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First Principle Description of CdTe Cluster

A.K. Dwivedi[1], S.I. Ansari[2], Preeti Porov[3], V.N. Mishra[4]
[1]*Department of Chemistry,Kisan College, Sohsarai, Nalanda Bihar, India*
[2,4]*Department of Physics, "Shree Ramswaroop" Memorial College of Engineering and Management, Lucknow (UP), India,*
[3]*Department of Applied Sciences GITM Lucknow, India*

Abstract-- **Cadmium Telluride (CdTe) is a Silicon-compatible optical material, whose nano crystals are being used as quantum dots for a varied range of applications in bio-imaging and bio-sensing. The present communication deals with the calculation of molecular geometries electric polarizabilities and dft based reactivity descriptors such as molecular chemical potential, chemical hardness, global electrophilcity index, as well as homo lumo energies and band gap of cadmium telluride clusters $(CdTe)_n$; n =1-8, using ab initio and density functional theory. An increase in mean polarizability, chemical hardness, binding energy and band gap with the cluster size has been observed. It is also observed that chemical potential, global electrophilcity index are decreases with cluster size. The molecule [CdTe]2, [CdTe]4, [CdTe], [CdTe]8 are found to be more stable than CdTe, [CdTe]3, [CdTe]5, [CdTe]7.**

I. INTRODUCTION

Semiconductor nanocrystals, frequently known as quantum dots [1], have been used widely for a varied range of applications in bio-imaging and bio-sensing. These quantum dots (QDs) are generally composed of atoms from groups II and VI or groups III and V of the periodic table. The diameters of QDs typically are between 1 and 10 nm, and each dot contains a relatively small number of atoms in a discrete cluster [2]. Cadmium telluride (CdTe) is a crystalline compound formed from cadmium and tellurium with a zinc blende (cubic) crystal structure. In the bulk crystalline form it is a direct band gap semiconductor. Recently Zhang Yun et. al. [3] have used cadmium telluride quantum dots as a proton flux sensor and have successfully applied it to detect H9 avian influenza virus. Sander F. Wuister et. al. [4] have used Efficiently luminescing colloidal CdTe quantum dots (QDs) for the preparation of mono-dispersed and mixed size QD solids. In recent years, quantum dots (QDs) have been emerging as an attractive alternative to traditional fluorescent organic dyes for biological labeling owing to their unique, size-tunable spectral properties and excellent photostability.[5,6] One challenge in the application of QDs, however, is their stability and biocompatibility in biological systems.

As an important kind of visible light emitting, CdTe QDs have been widely used in biological labeling, such as living-cell imaging[7,8] and cancer marker targeting.[9,10] QDs provide a versatile nanoscale scaffold fodesigning multifunctional nanoparticles with both imaging and therapeutic functions. Structurally, QDs also possess large surface areas for the attachment of multiple diagnostic and therapeutic agents.[11,12]

With the increasing interest in Cadmium Telluride nano crystals as non linear optical devices, quantum dots and nanosensors [3,4], the present communication deals with the calculation of molecular geometry, dipole moment electric polarizability and dft based reactivity descriptors such as molecular chemical potential, chemical hardness, global electrophilcity index, as well as homo lumo energies of Cadmium Telluride clusters $(CdTe)_n$, n=1-8 in gas phase using HF and density functional theory based methods. An intresting issue is HSAB principle and MPH theory. Which are concerned with the study of rationalizing the chemical reaction[13]. It is necessary to explore the possible relationships of these reactivity descriptor with observable calculation. To rationalize the quantitative definition of the descriptor, several studies have been carried out to show the correlation between electronic properties and polarisability[14,15]. The PMH asserts that the molecular system present highest value at equilibrium. At this stage many studies shows that PMH may told even that chemical potential and external potential vary during chemical process[16,17].

II. COMPUTATIONAL DETAILS

Quantum chemical study of the CdTe clusters has been performed within the framework of Hartree Fock and the density functional theory [18] with (B3LYP) [19-21] and B3pw91 methods employing LANL2DZ and LANL2MB basis set using the Gaussian 09 program package [22]. The Gaussian 09 program was used to calculate the dipole moment (μ), and polarizability (α) of the clusters based on the finite field approach. Following Buckingham's definitions [23], the total dipole moment and the mean polarizability in a Cartesian frame is defined by

$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2}$

$\langle\alpha\rangle = 1/3\,[\,\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\,]$

Density functional theory[24-27] based reactivity descriptors may be useful in the prediction of correlation of stability and polarizability of molecules. Ionization potential (I), electron affinity (A), electronegativity (ζ), chemical hardness (η) and chemical potential (μ) are termed as global reactivity descriptors. Parr et al.[28] have defined a new descriptor to quantify the global electrophilic power of the molecule as electrophilicity index (ω), which provides a quantitative classification of the global electrophilic nature of a molecule within a relative scale.

