-In-Ni diatoms. Table 6 summarizes the binding energy (E_b) values calculated from the following equation:

$$E_b = (E(\text{diatom (lowest spin state)}) - E(\text{atomA (lowest spin state)}) - E(\text{atomB (lowest spin state)}))$$

The value of binding energy gives information about the power of chemical bond in clusters since it might help to explain the reactivity of the system [65].

Table 6. Calculated binding energy values for the homonuclear and heteronuclear diatoms.

Diatom	E _A (lowest spin state) a.u.	E _B (lowest spin state) a.u.	E _{AB} (lowest spin state) a.u.	E _B (eV)
Mn ₂	-103.7906 (Mn-sextet)	-103.7906 (Mn-sextet)	-207.6899 (Mn ₂ -11-et)	2.9559
In ₂	-189.1796 (In-doublet)	-189.1796 (In-doublet)	-378.4058 (In ₂ -triplet)	1.2695
Ni ₂	-169.4496 (Ni-triplet)	-169.4496 (Ni-triplet)	-338.9438 (Ni ₂ -triplet)	1.2116
MnIn	-103.7906 (Mn-sextet)	-189.1796 (In-doublet)	-293.0125 (MnIn-quintet)	1.1544
InNi	-189.1796 (In-doublet)	-169.4496 (Ni-triplet)	-358.6996 (InNi-doublet)	1.9172
MnNi	-103.7906 (Mn-sextet)	-169.4496 (Ni-triplet)	-273.3440 (MnNi-octet)	2.8249

Table 7 reports calculated values of the frontier orbitals and their gap energies in ground state and the most stable state for homonuclear (Mn₂, Ni₂, In₂) and heteronuclear (MnNi, MnIn, NiIn) diatoms. The

homonuclear (Mn₂, Ni₂, In₂) diatoms have much more charge transfer in their structure since their HOMO-LUMO gap values are smaller than the heteronuclear (MnNi, MnIn, NiIn) diatoms.

Table 7. HOMO and LUMO energies (Hartrees), HOMO-LUMO Gap (E_g) Energies (eV) for the ground state (with minimum multiplicity) and also for the most stable state (with minimum total energy) of the diatoms.

Cluster	2S+1	HOMO(α)	LUMO(α)	E _g (α)	HOMO(β)	LUMO(β)	E _g (β)
Mn ₂	1	-0.162	-0.075	2.367			
Mn ₂	11	-0.166	-0.057	0.109	-0.133	-0.084	0.049
Ni ₂	1	-0.201	-0.125	2.068			
Ni ₂	3	-0.213	-0.187	0.707	-0.094	-0.086	2.558
In ₂	1	-0.108	-0.071	1.007			
In ₂	3	-0.127	-0.087	1.088	-0.267	-0.78	7.265
MnNi	2	-0.178	-0.091	2.367	-0.141	-0.028	3.837
MnNi	8	-0.162	-0.056	2.884	-0.200	-0.094	5.442
MnIn	1	-0.163	-0.069	2.558			
MnIn	5	-0.198	-0.063	3.674	-0.133	-0.122	3.619
NiIn	2	-0.170	-0.073	2.640	-0.168	-0.073	4.572

Following Koopmans' theorem [66] one can define ionization potential and electron affinity of a species in terms of frontier molecular orbital energies, respectively, as follows: $I = -E_{\text{HOMO}}$ and $A = -E_{\text{LUMO}}$. Here E_{HOMO} and E_{LUMO} represent the highest occupied molecular orbital and the lowest unoccupied molecular orbital energies, respectively. These quantities are commonly used to define some physical and/or chemical quantities [67], such as the global hardness $\eta = (I - A)/2$, the global softness $S = 1/(2\eta)$, the electronic chemical potential $\mu = -(I + A)/2 = -\chi$ (χ is electronegativity), and the global electrophilicity index $\omega = \mu^2 / (2\eta)$, which measures the affinity of species to attract electrons. Another electronic quantity called HOMO-LUMO gap, which reflects the ability for electrons to jump

from the highest occupied to the lowest unoccupied molecular orbital, as well as the ability for the species to participate in the chemical reactions to a certain extent. A large gap value stands for a high chemical stability.

