

# Ab-Initio Quantum Calculations of Some Molecular and Physical Properties of Alamine-Templated Gold Metal Nanoclusters for Application in Biosensing

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## Abstract

Alamine derived nanoclusters with Gold carriers for Biosensing are studied using ab-initio Quantum Chemical calculations. Density functional computations at the Becke3LYP (B3LYP) are arrived at with the aid of LANL2DZ basis set. The molecular structure, dipole moment, quadrupole moment, charge transfer, polarizability and energy are studied. The Alamine DNA basis shows that the properties of pure Alamine are greatly influenced with the addition of Gold nanoclusters. The computed dipole moments are high showing that the nanocluster molecules are polar and the charge distribution is not symmetrical. The quadrupole moment showed that the molecules are a bit elongated along the ZZ axis. The total energies indicate that the Alamine molecules are slightly more stable with increase in the number of Alamine segments in the Gold four chains.

**Keywords:** Alamine, Molecular, Physical, Biosensing, Density Functional Theory.

## INTRODUCTION

Ab-initio molecular theory is concerned with predicting the properties of atomic and molecular systems. It is based upon the fundamental laws of Quantum Mechanics and uses a variety of mathematical transformations and approximation techniques to solve the fundamental equations. Nanoparticles can be defined as particulate substances of nanoscale dimensions (usually <100 nm). Particles <100 nm are called ultrafine particles in Atmospheric Science, though most atmospheric nanoparticles are usually <50 nm. Environmental or atmospheric nanoparticles contain semi-volatile alkanes that originate from fuels and lubricants whereas components of manufactured or engineered nanoparticles vary, depending on the type of product. It should be noted that

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nanoparticles are also used in drug-delivery systems (DDS), because nanoparticles can evade phagocytosis and efficiently reach the target points (Alzate *et al.*, 2005).

Noble metal nanoclusters containing a few to several hundred atoms with sizes ranging from sub-nanometer to ~2nm occupy an intermediate size regime that bridges larger Plasmonic nanoparticles and smaller metal complexes (Levine, 1991; Ma, 2004; Liu *et al.*, 2007). With strong quantum confinement, metal nanoclusters exhibit molecule-like properties and are of interest in this study.

With the advent of Modern Physics, new fundamental types of materials have been created. Various types of forces operating in different classes of solids are exploited in the design of molecular materials (Xiaochao *et al.*, 2015). A variety of fabrication techniques have been developed with the desired properties. The quest for more efficient and cheaper materials for use in industry has led to the discovery of molecular materials. Noble metal nanoclusters can be synthesized within a single stranded DNA template. Compared to other ligand protected metal nanoclusters, DNA-templated metal nanoclusters manifest intriguing physical and chemical properties that are heavily influenced by the design of DNA templates. For example, DNA-templated silver nanoclusters can show bright fluorescence, tunable emission colors, and enhanced stability by tuning the sequence of the encapsulating DNA template. Gold Nanoclusters (AuNCs) can be applied to Biosensing, Biolabeling, and Bioimaging (Stancheva, 2012).

AuNCs can be used as nanoproboscopes and have the following advantages:

- i. Good stability and monodispersity in physiological environments (providing enhanced sensitivity and increased tracking lifetime)
- ii. Ultrasmall size which can be easily absorbed by cells
- iii. The biological functions of bioentities conjugated with AuNCs will not be disturbed
- iv. Photoluminescence in the form of fluorescence (decreasing the core size, fluorescence is depicted by a blue-shift from the NIR region to ultraviolet)
- v. The fluorescence Quantum Yield (QY) of AuNCs is much higher than bulk gold and gold NPs in magnitude
- vi. Compared with the harsh synthetic steps and tedious surface modification of quantum dots, it is much more achievable to prepare AuNCs and the functional groups induced by the templates and stabilizers are much convenient for coupling with the dyes, peptide, DNA, and other markers;
- vii. Owing to the low content of metal, AuNCs have good biocompatibility for lots of *in vitro* and *in vivo* applications.