III. THEORETICAL BACKGROUND

Parr and co-workers [24] interpreted that chemical potential (μ) could be written as the partial derivative of the system's energy with respect to the number of electrons at a fixed external potential v(r) :

$$\mu = (\partial E/\partial N)_{v(r)} \qquad \text{----(1)}$$

Iczkowski and Margrave [29] proposed to define electronegativity as

$$\zeta = -\,(\partial E/\partial N)_{v(r)} \qquad \text{-----(2)}$$

for a fixed nuclear charge.

The working formulas in DFT for calculating chemical potential (μ), electronegativity (ζ) and hardness (η) are as follows:

$$\mu \approx -(I+A)/2\ ;\ \zeta \approx (I+A)/2\ ;\ \eta \approx (I-A)/2 \qquad \text{------(3)}$$

The ionization potential and electron affinity can be replaced by the HOMO and LUMO energies, respectively, using Koopmans' theorem [30] within a Hartree-Fock scheme yielding and so on.

$$\zeta = -\,(\varepsilon_{HOMO} + \varepsilon_{LUMO}) \qquad \text{-----(4)}$$

The ionization potential and electron affinity may be better expressed as:

$$I \approx E(N-1) - E(N) \qquad \text{--------(5a)}$$

$$A \approx E(N) - E(N+1) \qquad \text{--------(5b)}$$

Parr et al.[28] have introduced the global electrophilicity index (ω) as a measure of energy lowering due to maximal electron flow between a donor and an acceptor in terms of the chemical potential and the hardness as

$$\omega = \mu^2/2\eta \qquad \text{---------(6)}$$

Binding energy of the cluster be also defined as given below:
binding energy per atom$\{E_b\}$= $\{-E(CdTe)_n + n(Cd) + n(Te)\}/2n$

IV. RESULTS AND DISCUSSION

The calculated molecular geometries for the CdTe and its clusters are shown in Fig. 1. These geometries are true minima. The Cd–Te bond lengths and bond angles at B3LYP/ LANL2DZ are presented in Fig. 1. We show in Fig. 2 the HOMO and LUMO of $(CdTe)_n$; n=1,3,5,7 and$(CdTe)_n$; n=2,4,6,8 in Fig. 3. The calculated values of dipole moment, homo and lumo energies, chemical potential, chemical hardness mean polarizability, global electrophilcity index and binding energy are shown in Table 1, 2, 3 and 4. As basis set increase molecular geometry is invariant, but as size increase the point group symmetry changes C*V, C.S, C.S to C1. The point group of $(CdTe)_n$; n=1,2,3,4,5,6,7,8 are C*V, C.S, C.S, C1, C1, C1, C1, C1 respectively.

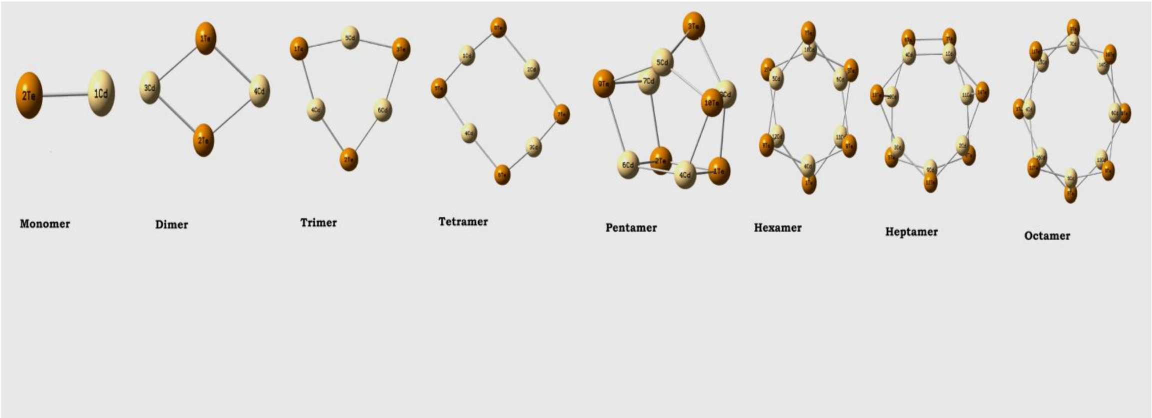


Figure 1. Molecular Geometries of monomer, dimer, trimer and tetramer of CdTe at B3LYP/LANL2DZ basis set. (Bond lengths are in Å)

