# **CURRICULUM VITAE**

I.	<ul> <li>(a) <u>Name</u>:</li> <li>(b) <u>Date of birth</u>:</li> <li>(c) <u>Department</u>:</li> <li>(d) <u>Faculty:</u></li> </ul>	Isaiah Ajibade <u>Adejoro</u> 24 May, 1960 Chemistry Science	
II.	<ul> <li>(a) <u>First Academic Appointment</u>:</li> <li>(b) <u>Present Post (with date):</u></li> <li>(c) <u>Date of Last Promotion</u>:</li> <li>(d) <u>Date Last Considered (in cases</u> where promotion was not through):</li> </ul>	Assistant Lecturer (3 January, 2000) Reader (1 October, 2014) 1 October 2014 Not Applicable	
III.	<u>University Education (with dates)</u> : University of Ibadan; Undergraduate, University of Ibadan; Postgraduate, University of Ibadan; Postgraduate,	1982 – 1986 1987 - 1988 1999 – 2005	
IV.	Academic Qualifications (with dates and granting B.Sc (Chemistry) University of Ibadan, M.Sc (Physical Chemistry), University of Ibadan PhD (Physical/Computational Chemistry), Univ	, 1986 , 1988	
V.	Professional Qualifications and Diplomas (with d	ates): Nil	
VI.	Scholarships, Fellowships and Prizes (with dates)in respect of Undergraduate and Postgraduate work only):Nil		
VII.	<u>Honours, Distinctions and Membership of Learned Societies</u> : Professional Member, Institute of Chartered Chemists of Nigeria (ICCON) Member, Chemical Society of Nigeria (CSN)		
VIII.	Details of Teaching/Work Experience:(a) Work Experience(i) Assistant Lecturer(ii) Lecturer II2002 - 2005(iii) Lecturer I2005 - 2010(iv) Senior Lecturer2010 - 2014(v) Reader2014 - date		

- (b) <u>Teaching Experience</u>
  - (i) Undergraduate courses:

CHE 157 - Physical Chemistry for 100 level students	(with 5 others)		
CHE 195 - 100 level Practical Chemistry	(with 8 others)		
CHE 357 - Introductory Quantum Chemistry, Statistical			
Thermodynamics/Electrochemistry	(with 3 others)		
CHE 451- Advanced Chemical Kinetics	(with 1 other)		
CHE 457- Quantum Mechanical Treatment of			
Chemical Bonding and kinetics			
CHE 481- Chemistry Seminar			

- (ii) Postgraduate courses: 2005 till dateCHE 754 Special Topics in Physical Chemistry
- (iii) Supervision of projects: 2000 to date 26 undergraduate students 20 M.Sc graduates.
  3 PhD graduates Currently: 6 PhD students.

#### (c) Administrative duties:

Member Examinations Committee (2004) Member Departmental Registration Committee (2000-2017) Member Departmental Small Scale Industry Committee (2003) Liaison Officer for Student Chemical Society (2002) Departmental Store Officer (2012-2015) Member Faculty Board of Technology (2005-2007) Senate Member representing Congregation (2005 - 2008) Senate Member representing Congregation (2011 – 2017) Senate representative on Business Committee (2011 – 2013) Assistant Warden - Kuti Hall (2012- 2015) Senate Representative on the Board of Osun State College of Technology, Esa-Oke (2014 – 2016) Senate Representative on the Board of the University Library (2014 – 2017) Warden - Kuti Hall (2015- 2018)

### IX <u>Research:</u>

- (a) Completed:
  - Semi-empirical Quantum Mechanical Orbital Method using MOPAC: Calculation of the Arrhenius Parameters for the Pyrolysis of Some Alkyl acetates
  - (ii) PM3 Study of the Effects of  $\alpha$ -Methylation on the Gas-phase Kinetics of Thermal Decomposition of Ethyl Acetates.
  - Study of Structural and electronic properties of 4-H- cyclopenta-[2,1-b,3;4-b#] dithiophene S-Oxide (BTO) with an S, S=O, O and SiH<sub>2</sub> and BH<sub>2</sub> bridge: semi-empirical and DFT Study.)
  - (iv) Theoretical Study on the Structural and Electronic Properties of New Materials based on Benzothiodiazole and Pyrrole derivatives.
  - (v) Study of Characterization of a novel polymeric Zinc (II) complex containing the anti-malarial Quinine as ligand: A Theoretical approach (Semi-empirical and DFT methods).
  - (vi) Theoretical Investigation on the Structural and Electronic Properties of Conjugated Organophosphorus Compounds.
  - (vii) Study of the Kinetics of some six centre pyrolytic elimination reaction and thermal rearrangements by the semi-empirical quantum mechanical molecular orbital methods.
  - (viii) Molecular Docking Studies of Lonchocarpus Cyanescens Triterpenoids as Inhibitor for Malaria.
- (b) In progress:
  - (i) The theoretical study of the effects of acid portion on the kinetics of the thermal decomposition of isopropyl acetate and isopropyl trimethylacetate was started in 2016. So far, we have concluded data collection and we are presently on data analysis.
     The application of this research will be used in reaction mechanism formulation.
  - (ii) Computational modeling of the kinetics of the multipath thermal decomposition of s-butyl acetate was started in 2015. Result so far is showing that the pyrolysis of s-butyl acetate yields different products via different routes. We have been able to formulate a procedure to study this complex pyrolytic elimination reaction.