Electronic properties of the homonuclear and heteronuclear diatoms changing by the spin multiplicity are shown in Table 8. As seen from the Table 8 the softness of the homonuclear diatoms have the largest values when they are at the minimum multiplicity states, whereas the heteronuclear diatoms have the largest values when they are at minimum energy state. Also electronegativity for the homonuclear diatoms have the lowest values when they are at their minimum multiplicity states.

Table 8. Electronic properties of the homonuclear and heteronuclear diatoms changing by the spin multiplicity (only for α-spin case). All units are in eV.

Cluster	Multiplicity	HOMO _α	LUMO _α	ΔE _α	I _α	A _α	χ _α	η _α	S _α	μ _α	ω _α
Mn ₂	1	-0.16	-0.07	0.09	0.16	0.07	0.12	0.04	26.67	-0.12	0.1872
	3	-5.45	-2.21	3.24	5.45	2.21	3.83	1.11	0.91	-3.83	6.6324
	5	-4.91	-2.25	2.66	4.91	2.26	3.58	1.13	0.89	-3.58	5.6920
	7	-4.93	-3.92	1.01	4.93	3.92	4.43	1.96	0.51	-4.43	4.9966

	9	-0.23	-0.11	0.12	0.23	0.11	0.17	0.06	17.70	-0.17	0.2664
	11	-4.52	-1.56	2.96	4.52	1.56	3.03	0.78	1.28	-3.03	5.9138
Ni ₂	1	-0.20	-0.12	0.08	0.20	0.12	0.16	0.06	16.00	-0.16	0.2126
	3	-0.21	-0.19	0.02	0.21	0.19	0.20	0.09	10.70	-0.20	0.2139
	5	-4.18	-1.32	2.86	4.18	1.32	2.76	0.66	1.52	-2.76	5.7423
	7	-3.37	-2.19	1.18	3.37	2.19	2.78	1.10	0.91	-2.78	3.5334
	9	-4.24	-2.31	1.93	4.24	2.31	3.27	1.15	0.87	-3.27	4.6419
In ₂	1	-0.11	-0.07	0.04	0.11	0.07	0.09	0.04	28.17	-0.09	0.1128
	3	-0.13	-0.09	0.04	0.13	0.09	0.11	0.04	22.99	-0.11	0.1316
	5	-4.26	-1.22	3.04	4.26	1.22	2.74	0.61	1.64	-2.74	6.1687
	7	-3.33	-2.35	0.98	3.33	2.35	2.84	1.18	0.85	-2.84	3.4362
	9	-4.23	-1.89	2.34	4.23	1.89	3.06	0.95	1.06	-3.06	4.9556
MnNi	2	-0.18	-0.09	0.09	0.18	0.09	0.13	0.05	21.98	-0.13	0.1988
	4	-4.61	-2.51	2.11	4.61	2.51	3.56	1.25	0.80	-3.56	5.0562
	6	-4.84	-2.43	2.41	4.84	2.43	3.64	1.21	0.82	-3.64	5.4408
	8	-0.16	-0.06	0.11	0.16	0.06	0.11	0.03	35.71	-0.11	0.2122
	10	-3.15	-2.06	1.08	3.15	2.06	2.61	1.03	0.97	-2.61	3.2912
MnIn	1	-0.16	-0.07	0.09	0.16	0.07	0.12	0.04	28.99	-0.12	0.1950
	3	-4.67	-2.35	2.32	4.67	2.35	3.51	1.17	0.85	-3.51	5.2413
	5	-0.20	-0.06	0.14	0.20	0.06	0.13	0.03	31.75	-0.13	0.2703
	7	-3.37	-2.00	1.37	3.37	2.00	2.68	1.00	1.00	-2.68	3.6060
	9	-3.75	-2.60	1.15	3.75	2.60	3.17	1.30	0.77	-3.17	3.8752
NiIn	2	-0.17	-0.07	0.10	0.17	0.07	0.12	0.04	27.40	-0.12	0.2022
	4	-3.33	-2.16	1.16	3.33	2.16	2.75	1.08	0.92	-2.75	3.4844
	6	-3.84	-2.52	1.32	3.84	2.52	3.18	1.26	0.79	-3.18	4.0145
	8	-4.274	-1.40	2.87	4.27	1.40	2.83	0.70	1.43	-2.83	5.7393
	10	-3.52	-2.50	1.02	3.52	2.50	3.01	1.25	0.80	-3.01	3.6189

Table 9. Electronic properties of the homonuclear and heteronuclear diatoms changing by the spin multiplicity (only for β -spin case). All units are in eV.