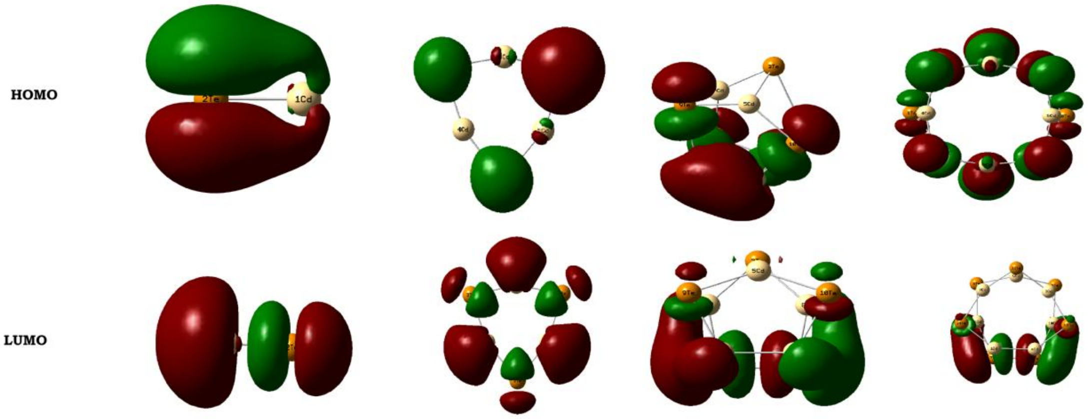


Figure 2: HOMO and LUMO of CdTe Clusters monomer, trimer, pentamer and heptamer.

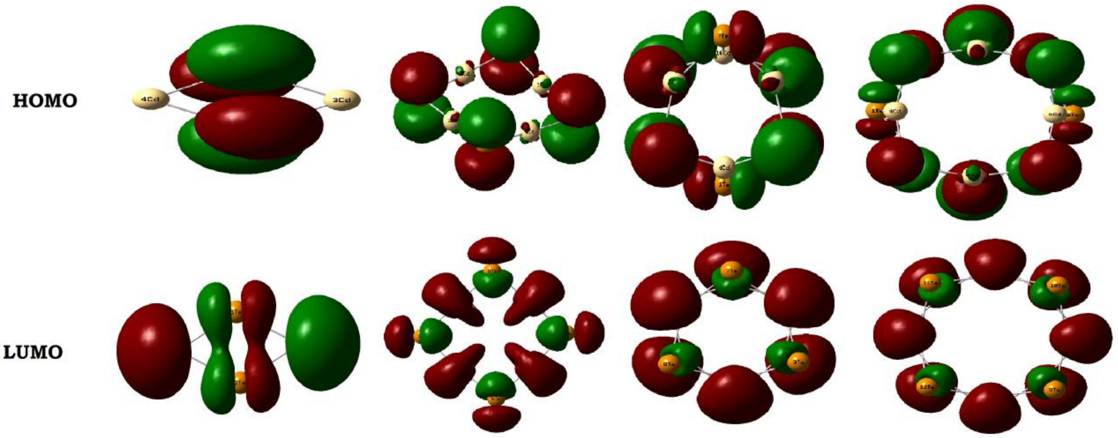


Figure 3: HOMO and LUMO of CdTe Clusters dimer, tetramer hexamer and octamer.

V. BINDING ENERGY AND HOMO LUMO ANALYSIS

The binding energy curve for CdTe cluster is shown in fig[**8,15**] for different basis set with cluster size. The binding energy per atom of the cluster is defined with respect to free atoms follow the mathematical equation: $E_b=-[E_{cluster}- n(E_{Cd})- n (E_{Te})]/2n$ where $E_{cluster}$, E_{Cd}, E_{Te} are optimized of cluster, free cadmium and free tellurium atom. Its also find that binding energy per atom with cluster size monotonically increases. it also find that even molecule [dimer, tetramer hexamer and octamer] are more relevant stable than odd molecule [monomer, trimer, pentamer and heptamer]. It shown in table 1,2,3,4 and a graph Eb Vs cluster size is given in fig. [**8,15**]. The max. binding energy is obtained 4.584 ev per atom for (CdTe)8.

Where as it varries from 0.545 ev to 4.584 ev for LANL2DZ and 0.26 ev to 4.344 ev for LANL2MB basis. The stabilityof the compound is usually measeredin terms of binding energy, bond length, bond dissociation energy, frontier orbital energy and their gap. We use also frontier orbital energy and band gap to evaluate stability. Fukui et al.[31] describe the eminent role played by HOMO and LUMO as agoverning body of chemical reaction. Several studies show that band gap[E homo-lumo] is a very important stabilty indexof molecules [32-35]. A large band gap implies high stability where as a small band gap implies lower stability. Therefore high stability concludes small chemical reactivity and lower stability means higher reactivity or we can say smaller band gap means easier electron transition and lesser stability.