Fluorescent AuNCs are promising materials for fluorescent biolabels and light-emitting sources in nanoscale. These materials can be applied in biological labeling, imaging, detection, and so on. The precondition for making the applications possible is appropriate surface modification for AuNCs, which can eventually influence their stability, biocompatibility, targeting, and other properties (Coates, 2000; Clarkson, 2003). Functionalizing AuNCs is a process that involves surface chemistry and bioconjugation, which should ensure AuNCs survival in these conditions.

The aim of this study is to determine the molecular, opto-electronic and vibrational properties of some DNA-templated noble metal nanoclusters for application in biosensing. The windows version of Gaussian software was used to predict the molecular, optical and electronic properties of Alamine Gold nanocluster molecules.

## **Research Methodology**

### **Materials**

The following materials were used:

- i. Gaussian Software with specification Gaussian 09 Revision-A.02-SMP (09W), 2009
- ii. Gauss View software with specification Gauss View 5.08, 2008
- iii. Pavilion HP laptop with specification Intel (R) Core (TM) i5 4210U CPU@ 1.70GHz 2.40GHz 12.0GB 64-bit Operating System x64-based processor Windows 8.1

### **Methods**

#### **Gaussian Package**

The Gaussian package is a computational Physics and Chemistry program. The name comes from the fact that it uses Gaussian type basis functions (Herbert, 2002; Kimberly & Ernest, 2011). It is used for electronic and geometric structure optimization (single point calculation, geometry optimization, transition states and reaction path modeling); and molecular properties and vibrational analysis (IR, Raman, NMR vibrational frequencies and normal modes; electrostatic potential, electron density, multipole moments, population analysis, natural orbital analysis, magnetic shielding induced current densities, static and frequency-dependent polarizabilities and hyperpolarizabilities) using both DFT and ab initio methods (Kukhta *et al.*, 2011).

#### **Geometry and Vibrational frequency Optimization**

Geometry optimization is done by locating both the minima and transition states on the potential surface of the molecular orbital (Ochterski, 1993). It can be optimized in Cartesian coordinates that are generated automatically from the input Cartesian coordinates. It also handles fixed constraints on distances, bond angles and dihedral angles in Cartesian or (where appropriate) internal coordinates (Lee & Parr, 1988; Makashir & Kurian, 1999). The process is iterative, with repeated calculations of energies and gradients and calculations or estimations of Hessian in every optimization cycle until convergence is attained.

One of the most computationally demanding aspects of calculating free energy using electronic structure theory is the calculation of the vibrational energy and entropy contributions (Anderson, 2012). The computational expense is incurred by the calculation of the matrix of second energy-derivatives (i.e. the Hessian or force constant matrix) which yields harmonic vibrational frequencies upon diagonalization (Parr & Yang, 1989).

#### **Computation of Molecular Properties**

The molecular structures and geometries of Gold templated Alamine nanoclusters are completely optimized using Density Functional Theory which is a cost effective method for inclusion of electron correlations with the three-parameter density functional generally known as Becke3LYP (B3LYP), which includes Becke's gradient exchange corrections (Becke, 1993), the Lee *et al.* (1988) correlation functional and the Vosko, Wilk and Nusair correlation functional with suitable basis sets. At the first step, geometry optimizations are carried out then, the IR and Raman frequencies are calculated using the Hessian which is the matrix of second derivatives of the energy with respect to geometry (Hinchliffe, 1988; James, 2007).

The optimized molecular structures are tested by computing the second derivatives and checking that all the harmonic vibrational frequencies are found to be real at all level of calculations. All calculations will be performed using Windows version of Gaussian 03W suit of ab initio quantum mechanical software (Gaussian 03 Revision C.02, 2004).

