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The Ag_xSi_y(x=1-5, y=1-5) Clusters with Electronegativity, Molecular Orbitals and SCF Density

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Abstract: In this work I calculated the optimization geometry of Ag_xSi_y clusters with PBE/LANL2DZ level of theorie and I plot the molecular orbitals and SCF density. For the proprieties of clusters I claculated the electronegativity for employed the results in the chemical reaction. The HOMO and LUMO for neutral clusters are very different that anion and cation and not all atoms are greater density of electron. The SCF density in the structure of cluster are sferical density. The 8.36 and 7.26 eV are the mayor values obtained for the electronegativity.

Keywords: Ag_xSi_y Clusters, Electronic Proprieties, HOMO and LUMO, Electronegativity

1. Introduction

Although chemical reactivity is characterized by global reactivity parameters like electronegativity or hardness, the selectivity is usually understand in terms of local functions like the Fukui function f(r) and local softness s(r). These global and local descriptors of reactivity have been popularized within the framework of conceptual density functional theory, a field to which reviews have been dedicated recently.

The interaction between electrophiles (agents with deficit of electrons) and Ag_xSi_y are view in the orbital molecular picture and electronegativity. The volumen more greater of the HOMO and LUMO are show the active site. A soft molecule has an easily electron distribution and in this work the structure are soft. The quantities χ and η are global proprieties, characteristic of the entire molecule, and nota f particular orbitals or atoms.

In the literature are many article when are elucidate the reactive sites of molecule [1-6].

2. Results and Discussion

In this work are optimized de geometry of Ag_xSi_y cluster for determine your electronic proprieties with Gaussian 2003 programa employed the PBE/LANL2DZ level of theory what introduce the relativistic effects in structure. This effect are view in preview paper in the bonding and IP and AE proprieties. The relativistic effect are view in the color of the cluster. The HOMO and LUMO orbitals are determine the reactive site for this molecule with another molecule. Are employed the OM theory for view the difference with another calculus in the preview article. Are studie the global proprietie and electronegativity. Ab initio effective core potentials (ECPs) have been generated to replace the Coulomb, exchange, and core-orthogonality effects of the chemically inert core electron in the transition metal atoms.

In LANL2DZ the relativistic mass-velocity and Darwin effect on the valence electrons are incorporated in the relativistic ECP's generated for the havier (Z>36) elements.

3. Orbital Molecular

3.1. Neutral Dimers, Neutral Anions and Cat1ions

The function Fukui are relacioned with the density of HOMO and LUMO when are worthless the relaxation efects [6]:

$$f^{+}(r)=\rho_{LUMO}(r) \text{ site nuclephile}$$

$$f^{-}(r)=\rho_{HOMO}(r) \text{ site electrophile}$$

$$f^{0}(r)=1/2(\rho_{LUMO}(r)+\rho_{HOMO}(r)) \text{ site radical}$$

Here ρ_{LUMO} and ρ_{HOMO} are the normalized electron densities of the fronter orbitals. If electron transfer is important, than chemical reaction occurs at the site where f has its largest value.

In Fig. 1 a) A and B the site active are around of Si atom, are observed the greater orbital. The energy of α HOMO with one electron are near with α LUMO, for this reason are soft structure.

For anion structure, Fig. 1 b)A and B, are observed un little displesured of electron near of the silver atom because are two electrons.

I speak of cation, Fig. 1 c) A and B, the silver are great density of electron that silicio for HOMO.

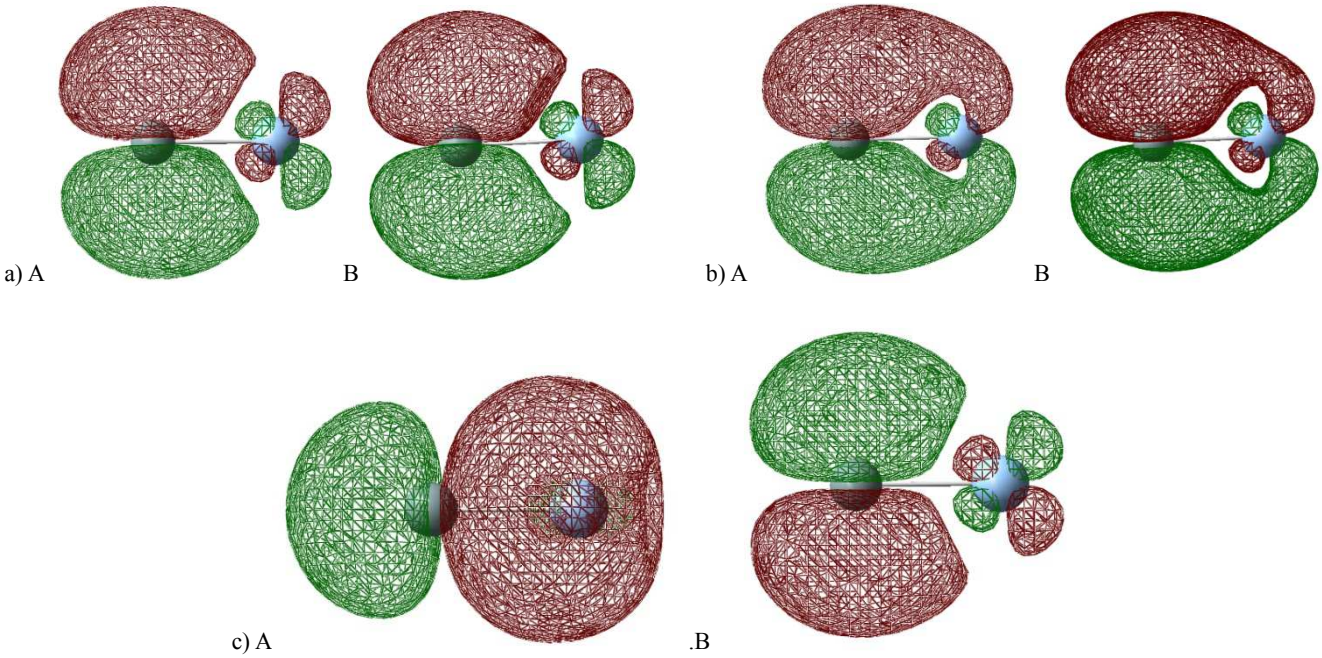
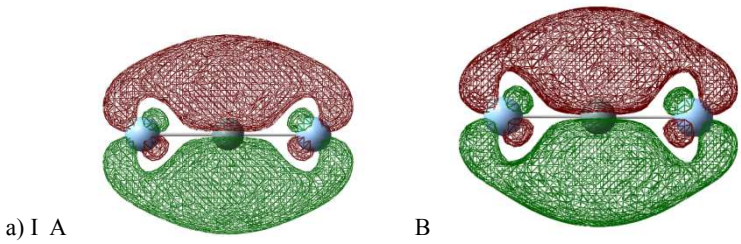
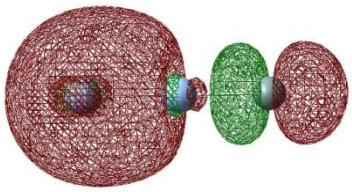
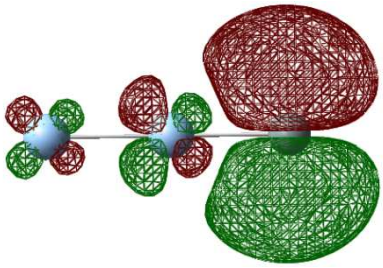


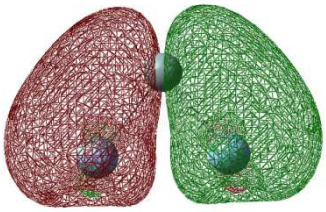
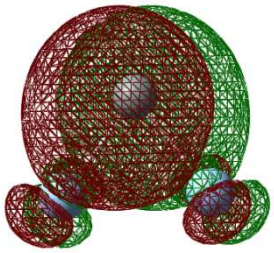
Fig. 1. *The structure with orbital molecular of dimer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations. Isovalue 0.02.A are HOMO and B are LUMO.*

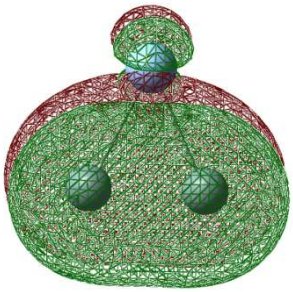
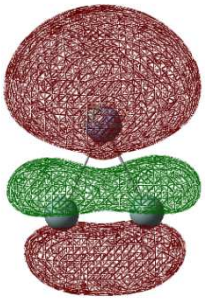
3.2. Neutral Trimer, Neutral, Anions and Cations