Variations of HOMO LUMO band gap is also shown in Fig. [**9, 16**]. It decreases with cluster size from 6.0138 ev to 2.3846ev for hartee fock theory. Whether it increases for DFT functional with cluster size from 1.2517 ev to 2.3946 ev. It also well known that relative stability of cluster can be predicted by calculating average binding energy, embedded energy and HOMO LUMO energies.[36]

Table : 1

Cluster	**method**	LANL2DZ							
		Dipol moment d in debye	**Homo in e.v.**	**Lumo in e.v.**	**Chemical potential µ in e.v.**	**Hardness η in e.v.**	**Mean α in a. u.**	**ω in e.v.**	**Binding energy in e.v.**
Monomer	HF	6.4892	-7.6192	-1.6055	-4.613	-3.006	87.99	-3.54	-0.545
	B3LYP	5.3258	-5.4967	-4.2450	-4.87	-0.626	79.14	-15.559	-0.830
	B3PW91	5.7277	-5.5512	-4.2178	-4.89	-0.667	89.27	-17.925	-0.955
Trimer	HF	0.0002	-8.2451	-0.3538	-4.300	-3.551	197.64	-2.603	-1.767
	B3LYP	0.0052	-6.0410	-2.9116	-4.477	-1.564	227.21	-6.407	-1.875
	B3PW91	0.0004	-6.1498	-2.7756	-4.463	-1.687	221.21	-5.903	-2.09
Pentamer	HF	2.6318	-7.2927	-0.5442	-3.9185	-3.374	343.559	-2.2683	-3.768
	B3LYP	3.5295	-5.4695	-3.2654	-4.3675	-1.102	386.816	-8.6540	-3.706
	B3PW91	0.9033	-5.6056	-3.2110	-4.4083	-1.197	378.877	-8.1154	-4.192
Heptamer	HF	4.3212	-7.7009	-0.5986	-4.1498	-3.551	482.264	-2.4247	-4.026
	B3LYP	4.2178	-5.7416	-3.5103	-4.6260	-1.115	551.931	-9.5903	-3.858
	B3PW91	4.0563	-5.7961	-3.5375	-4.7620	-1.129	531.428	-10.0401	-4.344

Table : 2

Cluster	**method**	LANL2DZ							
		Dipol moment d in debye	**Homo in e.v.**	**Lumo in e.v.**	**Chemical potential µ in e.v.**	**Hardness η in e.v.**	**Mean α in a. u.**	**ω in e.v.**	**Binding energy in e.v.**
Dimer	HF	7.2138	-7.1839	-1.1429	-4.164	-3.020	161.40	-2.870	-1.01
	B3LYP	0.0116	-5.0886	-3.5103	-4.300	-0.789	172.27	-11.717	-1.3775
	B3PW91	0.0035	-5.0341	-3.5919	-4.313	-0.721	169.53	-12.900	-1.5375
Tetramer	HF	0.0006	-8.1907	-0.2177	-4.2042	-3.9865	275.98	-2.2169	*-4.215*
	B3LYP	0.7442	-6.0410	-2.8300	-4.4355	-1.6055	322.618	-6.1270	*-3.850*
	B3PW91	0.8332	-6.2042	-2.7484	-4.4763	-1.7280	312.639	-5.7978	*-4.275*
Hexamer	HF	0.0002	-8.0274	-0.6259	-4.3266	-3.700	387.738	-2.5292	-4.172
	B3LYP	1.9340	-6.1498	-3.1021	-4.6260	-1.524	444.209	-7.0219	-4.073
	B3PW91	1.8859	-6.2887	-2.9389	-4.5988	-1.659	431.137	-6.3706	-4.592
Octamer	HF	0.0020	-8.0546	-0.5714	-4.3130	-3.7416	535.242	-2.4858	-4.283
	B3LYP	2.5036	-6.1770	-3.1293	-4.6532	-1.5238	623.0997	-7.1047	-4.078
	B3PW91	2.4570	-6.3131	-2.9933	-4.6532	-1.6599	602.755	-6.5222	-4.584

Table: 3

Cluster	method	LANL2MB							
		Dipol moment d in debye	**Homo in e.v.**	**Lumo in e.v.**	**Chemical potential µ in e.v.**	**Hardness η in e.v.**	**Mean α in a. u.**	**ω in e.v.**	**Binding energy in e.v.**
Monomer	HF	5.0194	-7.7553	-1.5238	-4.64	-3.115	86.37	-3.456	-0.260
	B3LYP	4.6491	-5.6327	-4.4899	-5.062	-0.571	70.72	-22.437	-0.525
	B3PW91	4.9917	-5.6872	-4.5171	-5.102	-0.585	71.34	-22.248	-0.620
Trimer	HF	0.0002	-8.2723	-0.8708	-4.572	-3.700	190.35	-2.824	-1.168
	B3LYP	0.0008	-6.1770	-3.3742	-4.776	-1.401	214.20	-8.140	-1.406
	B3PW91	0.0005	-6.3131	-3.3198	-4.816	-1.496	207.99	-7.752	-1.59
Pentamer	HF	2.6318	-7.2927	-0.5442	-3.9185	-3.3742	343.559	-2.2683	-3.768
	B3LYP	3.2693	-5.8504	-3.5647	-4.7076	-1.1429	352.601	-9.6953	-2.976
	B3PW91	3.1819	-5.9321	-3.5103	-4.7212	-1.2109	340.423	-9.2038	-3.393
Heptamer	HF	4.3212	-7.7009	-0.5986	-4.1498	-3.5511	482.264	-2.4247	-4.026
	B3LYP	3.7799	-6.0682	-3.7280	-4.8991	-1.1701	513.416	-10.2519	-3.086
	B3PW91	3.63132	-6.2042	-3.7824	-4.9933	-1.2109	493.366	-10.2953	-3.504