## Results and Discussion

### Optimized Molecular Structure and Bond Lengths

Geometry optimizations usually attempt to locate minima on the potential energy surface, thereby predicting equilibrium structures of molecular systems (Gaussian 03, Revision C.02, 2004). At the minima, the first derivative of the energy (gradient) is zero. Since the gradient is the negative of the forces, the forces are also zero at such a point (stationary point). In Gaussian, a geometry optimization begins at the molecular structure specified at the input and steps along the potential energy surface (Foresman, 1996; Colon *et al.*, 2004). It computes the energy and gradient at that point, and determines which direction to make the next step. The gradient indicates the direction along the surface in which the energy decreases most rapidly from the current point as well as the steepness of that slope (Ochterski *et al.*, 2007; Naoto *et al.*, 2007). The optimized parameters are the bond lengths (in Armstrong), the bond angles and the dihedral angles for the optimized molecular structure. Atoms in the molecule are numbered according to their order in the molecule specification section of the input in Gauss View (Perdew & Wang, 1992).

The optimized molecular structures of various Alamine and Gold derived nanocluster molecules are shown in Figure 3.1.

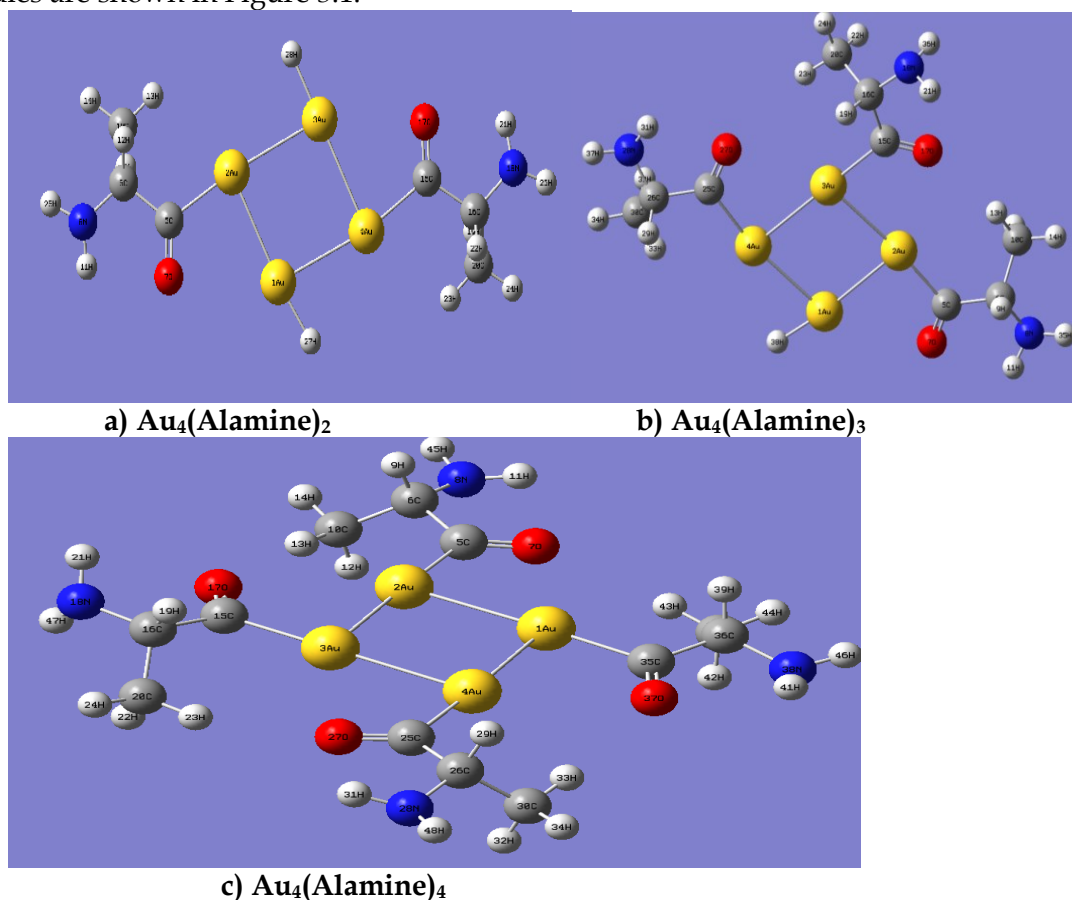


Fig. 3.1: Optimized Structures of various Alamine and Gold derived nanoclusters

Table 3.1 shows the mean bond length of Alamine derived nanoclusters. The Au-Au bonds have the highest length and hence are the weakest. The N-H bonds are the strongest with the least bond lengths. The mean Au-Au bond length decreases with increase in the number of Alamine molecules to the gold nanocluster chain. A comparative analysis of the optimized parameters obtained in this study and that of Kukhta *et al.* (2008) reveal a different trend.

**Table 3.1:** Optimized Mean Bond Lengths (Å) of Alamine derived nanoclusters

Bond type	Au <sub>4</sub> (Alamine) <sub>2</sub>	Au <sub>4</sub> (Alamine) <sub>3</sub>	Au <sub>4</sub> (Alamine) <sub>4</sub>
Au - Au	2.9267	2.7514	1.7563
Au - H	1.7390	1.6400	-
Au - C	2.0439	2.0700	2.1100
C - C	1.5403	1.5485	1.4906
C - O	1.2863	1.2399	1.3061
C - N	1.4546	1.4564	1.4490
C - H	1.1014	1.1007	1.0900
N - H	1.0124	1.0149	1.0000
O - H	-	-	1.0000