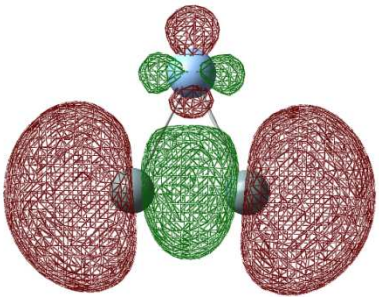
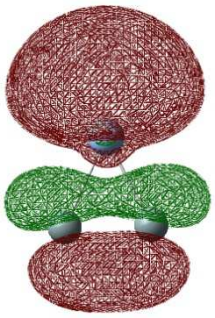
In Fig.2 a) I A and B the structure are comport in what manner of radical for the distributed between free atoms the electrons. In Fig. 2 a) all clusters are HOMO with 2 electrons. For Fig. 2 a) II A and B the silicio are concentred de density of electron. In Fig. 2 a) III B the electron are around of Si, whilst in IIIA are comparted the density of electron and are antibonding. In Fig. 2 a) IV A are bonding with the mayor density of Si and in B are for silver atoms. In Fig. 2 b) I A and B the in A the rectivity are for Si and B for silver. In Fig. 2 b) IIA and B, for HOMO are antibonding and for LUMO bonding π for all atoms. The electron are comparted between the atoms, Fig. 2 II for HOMO and LUMO. In structure of cations the better traslape are for silver in A and silicio in B, Fig. 2 c) IA and B. For Fig. 2 c) IIA and B are identicaly with Fig. 2 a) III A and B. For HOMO in Fig. 2 c) III A are antibonding between free atoms and for LUMO bonding. In Fig. 2 c) IV A and B silicio are more reactive for traslape of orbitals with another structure or compound.

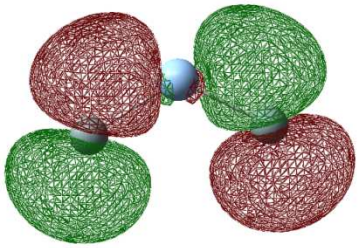
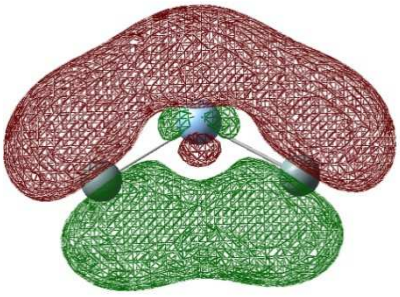


II A  B 

III A  B 

IV A  B 

b) I A  B 

II A  B 

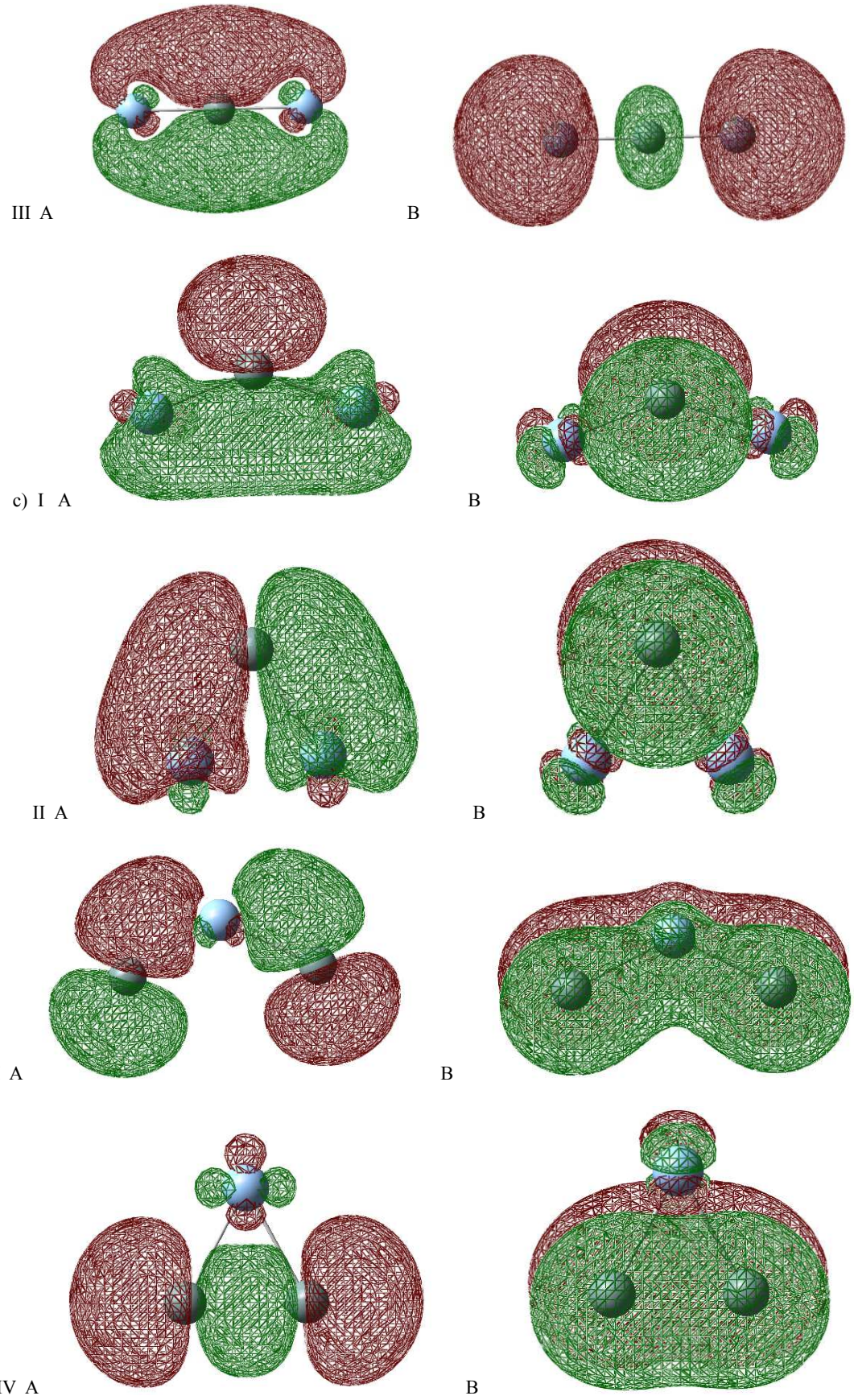
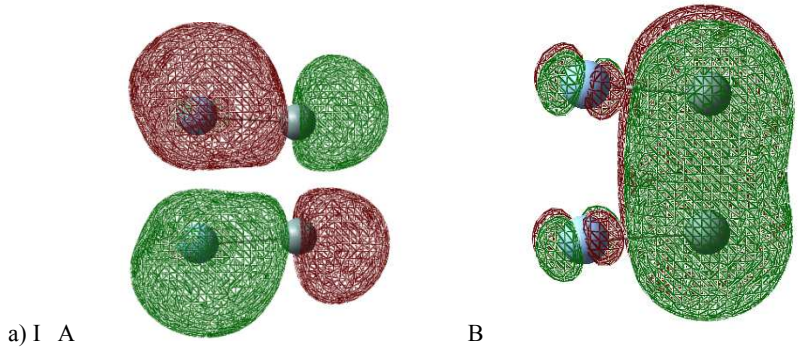


Fig. 2. *The structure with orbital molecular of trimer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations. Isovalue 0.02.A are HOMO and B are LUMO.*

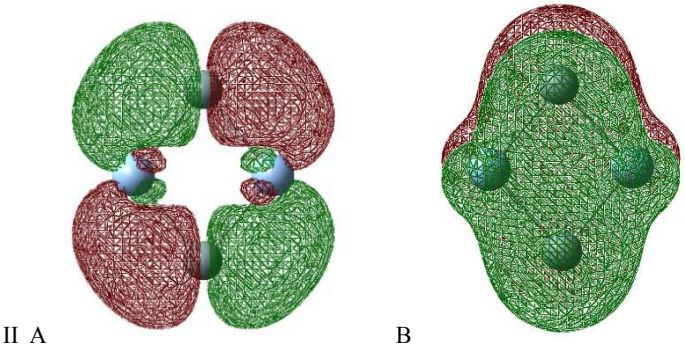
3.3. Tetramer, Neutral, Anions and Cations

Fig. 3 show the orbitals HOMO and LUMO for clusters with 4 atoms and this are soft. The Si are the orbital very large for better traslape in Fig. 3 a) IA and B. When are rombic structure for HOMO are antibonding and LUMO bonding when the charge are distributed between all atoms, Fig. 3 a) II A and B. In Fig. 3 a) III A and B the density of orbitals are distributed near of the basal atoms. In Fig. 3 IV A and B are observed de s-d interaction for this clusters. For anion cluster all structure are antibonding and all atoms contributed for density of electron in ataque with ataque with electrophiles or radical, Fig. 3 b). Fig. VII B are s-d traslape. Fig.3 b) IV A and VI A are biding. For cation clusters, Fig. 3 c) I and II A and B the two silver and two silicio are greater orbital molecular. In Fig. 3 c) III A and B are antibonding distributed the charge between all atoms. In Fig. 3 c) IV, V, VI, VII and VIII are antibonding for all atoms.