Table : 4

Cluster	method	LANL2MB							
		Dipol moment d in debye	**Homo in e.v.**	**Lumo in e.v.**	**Chemical potential μ in e.v.**	**Hardness η in e.v.**	**Mean α in a. u.**	**ω in e.v.**	**Binding energy in e.v.**
Dimer	HF	7.0837	-7.2111	-1.7143	-4.463	-2.748	163.72	-3.624	-0.645
	B3LYP	5.1197	-5.2246	-4.1634	-4.694	-0.530	166.91	-20.786	-1.09
	B3PW91	5.4977	-5.2791	-4.1089	-4.694	-0.612	164.05	-18.001	-1.225
Tetramer	HF	0.0000	-8.2723	-0.5987	-4.4355	-3.8368	273.211	-2.5638	*-3.024*
	B3LYP	0.5634	-6.2315	-3.0205	-4.6260	-1.6055	309.666	-6.6446	*-2.958*
	B3PW91	0.5646	-6.3675	-2.9933	-4.6804	-1.6871	300.006	-6.4922	*-3.282*
Hexamer	HF	0.0002	-8.0274	-0.6259	-4.3266	-3.7007	387.738	-2.5292	-4.172
	B3LYP	1.6704	-6.4491	-3.5919	-5.0205	-1.4286	402.344	-8.8217	-3.252
	B3PW91	1.6206	-6.5852	-3.5103	-5.0478	-1.5374	387.507	-8.2868	-3.695
Octamer	HF	0.0020	-8.0546	-0.5714	-4.3130	-3.7416	535.242	-2.4858	-4.283
	B3LYP	2.1644	-6.4764	-3.5647	-5.0205	-1.4558	582.369	-8.6569	-3.248
	B3PW91	2.1071	-6.6124	-3.4831	-5.0478	-1.5647	559.581	-8.1422	-3.681

VI. GLOBAL REACTIVITY DESCRIPTORS

Basic reactivity Descriptors are play a very important roll to get the rationalize molecule structure and chemical reaction[37]. DFT has provided the basis for rigorous mathematical definition of reactivity descriptors[25,38,39,40]. Such as chemical potential(μ) characterize the escape tendency of electron from equilibrium. The hardness(η) can be seen as resistance to charge transfer whether softness(S) has been quantitatively related to polarisabilty of system.

We can see the calculated value of descriptors in table 1,2,3,4 and their graph with respect to cluster size are shown in fig.[**???????**]. Which are determine to undermine the corresponding electrophilcity value by density functional theory. Chemical hardness has been established as an electronic quantity which may used to characterized the relative study of molecules and aggregate in many cases of PMH. Assuming that PMH holds in these systems, the hardness is expected to present a behavior with local maximum at numbers of magic clusters. Here tetramer and hexamer are more harder than neighbouring atoms means having more stability than them.

Fig.[**???**] plot the chemical hardness has lowest value 0.530 ev and 3.9865 ev as maximum value. Hardness increases with cluster size. More hardness means hard to react or more stable. It also confirmed by binding energy curve plot in fig[**???**] that trimer molecules are most stable. Its also found that it does not varry mare at level of basis set but has a significance change with theory. As hardness and softness are important factors of the charge transfer resistance and inversaly proportional to each other[41]. For atomic systems the softness is readily related with polarisabilty. The dipole plarisability (α) measures the distortion of the electron density of the molecules and the response of the molecule to the external electric field. As shown in fig[**??**] the mean polarisability is monotonically increases with cluster size and have maximum value 623.0997 a.u. for octamer.

The chemical potential (μ) characterizes the tendency of electron to escape from the molecule in the equilibrium state. Koopman's theorem has been used to calculate μ of the molecules [30].

In present calculation the chemical potential varies with size but it increase for even molecules of cluster. Fig [**???**] shows this tradition but odd molecules have more value than even clusters.

VII. GLOBAL ELECTROPHILCITY INDEX

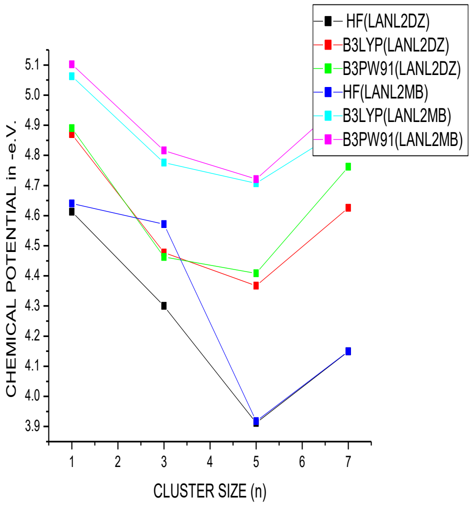
The generalized concept of philcity was proposed by Chattaraj et al[42]. The group concept of philcity is very useful in unraveling reactivity of various molecular system[43].