### Optimized Bond Angles

Table 3.2 shows the optimized mean bond angles of Alamine derived nanoclusters. A similar trend as in Table 3.1 is observed and Au-Au-Au bond angles are the least.

**Table 3.2:** Optimized Mean Bond Angles of Alamine Derived Nanoclusters molecule

Bond type	Au <sub>4</sub> (Alamine) <sub>2</sub>	Au <sub>4</sub> (Alamine) <sub>3</sub>	Au <sub>4</sub> (Alamine) <sub>4</sub>
Au - Au - Au	89.9990	89.9964	-
Au - Au - H	70.3503	88.3975	-
Au - Au - C	106.5951	87.9961	-
Au - C - C	123.3470	115.7555	120.0000
Au - C - O	120.6035	122.0412	120.0000
C - C - O	135.9598	122.1348	120.0000
N - C - C	111.4601	110.9559	111.1000
C - C - H	107.2266	108.4280	109.2840
C - C - C	111.3875	111.5160	108.7945
N - C - H	113.4974	112.2021	109.5000
C - N - H	116.6338	116.1639	120.0000
H - C - H	108.6763	108.5185	109.4424
H - N - H	116.5887	115.0068	120.0000

### Dipole Moments, Quadrupole Moments and Energies

#### Dipole Moments

The dipole moment is defined as the first derivative of the energy with respect to an applied electric field. It is a measure of the asymmetry in the molecular charge distribution and is given as a vector in three dimensions (Clarkson *et al.*, 2003). For Hartree-Fock computations, this is equivalent to the expectation values of X, Y and Z, which are the quantities reported in the output. The computed dipole moments (in Debye) at different levels of theory are shown in Tables 3.3. The dipole moment of the molecules gives the strength of the polarity of the molecule.

**Table 3.3:** Total Dipole moments (in Debye) of Alamine derived nanocluster molecules

$\text{Au}_4(\text{Alamine})_2$	$\text{Au}_4(\text{Alamine})_3$	$\text{Au}_4(\text{Alamine})_4$
1.8447	3.3469	4.9605

The dipole moment of the molecules gives the strength of the polarity of the molecules and  $\text{Au}_4(\text{Alamine})_4$  has the highest dipole moment showing that the addition of Alamine makes the polarity of the nanoclusters to increase.

### Quadrupole Moments

Quadrupole moments give a second order approximation of the total electron distribution, providing at least a crude idea of its shape. One of the components being significantly larger than the others would represent an elongation of the sphere along that axis. If present, the off-axis components represent trans-axial distortion (stretching or compressing of the ellipsoid) (Umar and Chifu, 2013).