In Fig. 3) III, V, 3 b) II, 3 b) X, 3 c) II and3c) VII the HOMO with one electron, are name SOMO.



a) I A B



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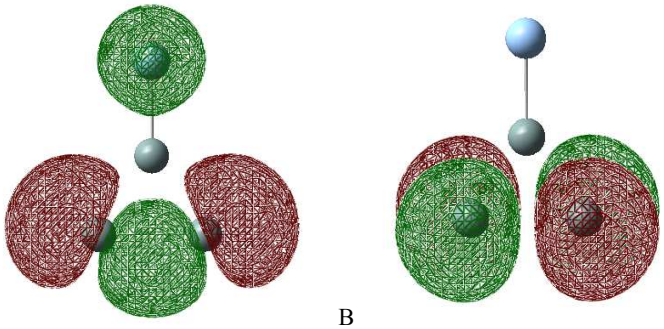
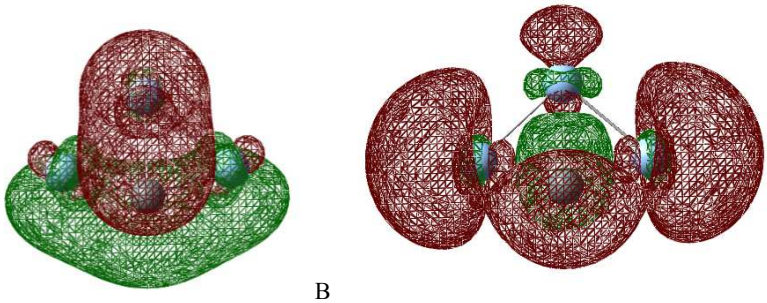
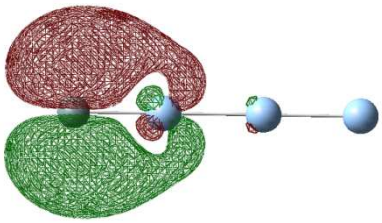
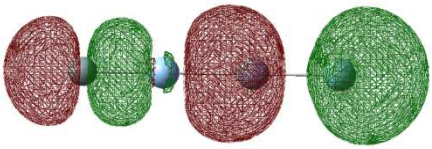
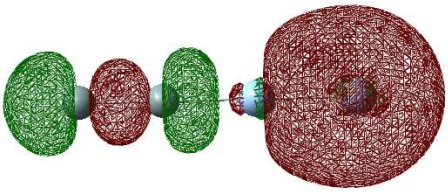
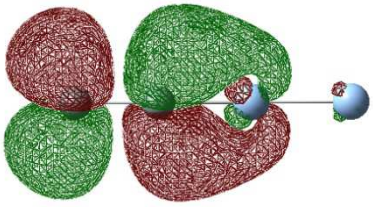


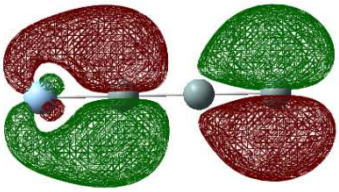
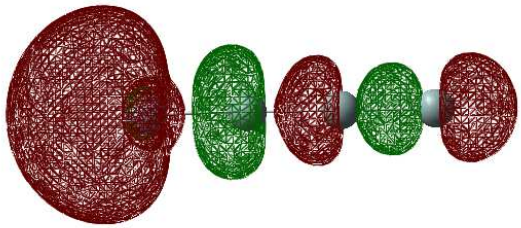
III A B

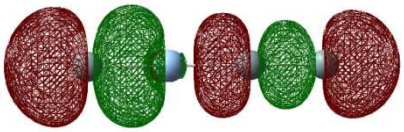
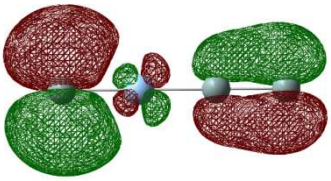


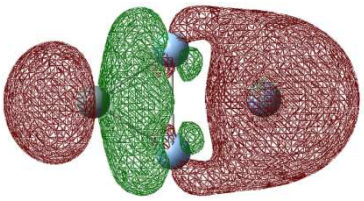
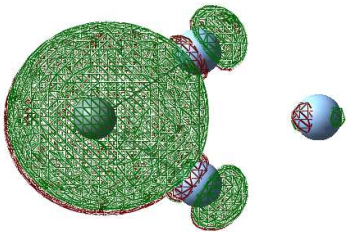
VI A B

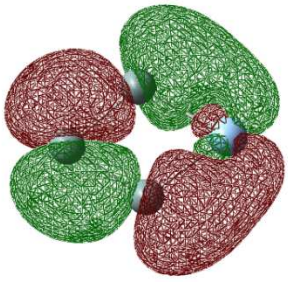
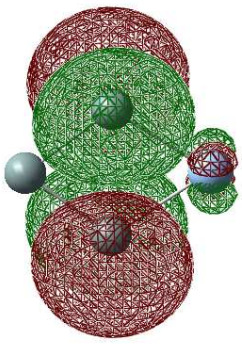
b) I A  B 

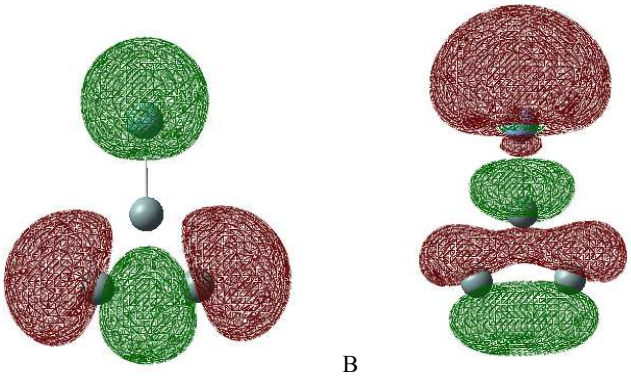
II A  B 

III A  B 

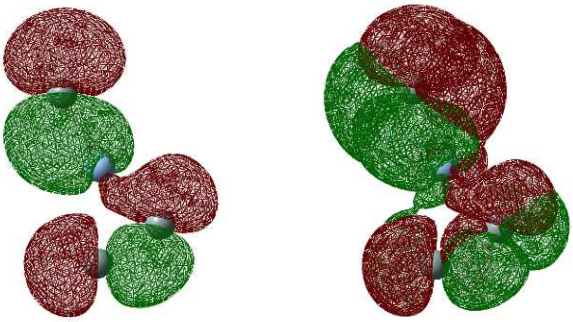
IV A  B 

V A  B 

VI A  B 



VII A B



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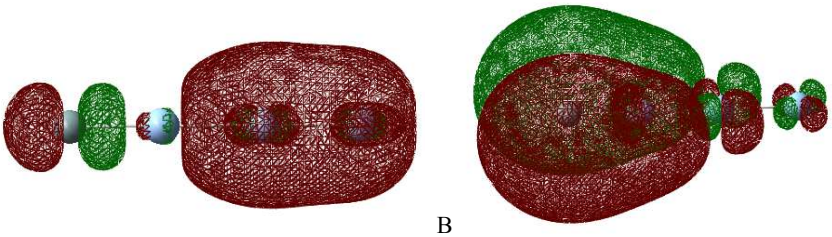
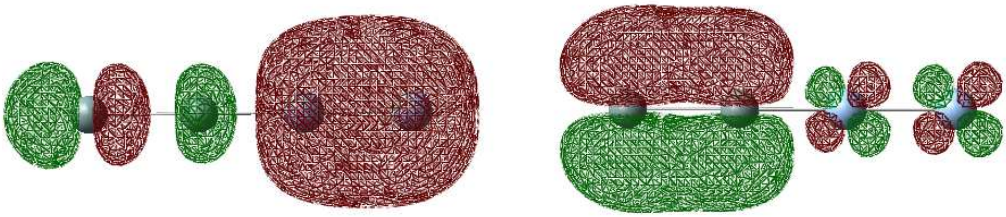


c) I A B



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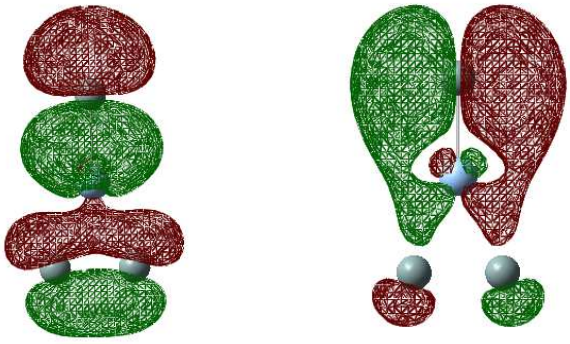