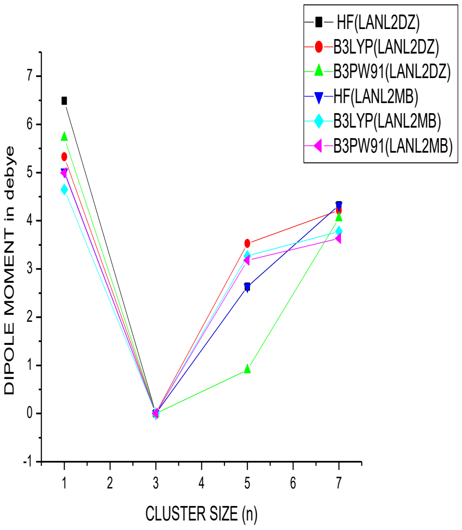
N=1,3,5,7

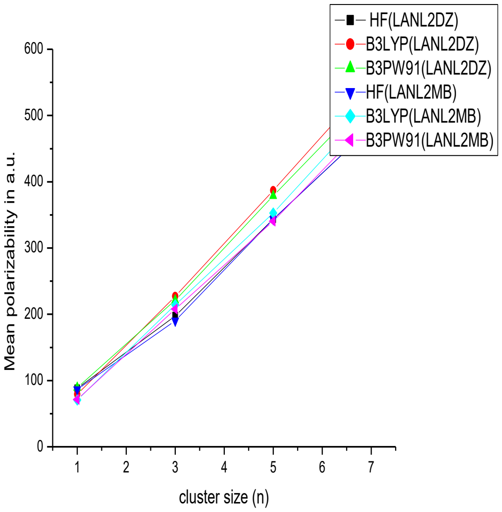
The condense philcity summed over a group of relevant atoms is defined as the group philcity. It can be expressed as:

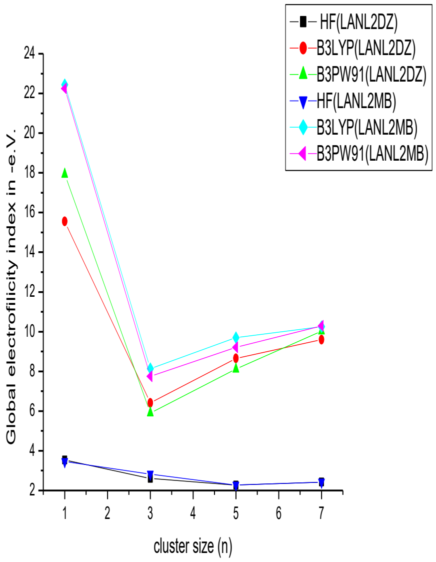
$$\omega = \mu^2/2\eta$$

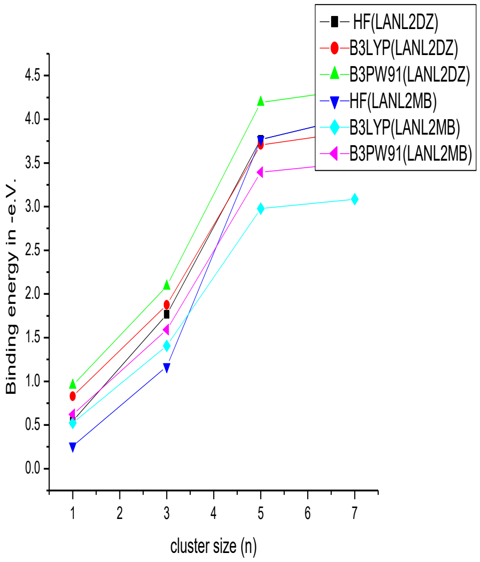
In present work we see that the global electrophilcity index is readily decreases with cluster size and is minimum for trimer molecules. It means it is less reactive for electrophilic, nucleophilic and radical attack conclude that it is more stable than rest of molecules. Fig [**??**] shows this tradition.