**Table 3.4:** Quadrupole moments (in Debye) for Alamine Derived Nanoclusters

	$\text{Au}_4(\text{Alamine})_2$	$\text{Au}_4(\text{Alamine})_3$	$\text{Au}_4(\text{Alamine})_4$
XX	-123.9607	-158.3446	-202.6710
YY	-159.8475	-185.9304	-188.1095
ZZ	-158.6152	-187.2625	-217.3095
XY	-4.1452	-15.0324	0.9701
XZ	0.0017	1.3392	-7.5197
YZ	-0.0003	2.0167	-3.0650

### Energies

All frequency calculations include thermochemical analysis of the molecular system. By default, this analysis is carried out at 298.15 K and 1 atmosphere of pressure, using the principal isotope of each element type in the molecular system. Predicted total, electronic, translational, rotational and vibrational energies in kcal/mol for the nanoclusters are listed in Table 3.5. The translational energy relates to the displacement of molecules in space as a function of the normal thermal motions of matter as in Young (2001). Rotational energy is observed as the tumbling motion of a molecule as a result of the absorption of energy within the microwave region. The vibrational energy component is a higher energy term and corresponds to the absorption of energy by a molecule as the component atoms vibrate about the mean center of their chemical bonds (Chifu *et al.*; 2018). The electronic component is linked to the energy transitions of electrons as they are distributed throughout the molecule, either localized within specific bonds, or delocalized over structures, such as an aromatic ring.

**Table 3.5:** Predicted thermal energies (kcal/mol) for Alamine Derived Nanoclusters

	$\text{Au}_4(\text{Alamine})_2$	$\text{Au}_4(\text{Alamine})_3$	$\text{Au}_4(\text{Alamine})_4$
<b>Total</b>	173.219	196.268	253.876
<b>Electronic</b>	0.000	0.000	0.000
<b>Translational</b>	0.889	0.889	0.889
<b>Rotational</b>	0.889	0.889	0.889
<b>Vibrational</b>	171.441	194.490	252.098

It is seen that the vibrational energy contributes the bulk of the total energy and that addition of more Alamine templates increases the stability of the molecules is found to be most stable  $\text{Au}_4(\text{Alamine})_4$ .

## Charge Transfer and Polarizabilities

### Charge Transfer

Within molecular system, atoms can be treated as a quantum mechanical system. On the basis of the topology of the electron density the atomic charges in the molecule can be explained. The electrostatic potential derived charges using the CHelpG scheme of Breneman at different atomic positions is given in Tables 3.6 and 3.7. The Mulliken population analysis partitions the charges among the atoms of the molecule by dividing orbital overlap evenly between two atoms. Whereas the electrostatic potential derived charges assign point charges to fit the computed electrostatic potential at a number of points on or near the Van der Waal surface. Hence, it is appropriate to consider the charges calculated by CHelpG scheme of Breneman instead of Mulliken population analysis.

### Polarizabilities

Polarization interactions are between two molecules, one with permanent dipole and the other with induced dipole. Even in a non-polar molecule, however, the valence electrons are moving around and there will occasionally be instances when more are on one side of the molecule than on the other. This gives rise to fluctuating or instantaneous dipoles. These instantaneous dipoles may be induced and stabilized as an ion or a polar molecule approaches the non-polar molecule (Alzate *et al*, 2005).

Polarizability refers to the way the electrons around an atom redistribute themselves in response to an electrical disturbance. The polarizability tensor components of the studied nanoclusters are listed on Table 3.6.

Table 3.6: Polarizabilities of Alamine derivatives

Orientation	Au <sub>4</sub> (Alamine) <sub>2</sub>	Au <sub>4</sub> (Alamine) <sub>3</sub>	Au <sub>4</sub> (Alamine) <sub>4</sub>
XX	414.031	433.618	496.728
XY	7.423	9.568	12.744
YY	262.166	372.084	476.170
XY	0.074	0.154	0.356
YZ	1.646	2.366	3.911
ZZ	122.336	162.626	185.205

There is increase in polarizability tensors with addition of Alamine molecules to the gold chain. The polarizability along the off-diagonal axis XZ, YZ and XY is very minimal in both cases. Kukhta *et al* (2011) showed a similar polarity trend in alpha alamine.