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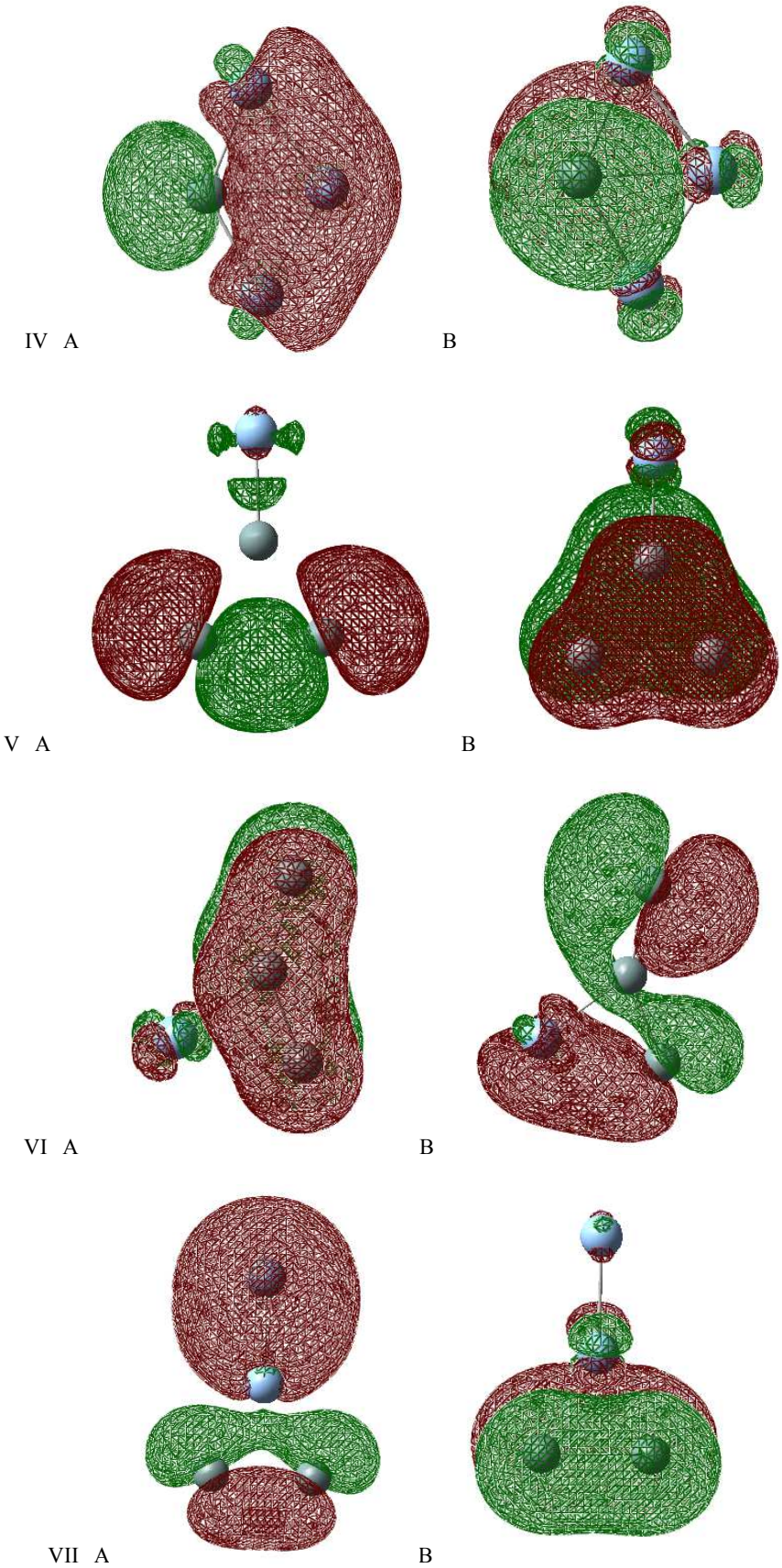
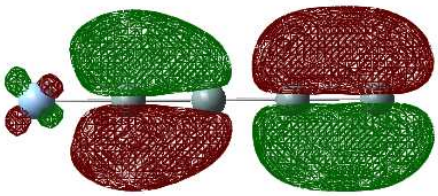


Fig. 3. *The structure with orbital molecular of tetramer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations. Isovalue 0.02.A are HOMO and B are LUMO.*

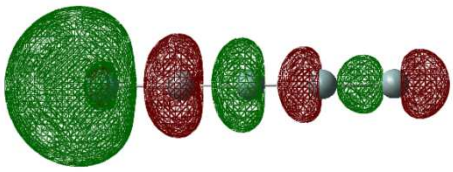
3.4. Pentamer, Neutral, Anions and Cations

In the majority structure the density of electron are distributed between par of atoms. Are look the Fig. 4 a) I A for HOMO IIA and B, III A and B, VI A and XA; Fig. 4 b) IA, II A and B, V A; Fig. 4 c) I A and B and III A. In Fig. 4 c) IV A and B are s-d traslape of orbitals.

In the Fig. 4 a) IA, IIA and B and III A and B are present the π boding. IA, II A, III A, IV A and V are one electron in HOMO. Fig. 4 a) VIII, IX; Fig. 4 b) II, IV; Fig. 4 c) II, III and IV are one electron in HOMO.



a) I A



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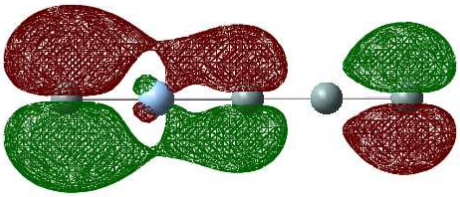
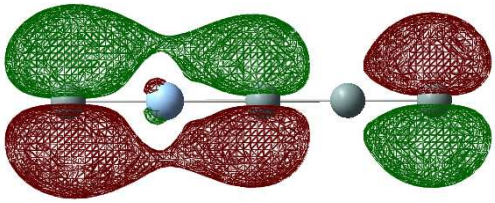
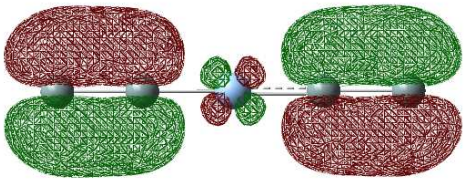


II A



B



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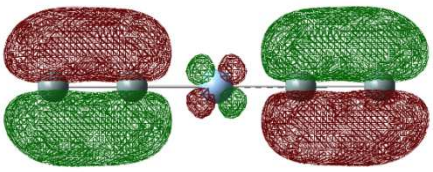

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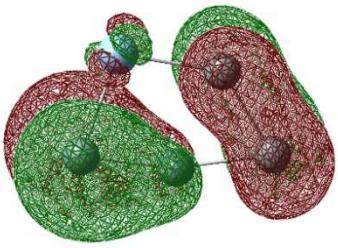

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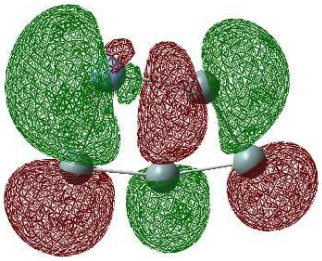

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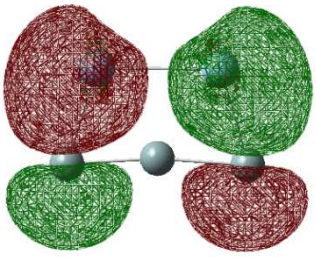

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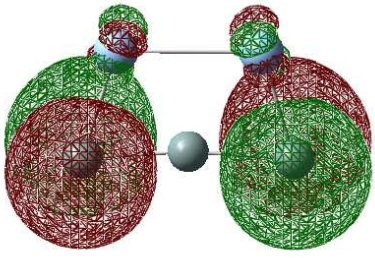

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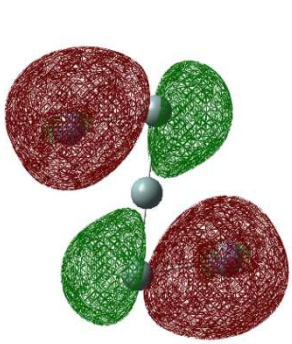

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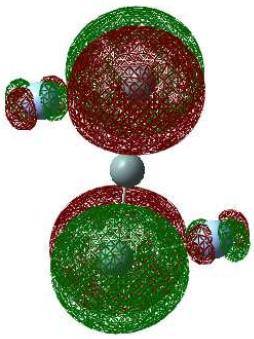

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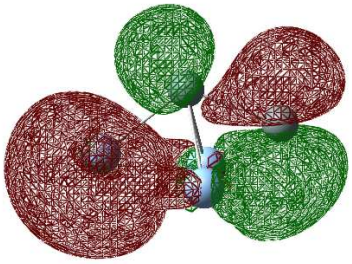