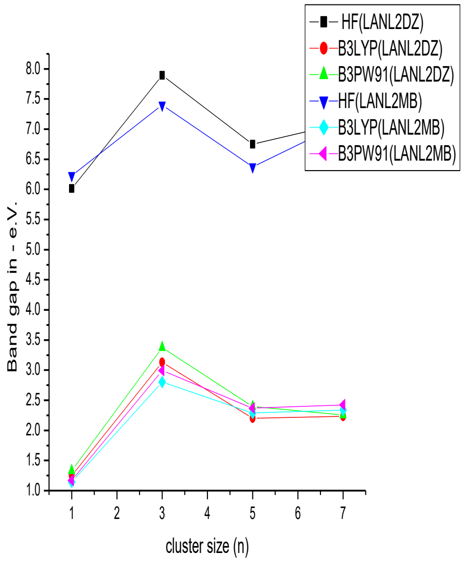


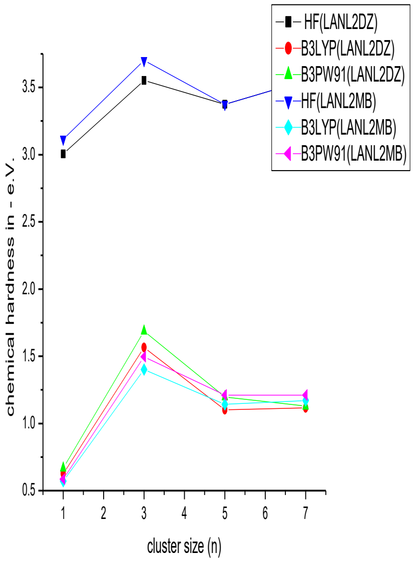




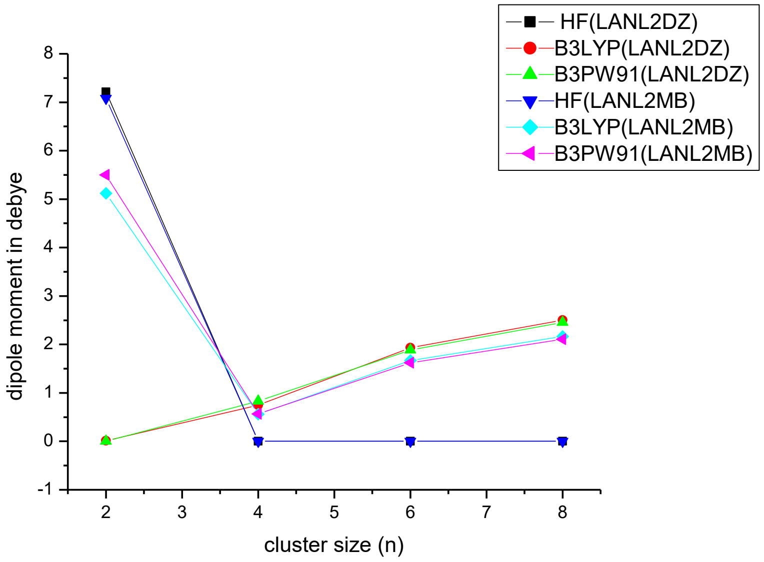

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
Global electrofilicity index in -e.V.
2
4
6
8
10
12
14
16
18
20
22
24
1
2
3
4
5
6
7
cluster size (n)

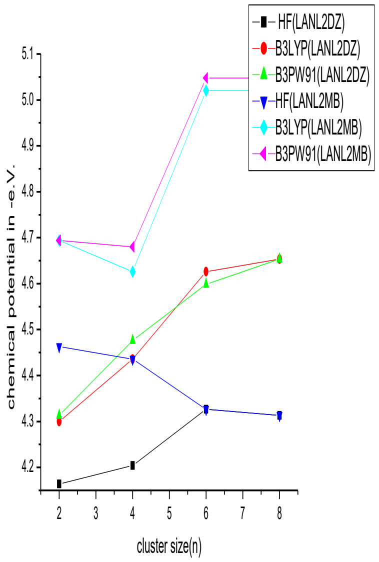

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
Binding energy in -e.V.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
1
2
3
4
5
6
7
cluster size (n)

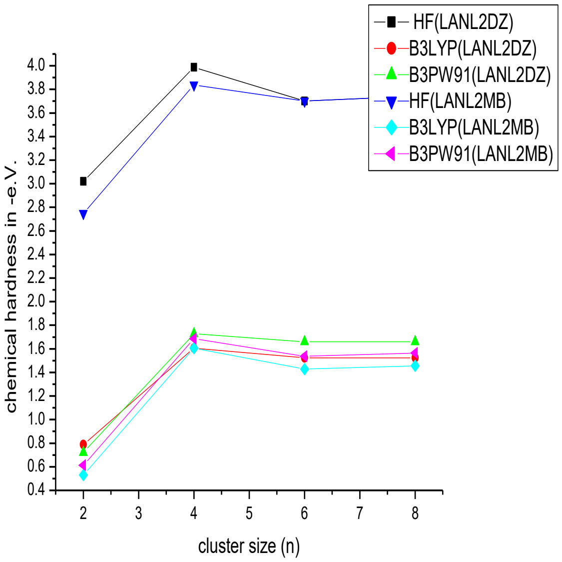

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
Band gap in - e.V.
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
1
2
3
4
5
6
7
cluster size (n)