Table 3.7: Mean Electrostatic Potential Derived Charges on different atomic positions for Alamine nanoclusters

	Au <sub>4</sub> (Alamine) <sub>2</sub>	Au <sub>4</sub> (Alamine) <sub>3</sub>	Au <sub>4</sub> (Alamine) <sub>4</sub>
Atom			
N	-0.653115	-0.626059	-0.632597
H	0.220691	0.240950	0.260090
C	-0.248640	-0.246062	-0.242727
O	-0.362408	-0.220198	-0.222935
Au	0.108303	0.048938	0.094262

Table 3.7 shows the mean electrostatic potential derived charges for Alamine derived nanoclusters. The bulk negative charge in this case resides on Nitrogen, Carbon and Oxygen atoms while Gold and Hydrogen are electropositive.

## CONCLUSION

The molecular geometry of Alamine derived nanoclusters with Gold carriers for biosensing are studied using ab-initio Quantum Chemical calculations. Density functional calculations at the Becke3LYP (B3LYP) are carried out using LANL2DZ basis set. The molecular structure, dipole moment, quadrupole moment, charge transfer, polarizability and energy are studied. The stability of the molecules studied clearly indicates that they are suitable for Biosensing.

## REFERENCES

- Alzate, L., Ramos, C., Hernández, S., & Mina, N. (2005), "Ab-Initio treatment of the behavior of TNT in soil". *Detection and Remediation Technologies for Mines and Minelike Targets VIII. Proceedings of SPIE.* . 5794. 1300-1309
- Anderson, A. (2012), *Vibronic Excitons in Molecular Systems*, M.Sc Thesis, Lund University
- Becke, A.D. (1993), "Density Functional Thermochemistry. III. The role of exact exchange", *Journal of Chemical Physics*, 98, 5648-5660
- Chifu E. Ndikilar, L.S. Taura, G. W. Ejuh & A. Muhammad; " RHF and DFT Study of the Molecular and Electronic Properties of (SiO<sub>2</sub>)<sub>n</sub> and (GeO<sub>2</sub>)<sub>n</sub> Nanoclusters ", *Modern Applied Science* 12(9): 108-118, 2018
- Clarkson, J., Smith, W., Batchelder, D., Smith, D. & Coats, A. (2003), "A theoretical study of the structure and vibration of 2,4,6-trinitrotoluene", *Journal of Molecular Structure.* **648**, 203-216
- Coates, J. (2000), "Interpretation of Infrared Spectra, A Practical Approach" in *Encyclopedia of Analytical Chemistry*, R.A. Meyers (Ed.), pp.10815-10837, John Wiley & Sons, Chichester
- Colon, Y., Ramos, C., Alzate, L., Santana, A., Hernández, S., Castro, M., Briano, J., Muñoz, M. & Mina, N. (2004), Adsorption of RDX on Clay. *Detection and Remediation Technologies for Mines and Minelike Targets VIII. Proceedings of SPIE*, 5415, 1419-1430
- Foresman, J. B. (1996), "Ab-Initio Techniques in Chemistry: Interpretation and Visualisation", Chapter 14 in *What Every Chemist Should Know about Computing*, ACS Books, Washington, D.C
- Friedrich, D. M, Mathies R., and Albrecht A. C. (2004), "Studies of excited electronic states of anthracene and some of its derivatives by photoselection and PPP-SCF calculations", *Journal of Molecular Spectroscopy*, 74, 90180
- Gaussian 03, Revision C.02 (2004), Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Montgomery, J. A., Vreven, Jr. T., Kudin, K. N., Burant, J. C., Millam, M., Iyengar, S. S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G. A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J. E., Hratchian, H. P., Cross, J. B., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Ayala, P. Y., Morokuma, K., Voth, G. A., Salvador, P., Dannenberg, J. J., Zakrzewski, V. G., Dapprich, S., Daniels, A. D., Strain, M. C.,