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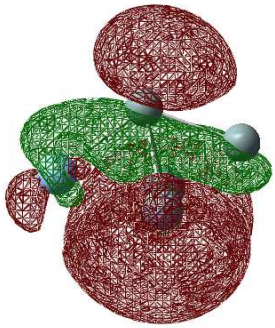

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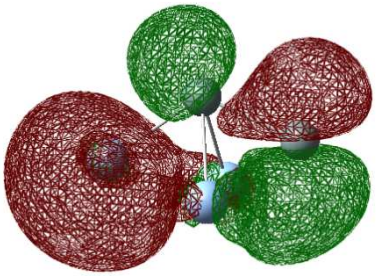

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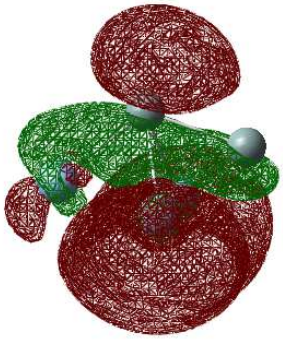

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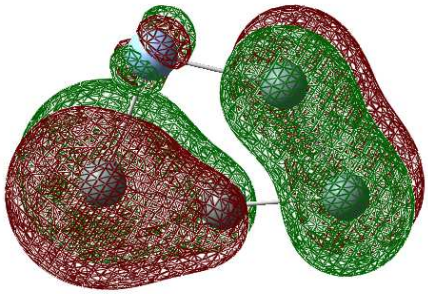

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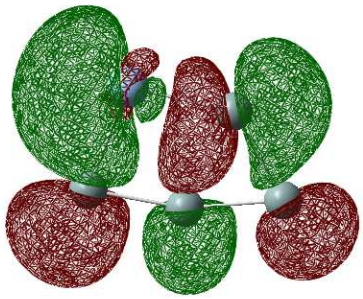

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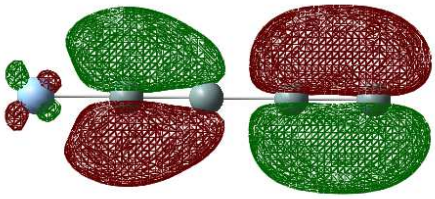

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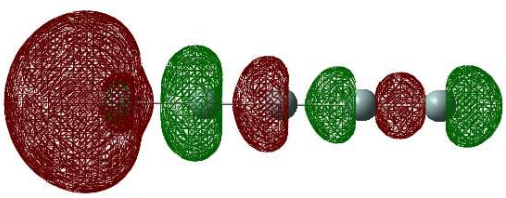

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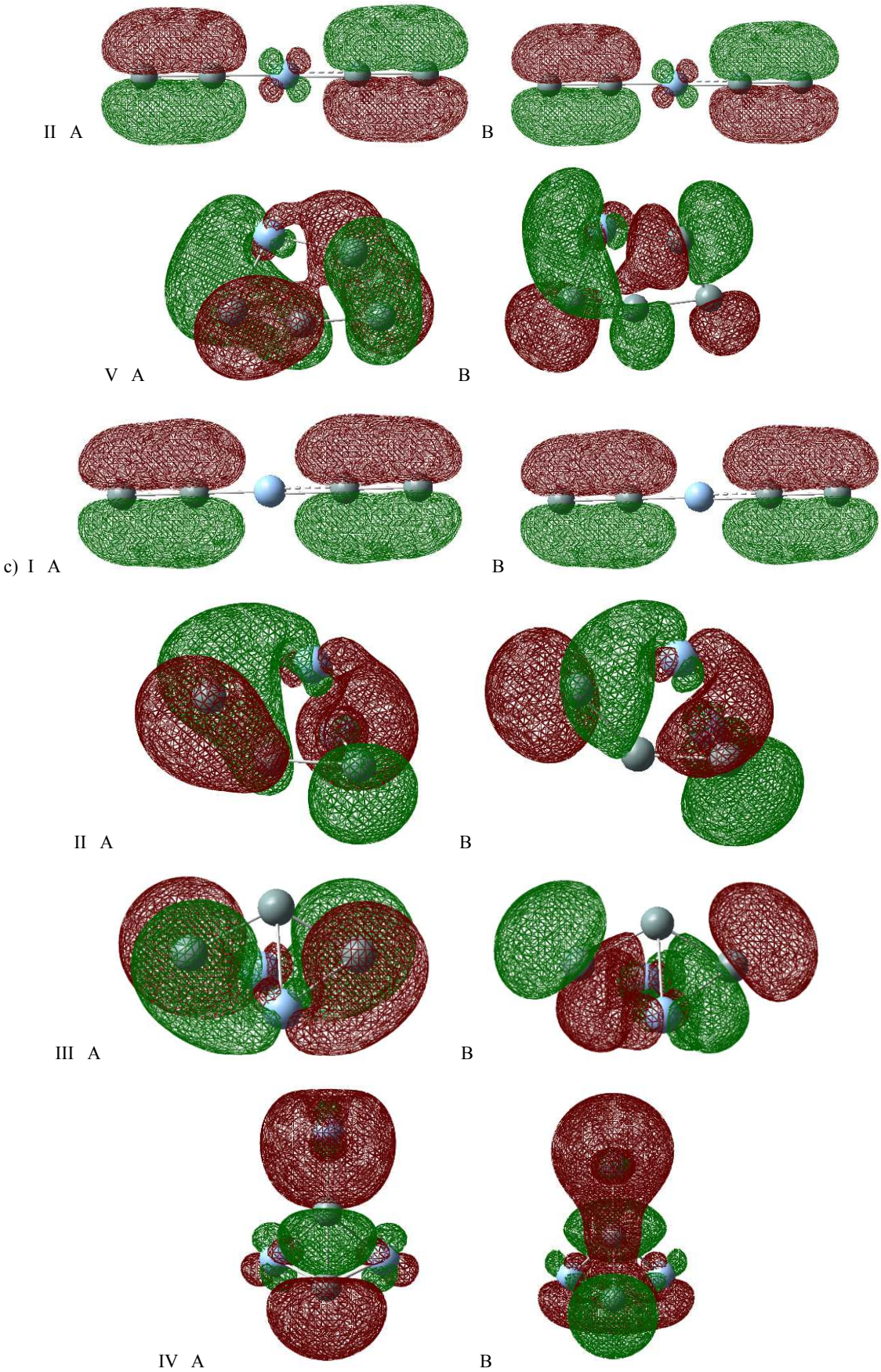


Fig. 4. *The structure with orbital molecular of pentamer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations. Isovalue 0.02. A are HOMO and B are LUMO.*

4. SCF Density

Are generating a cube of the electrostatic potential computed from the SCF electron density.

4.1. Neutral Dimers, Neutral Anions and Cations

With electrostatic potential the electron density are uniform distributed between of the atoms.