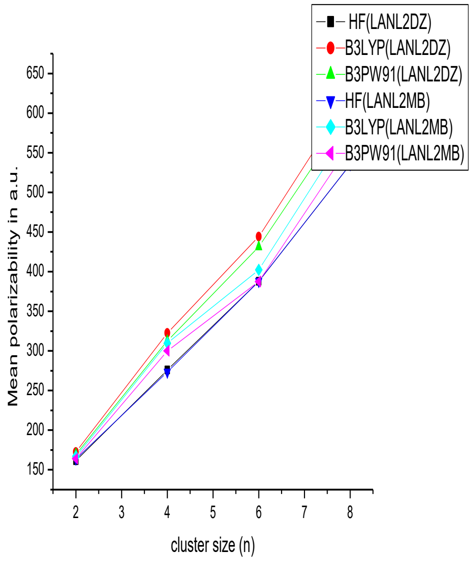

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
chemical hardness in - e.V.
0.5
1.0
1.5
2.0
2.5
3.0
3.5
1
2
3
4
5
6
7
cluster size (n)

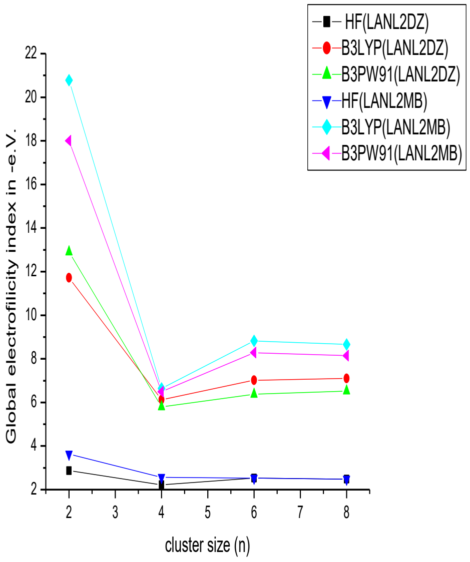
N=2,4,6,8

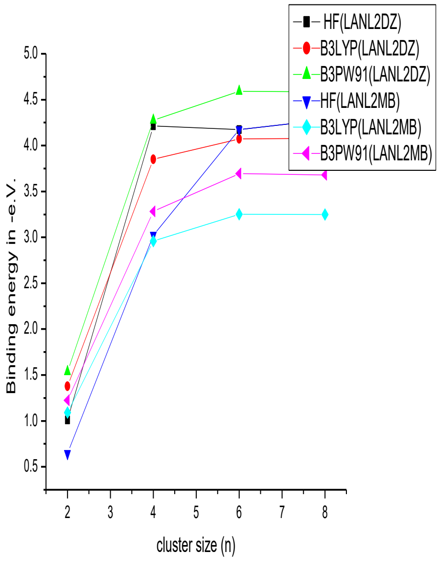

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
dipole moment in debye
-1
0
1
2
3
4
5
6
7
8
2
3
4
5
6
7
8
cluster size (n)

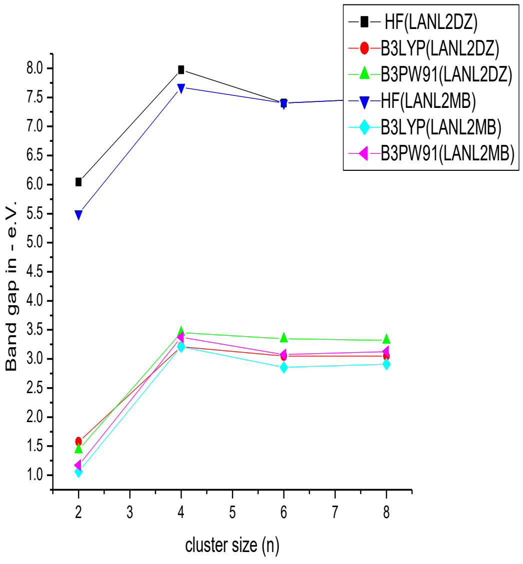

HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
chemical potential in -e.V.
4.2
4.3
4.4
4.5
4.6
4.7
4.8
4.9
5.0
5.1
2
3
4
5
6
7
8
cluster size(n)


HF(LANL2DZ)
B3LYP(LANL2DZ)
B3PW91(LANL2DZ)
HF(LANL2MB)
B3LYP(LANL2MB)
B3PW91(LANL2MB)
chemical hardness in -e.V.
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0
2
3
4
5
6
7
8
cluster size (n)









VIII. CONCLUSION

In summary a report on present calculation has been presented and molecular structure, binding energy and global reactivity descriptors have been discussed. Based on our results following conclusion can be made.

(a) With change in cluster size binding energy increases but even molecules (dimer, tetramer, hexamer and octamer) have more binding energy than odd molecules (monomer, trimer, pentamer and heptamer).

(b) With increase in cluster size chemical hardness increases and tetramer, hexamer shows himself as magic cluster.

(c) Mean polrisability increases with cluster size, whether dipole moment is declines with it.

(d) Chemical potential varries with size of cluster. As it increase for even molecules but odd molecules have more value than neighbour.

(e) Even molecules have more band gap. Hence they are more stable than odd, its also show a good agreement with previous conclusion of binding energy.

The present quantum chemical study may further play an important role in understanding of electric properties of CdTe clusters possessing potential non-linear optical properties and their future use in various devices.

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