Cluster	Multiplicity	HOMO _{β}	LUMO _{β}	ΔE_{β}	I _{β}	A _{β}	χ_{β}	η_{β}	S _{β}	μ_{β}	ω_{β}
In ₂	3	-7.29	-2.13	5.16	7.29	2.13	4.71	2.58	0.39	-4.71	4.2905
	5	-9.63	-5.67	3.96	9.63	5.67	7.65	1.98	0.51	-7.65	14.7703
	7	-21.15	-7.80	13.35	21.15	7.80	14.47	6.68	0.15	-14.47	15.6842
	9	-22.55	-21.59	0.96	22.55	21.59	22.07	0.48	2.08	-22.07	505.3350
Mn ₂	3	-3.84	-2.05	1.79	3.84	2.05	2.95	0.89	1.12	-2.95	4.2905
	5	-3.63	-1.94	1.68	3.63	1.94	2.78	0.84	1.19	-2.78	14.7703
	7	-3.92	-1.97	1.95	3.92	1.97	2.96	0.97	1.03	-2.95	15.6842
	9	-3.84	-1.77	2.06	3.84	1.77	2.80	1.03	0.97	-2.80	505.3350
	11	-3.62	-2.30	1.32	3.62	2.30	2.96	0.66	1.51	-2.96	4.2905
Ni ₂	3	-5.09	-2.34	2.75	5.09	2.34	3.72	1.37	0.73	-3.72	5.0300
	5	-5.60	-4.78	0.82	5.60	4.78	5.19	0.41	2.45	-5.19	32.9829
	7	-7.33	-5.86	1.46	7.33	5.86	6.60	0.73	1.37	-6.60	29.7524
	9	-9.97	-8.70	1.27	9.97	8.70	9.34	0.644	1.574	-9.34	68.6502
InNi	2	-4.57	-2.00	2.57	4.57	2.00	3.29	1.29	0.78	-3.29	4.1955
	4	-5.91	-3.55	2.36	5.91	3.55	4.73	1.18	0.85	-4.73	9.5008
	6	-9.30	-5.23	4.07	9.30	5.23	7.27	2.04	0.49	-7.27	12.9732
	8	-11.97	-7.32	4.65	11.97	7.32	9.64	2.32	0.43	-9.64	19.9874

	10	-18.39	-11.49	6.90	18.39	11.49	14.94	3.45	0.29	-14.94	32.3400
MnNi	2	-3.84	-2.33	1.51	3.84	2.33	3.09	0.75	1.32	-3.09	6.3173
	4	-2.62	-2.22	0.40	2.62	2.22	2.42	0.20	4.98	-2.42	14.6146
	6	-4.32	-2.12	2.20	4.32	2.12	3.22	1.10	0.91	-3.22	4.6957
	8	-5.47	-2.59	2.88	5.47	2.59	4.03	1.44	0.69	-4.03	5.6227
	10	-7.45	-4.33	3.12	7.45	4.33	5.89	1.56	0.64	-5.89	11.1121
MnIn	3	-4.40	-1.83	2.57	4.40	1.83	3.12	1.29	0.78	-3.12	6.3173
	5	-3.641	-3.35	0.29	3.64	3.35	3.49	0.15	6.81	-3.49	14.6146
	7	-3.88	-3.27	0.61	3.88	3.27	3.58	0.30	3.29	-3.58	4.6957
	9	-8.92	-3.88	5.04	8.92	3.88	6.40	2.52	0.40	-6.40	5.6227

III. CONCLUSION

For the different spin multiplicities the structures of Mn-In-Ni diatoms have been calculated at B3LYP/CEP-121G level. According to the results, the equilibrium structures of the Mn-In-Ni diatoms are in different multiplicities. The localization of the charge density of the diatoms are in central region, this indicates that bonding character of the diatoms are semimetallic.

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