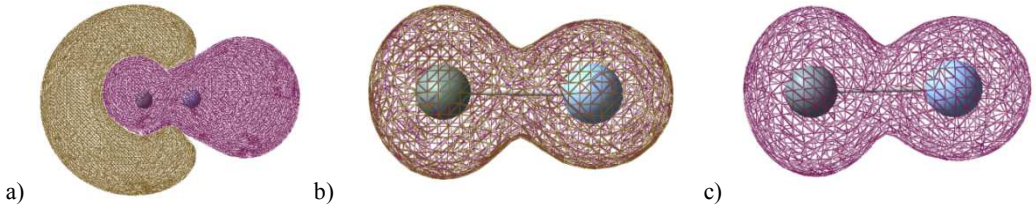
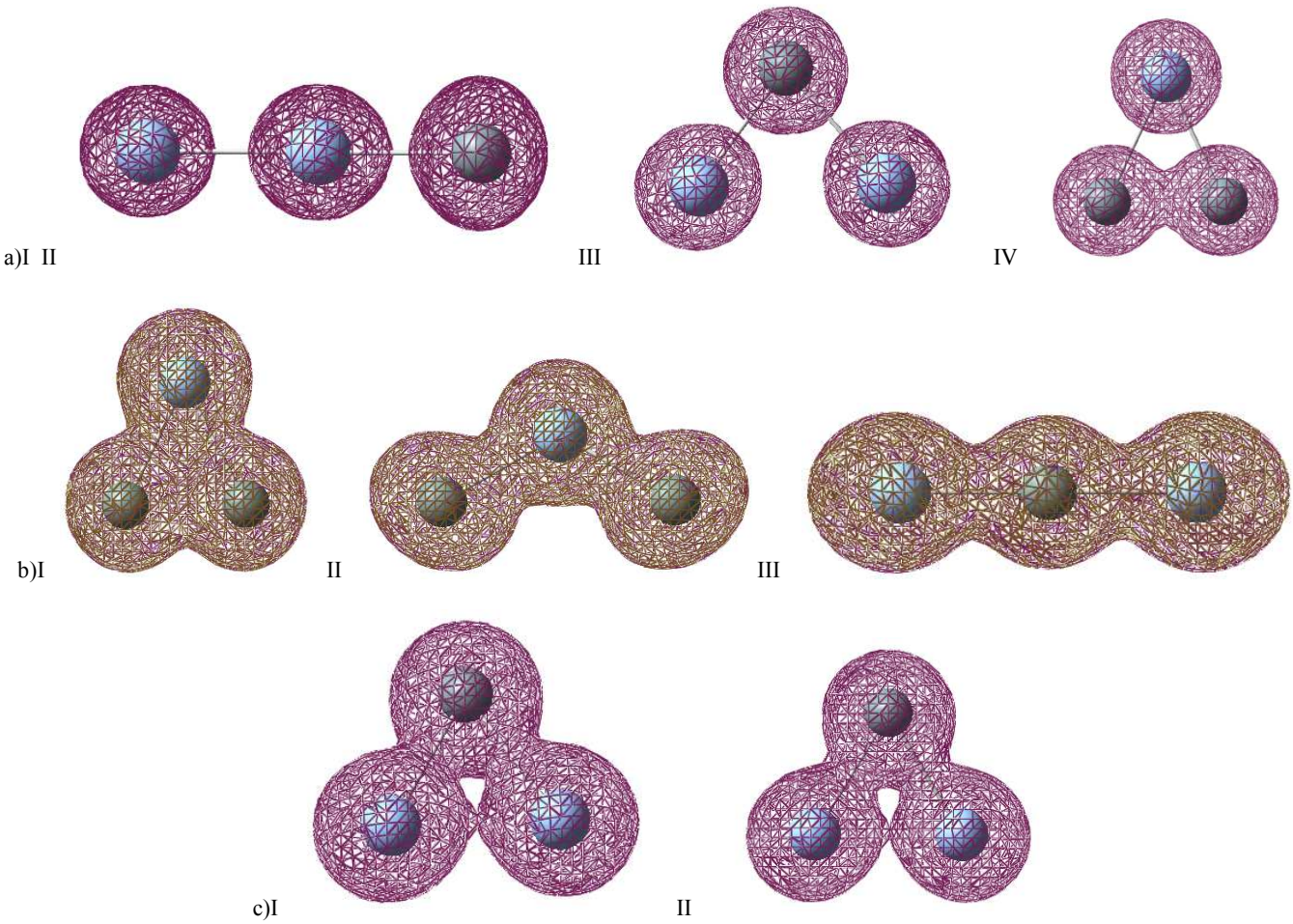


Fig. 5. *The structure with SCF density of dimer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations. Isovalue 0.004.*

4.2. Neutral Trimer, Neutral, Anions and Cations

For all cluster are uniform distributed the density and are not very important for chemical reaction.



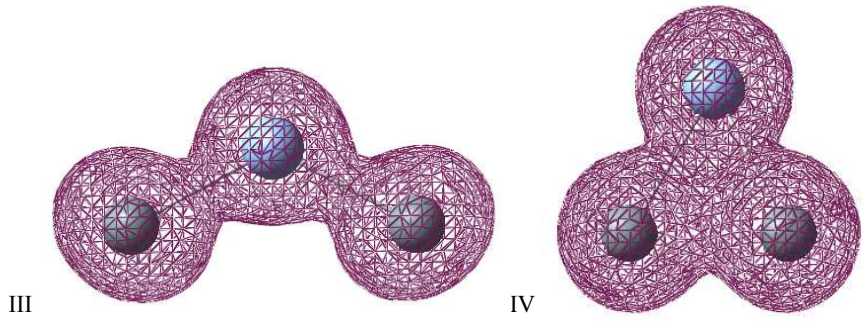
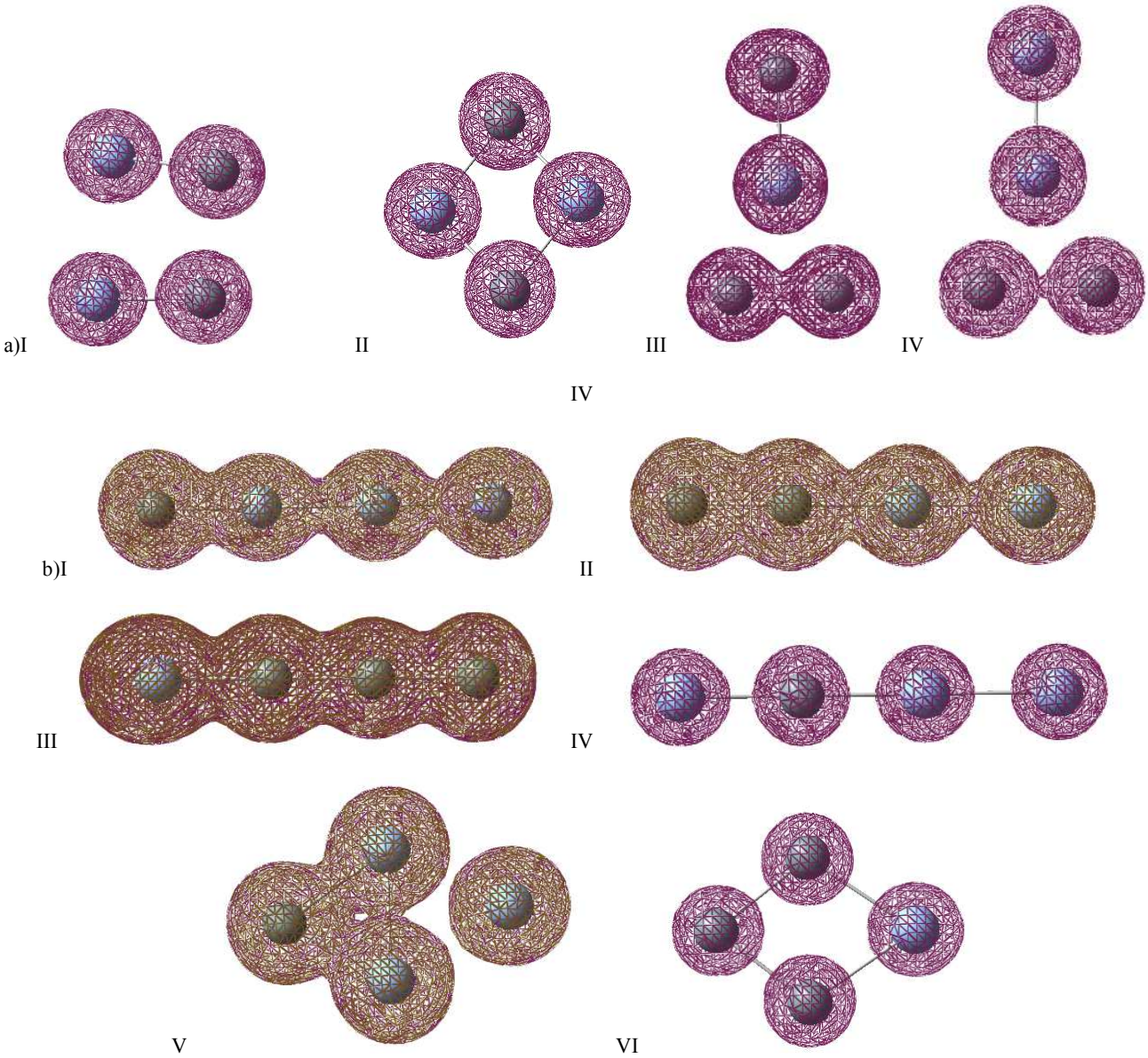
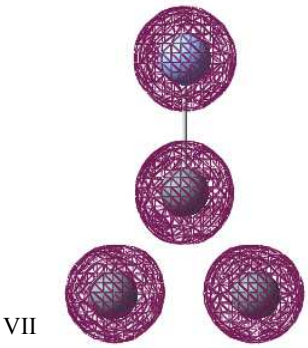


Fig. 6. *The structure with SCF density of trimer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations.*

4.3. Tetramer, Neutral, Anions and Cations

Around of each atoms the density are not important for the proprieties of the clusters.