- Farkas, O., Malick, D. K., Rabuck, A. D., Raghavachari, K., Foresman, J. B., Ortiz, J. V., Cui, Q., Baboul, A. G., Clifford, S., Cioslowski, J., Stefanov, B. B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R. L., Fox, D. J., Keith, T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C. & Pople, J. A., Gaussian, Inc., Wallingford CT, 2004.
- Herbert, N. (2002) "Polymers, Electrically Conducting" in Ullmann's Encyclopedia of Industrial Chemistry 2002 Wiley-VCH, Weinheim.
- Hinchliffe, A. (1988), Computational Quantum Chemistry, Wiley, New York
- James, W. (2007). Product engineering: molecular structure and properties. Oxford University Press.
- Kimberly, D. M. & Ernest, M.(2011), "Coordination Complexes as Catalysts: The Oxidation of Anthracene by Hydrogen Peroxide in the Presence of VO(acac)<sub>2</sub>" *Prokopchuk Journal of Chemical Education* 88 (8), 1155-1157
- Kukhta, A. V., Kukhta, I. N., Kukhta, N. A., Neyra, O. L. & Meza, E. (2011); "DFT study of the electronic structure of anthracene derivatives in their neutral, anion and cation forms" *Journal of Physics B*, 41, 205701
- Lee, C., Yang, W. & Parr, R. G. (1988), "Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density", *Physical Review B*, 37, 785
- Levine, I. N. (1991), Quantum Chemistry, 4<sup>th</sup> ed., Prentice Hall, Englewood Cliffs, NJ
- Liu, J., Jiang L. & Hu, W. (2009), "The Application of Anthracene and Its Derivatives in Organic Field-Effect Transistors", *Progress in Chemistry*, 2568-2577
- Ma, Y. (2004), *Determination of Non-Covalent Intermolecular Interaction Energy from Electron Densities*. Dissertation Ph.D. University New Orleans, New Orleans
- Makashir, P. S. & Kurian, E. M. (1999) "Spectroscopic and Thermal Studies on 2,4,6-Trinitrotoluene (TNT)". *J. Therm. Anal. Calorim.* 55. 173-185.
- Naoto, A., Masaaki, M., & Atsushi, N. (2007), "Comprehensive photoelectron spectroscopic study of anionic clusters of anthracene and its alkyl derivatives: Electronic structures bridging molecules to bulk" *Journal of Chemical Physics*. **127**, 234305
- Ochterski, J. W. (1993), Complete Basis Set Model Chemistries, Ph.D Thesis, Wesleyan University, Middletown
- Parr, R. G. & Yang, W. (1989), Density -functional theory of atoms and molecules, Oxford Univ. Press, Oxford
- Perdew, J. P. & Wang, W. (1992), "Accurate and Simple Analytic Representation of the Electron Gas Correlation Energy" *Physical Review B*, 45, 13244
- Skorokhodov, S. S., Krakovjak, M. G., Anufrieva, E. V. & Shelekhov, N. S. (2007), "Investigation of chemical behavior of anthracene derivatives as monomers and reagents in synthesis of macromolecules containing anthracene groups" *Journal of Polymer Science*, 15, 287-295
- Umar G. & Chifu E. N. "Electronic Structure and Properties of the Organic Semi Conductor Material Anthracene in Gas Phase and Ethanol: An ab initio and DFT Study", *The African Review of Physics* 7:253 - 263, 2012
- Wilson, E. B. Jr., Decious, J. C. & Cross, P. C. (1955), Molecular Dynamics. The Theory of Infrared and Raman Vibrational Spectra, McGraw-Hill
- Young, D. C. (2001), *Computational Chemistry: A Practical Guide foy Applying Techniques to Real-World Problems*. John Wiley & Sons, Inc. Chapter 24. London