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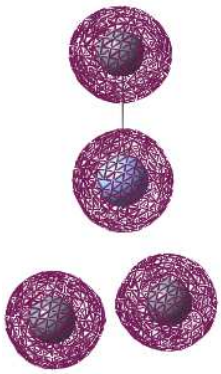

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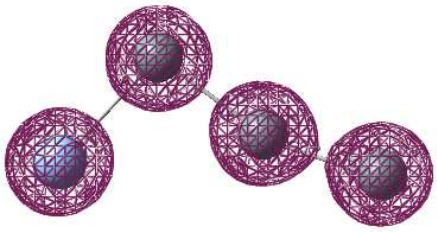

IX

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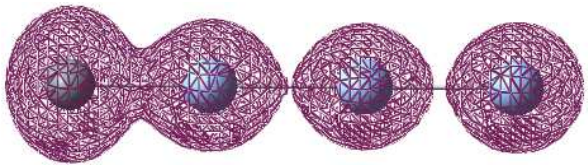

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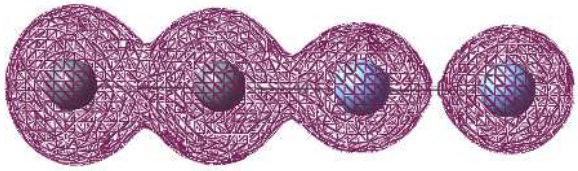

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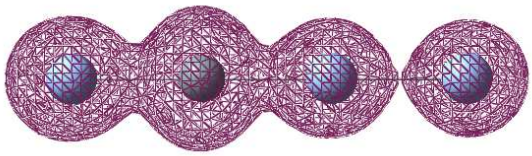

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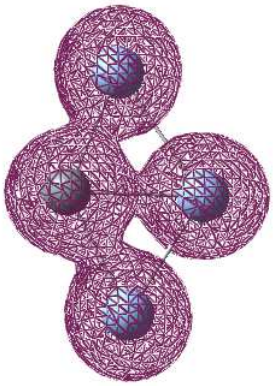

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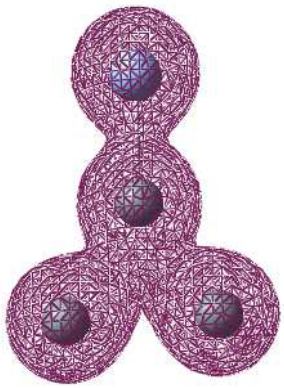

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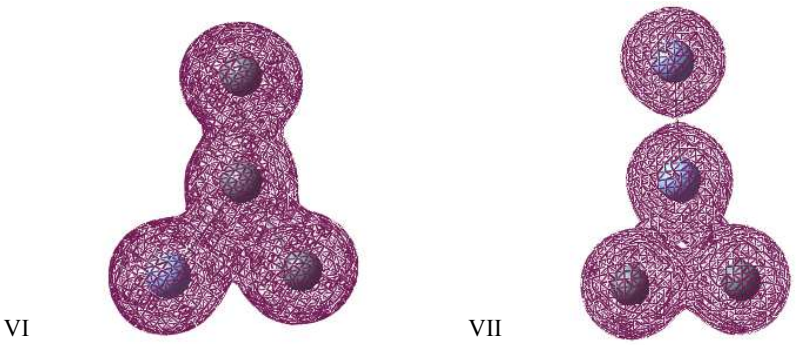
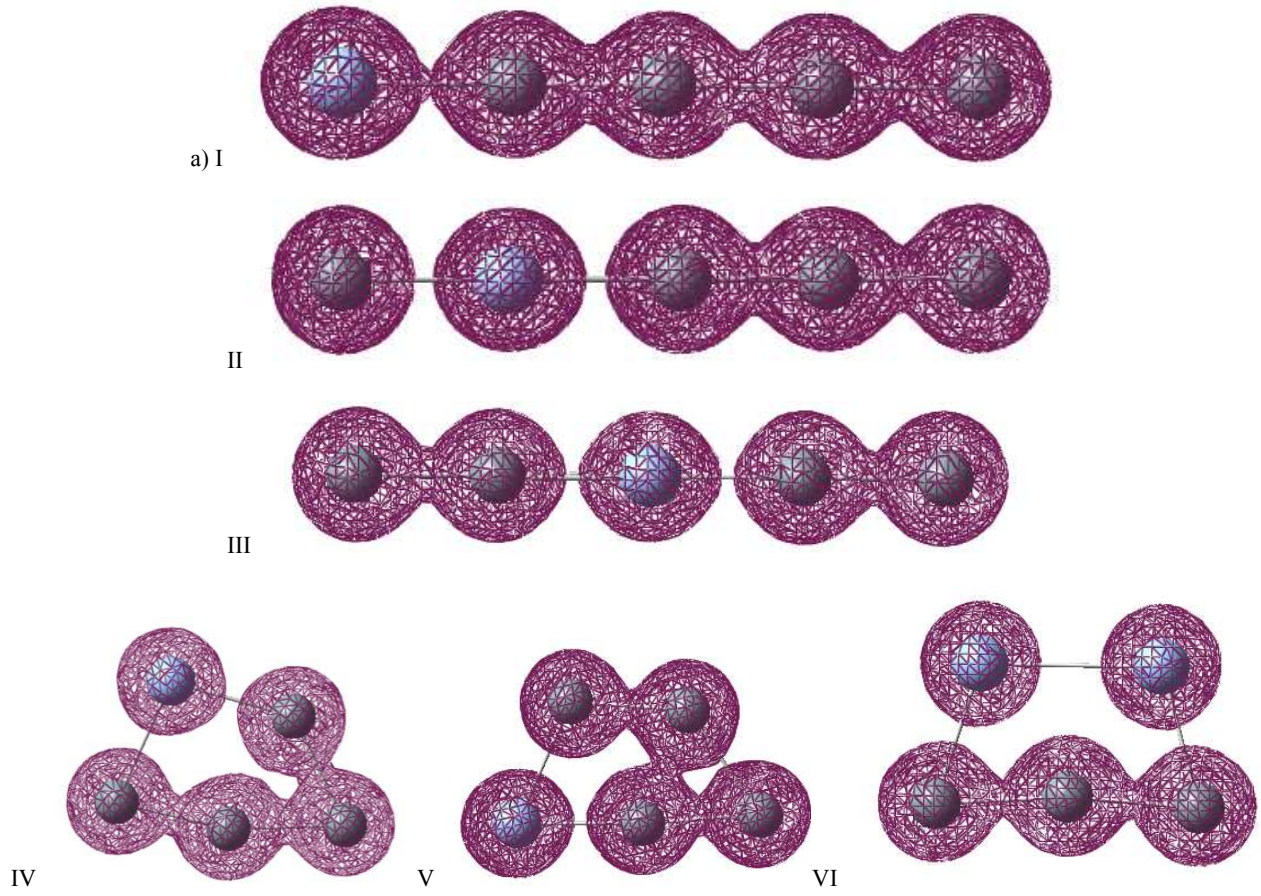


Fig. 7. *The structure with SCF density of tetramer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations.*

4.4. Pentamer, Neutral, Anions and Cations

The color and form of the density are speak of the surface of the potential electrostatic are sferic distribution., the color are not important of caracterization of the proprieties of cluster, all atoms are distributed in sferical density for all atoms.



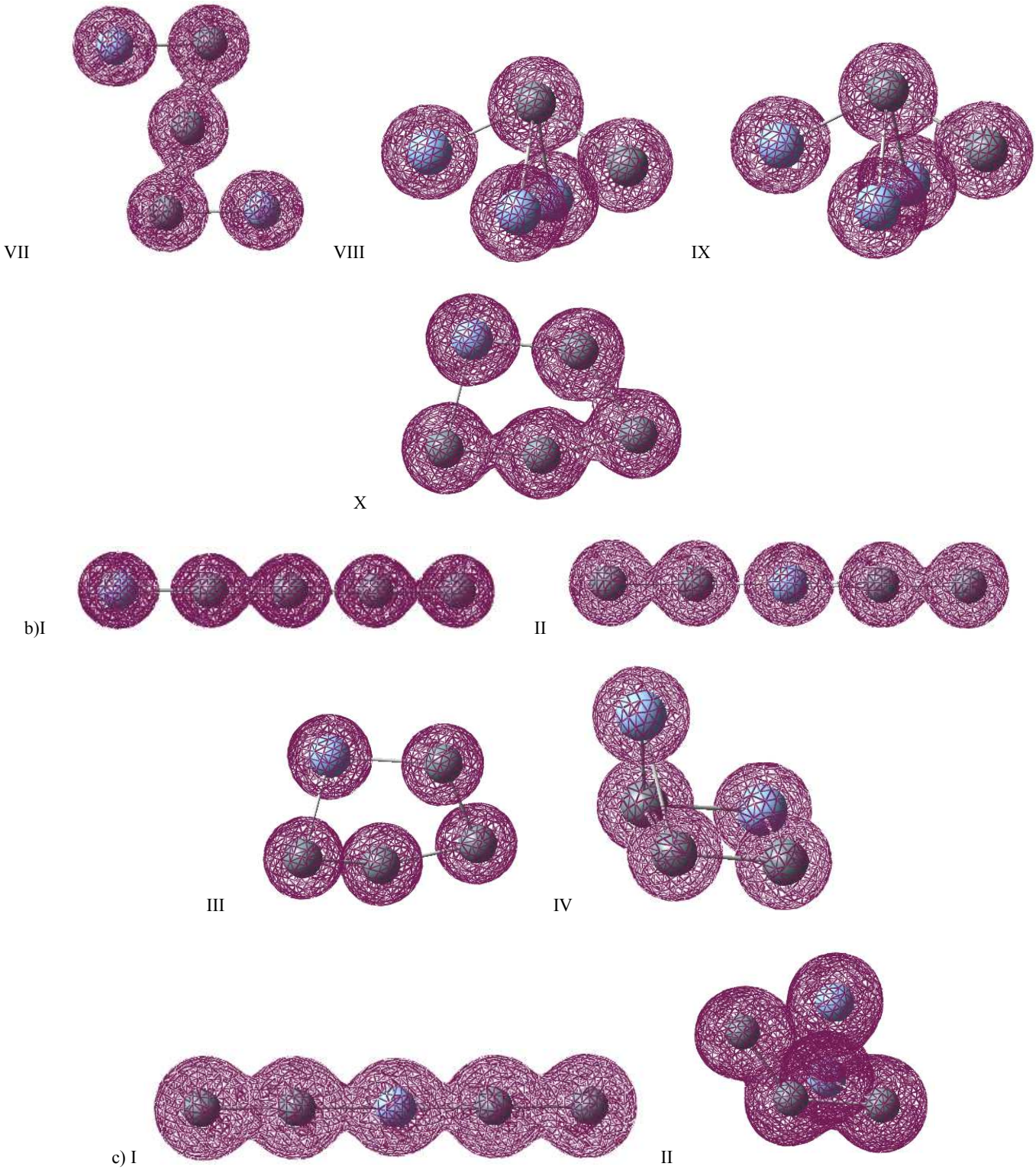


Fig. 8. *The structure with SCF density of pentamer clusters with PBE/LANL2DZ: a) neutral; b) anions; c) cations.*

5. Electronegativity

For calculation of electronegativity are used this formula: X=(I+A)/2, where I and A are ionization potential and electron affinity.

In Fig 9 are calculated with the adiabatic I and A when are optimized of geometry the neutral, anion and cation clusters.

For free and five atoms are greater electronegativity 8.36 and 7.26 eV.

The values when are employed I and A vertical with the optimized of geometri of neutral structure and single point for anion and cation the values are very near for all atoms except one value of 7.34 eV. The greter value show the

rectivity of this clusters. Are prefered the value obtained with I and A adiabatic.

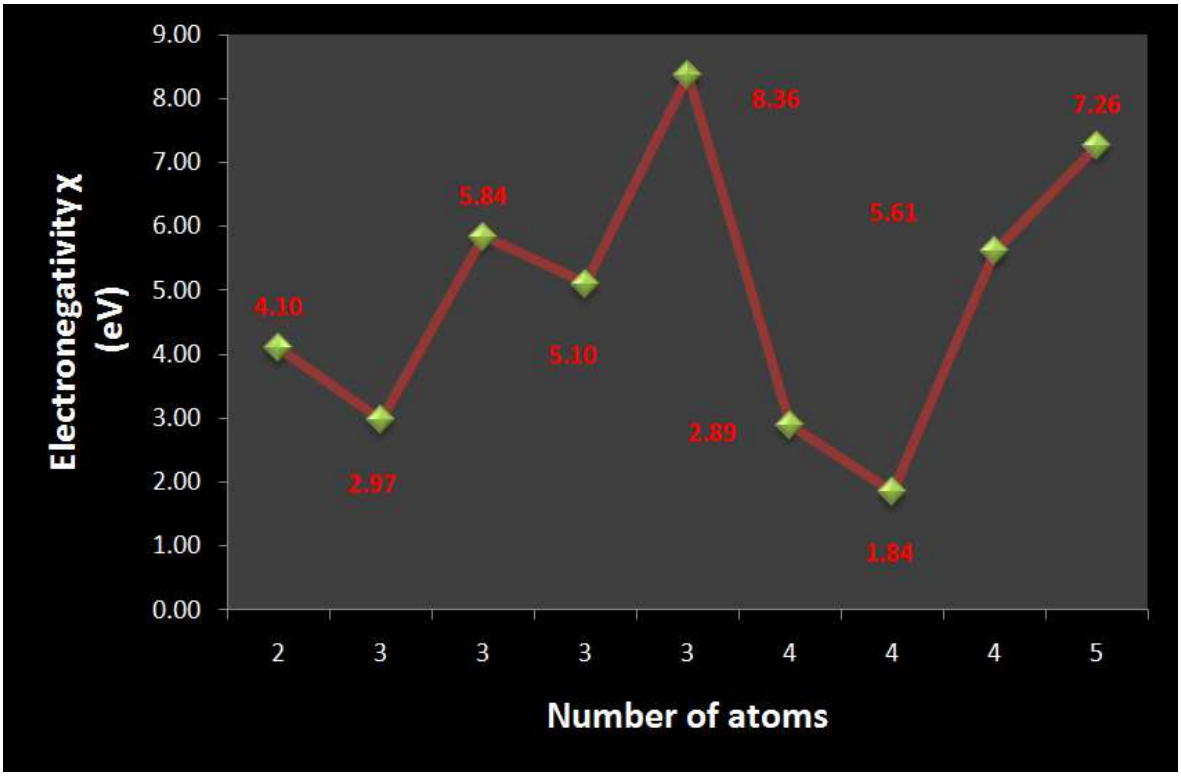


Fig. 9. *Electronegativity for Ag_xSi_y clusters with PI and AE adiabatic.*

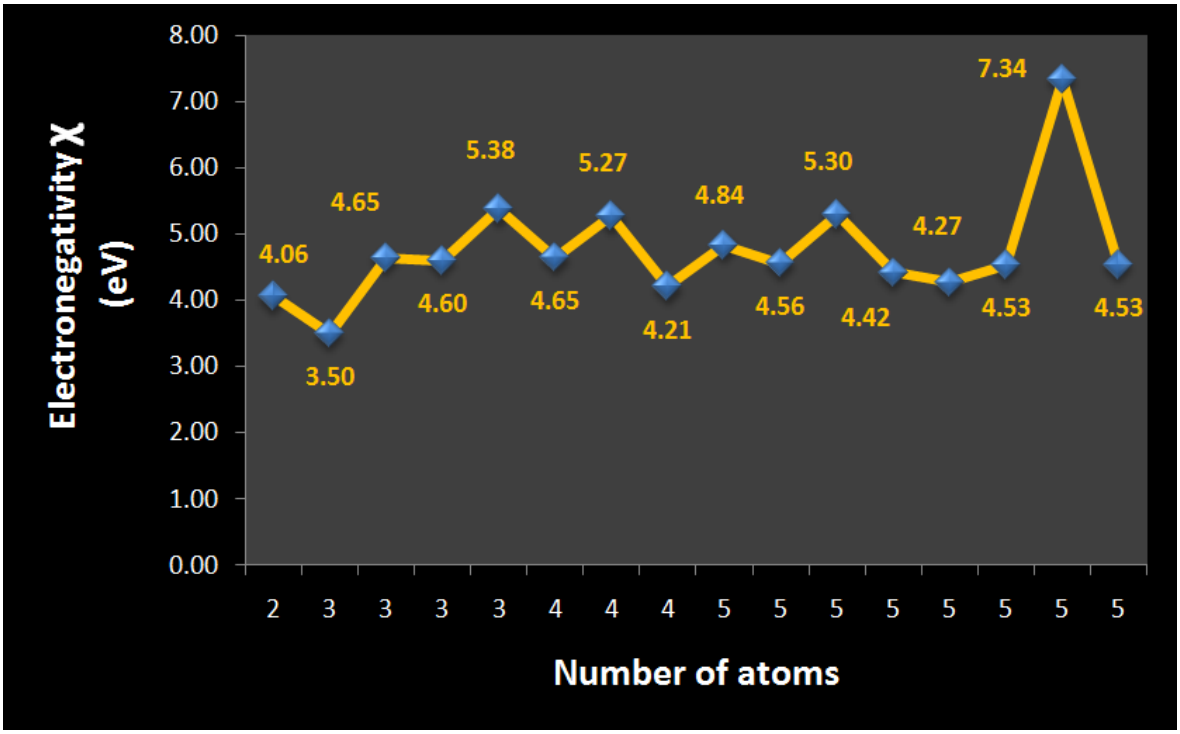


Fig. 10. *Electronegativity for Ag_xSi_y clusters with PI and AE vertical.*

6. Conclusions

The electronic proprieties are very important for many reaction and caracterisation of cluster for this reason in this paper I investigated the molecular orbitals, electronegativity and SCF density. I ploted the HOMO and LUMO for Ag_xSi_y clusters for nucleophilic and electrophilic site. All are soft and are variation for neutral, anion and cation clusters in density of electron. Are presented the bonding and

antibonding in this clusters. Are not distibuted uniform the charge in the clusters. In SCF density are view the sferical distributed the charge. Is better the electronegativity value for adiabatic inization potential and electronic affinity.

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