- (c) Project, Dissertation and Thesis
  - (i) **Adejoro, I. A.** (1988): Study of the pH dependence of the kinetics of the reaction of 5, 5'-dithiobis (2-nitrobenzoic acid) with sulphydryl groups of dog hemoglobin. (*M.Sc Project, University of Ibadan*)
  - (ii) Adejoro, I. A. (2005): Kinetics of some six centre pyrolytic elimination reaction and thermal rearrangements by the semi-empirical quantum mechanical molecular orbital methods. (*PhD Thesis, University of Ibadan*)

### X <u>Publications:</u>

- (a) <u>Books Already Published</u>: Nil
- (b) Chapters in Books Already Published:
- (c) Articles that have Already Appeared in Refereed Conference Proceedings:

#### V <u>Publications:</u>

- 1. Adeniyi, A. A. and **Adejoro, I. A.** (2011): Increasing the rate of Novel Drug Discovery through Exploration of Natural Products Biodiversity and Combinatorial Chemistry. *Proceedings of the 34<sup>th</sup> International Conference of the Chemical Society of Nigeria, Ilorin.* 195-198pp.
- 2 Adejoro, I. A., Akintemi, E. O., Ezekwe, C. C. and Adewole, F. S. (2015). Computational Study of the Gas-phase Substitution of Phenoxy in 2, 4-Dinitrodiphenylether with Dimethylamine. 2<sup>nd</sup> International Conference on Scientific Research and Innovation held by Faculty of Science, University of Ibadan, Nigeria. 1-9pp.
- 3. Okonjo, K. O. and **Adejoro, I. A.** (1993). Hemoglobin with Multiple Reactive Sulphydryl Groups: The Reaction of Dog Hemoglobin with 5, 5'-dithiobis (2-nitrobenzoate), *Journal of Protein Chemistry* Vol.12, No 1: 33-37.
- 4. Adejoro, I. A. and Bamkole, T. O. (2005). Semi-empirical Quantum Mechanical Orbital Method using MOPAC: Calculation of the Arrhenius Parameters for the Pyrolysis of Some Alkyl acetates. *Journal of Applied Sciences* Vol.5, No 9, 1559-1563.
- 5. Adejoro, I. A. and Bamkole, T. O. (2009). Kinetics and Mechanism of Elimination of Ethyl Acetate in the Gas phase: a Theoretical Study, *African Journal of Pure and Applied Chemistry*. Vol. 3, No 8, 140-144.
- 6. Odiaka, T. I., **Adejoro, I. A.** and Akinyele, O. F. (2009). Synthesis and Characterization of New tricarbonyl (1, 4-η-Cyclohexa-1, 3-Diene)-N-anilino iron complexes. *Inorganic Chemistry: An Indian Journal* Vol. 4, No. 4, 172-175.
- Adejoro, I. A. (2009). PM3 Study of the Effects of α-Methylation on the Gas-phase Kinetics of Thermal Decomposition of Ethyl Acetates. *Physical Chemistry: An Indian Journal* Vol. 4, No. 2, 82-87.
- 8. Adejoro, I. A. and Eke E. (2010). Theoretical Study of the Kinetics of the Pyrolytic Elimination Reaction of Ethyl Chloride. *E-Journal of Chemistry* Vol. 7, No 1, 271-274.

Nil

- Odiaka, T. I., Akinyele, O. F. and Adejoro, I. A. (2011). Synthesis And Characterization of Pyridino (1, 4-η-Cyclohexa-1, 3-Diene) Derivatives of Iron Tricarbonyl Complexes. *E-Journal of Chemistry*, Vol. 8, No. 3, 960-965.
- 10. Adejoro, I. A. and Adeniyi, A. A. (2011). Chemistry of benzobispyrrole-derived squaraines. *International Journal of the Physical Sciences* Vol. 6, No.27, pp. 6246-6256
- **11. Adejoro, I.** A., Odiaka, T.I. and Akinyele, O.F. (2011). Semi-Empirical (PM3) Studies Of New Pyridino-1-4-η-2- Methoxycyclohexa-1, 3-Diene Iron Tricarbonyl Complexes. *Inorganic Chemistry, An Indian Journal* Vol. 6, No.1, 1-5.
- Semire, B., Odunola, O. A. and Adejoro, I. A. (2011). Structural and electronic properties of 4-H- cyclopenta-[2,1-b,3;4-b#] dithiophene S-Oxide (BTO) with an S, S=O, O and SiH<sub>2</sub> and BH<sub>2</sub> bridge: semi-empirical and DFT Study. *Journal of Molecular Modeling*, Vol. 18, No. 6, 2755-2760.
- Semire, B., Adejoro, I. A. and Odunola, O. A. (2011). Conformational Analysis and Electronic Properties of Fluoromethylfuran Oligomers: Semi-empirical and DFT Study. *Ecletica Quimica*, Vol. 36, No.3, 26-30.
- Odiaka, T. I., Adejoro, I. A. and Akinyele, O. F. (2012). Semi-empirical (PM3) studies of novel Aminopyridino-1- 4-η-cyclohexa-1, 3-diene iron tricarbonyl complexes. *American Journal of Science and Industrial Research*, Vol. 3, No.1, 1-13. (United States of America) (Contribution: 45%) (Currently volume 9 in 2018)
- Adejoro, I. A., Odiaka, T. I. and Akinyele, O. F. (2012). Molecular Modeling and Computational Studies of Dimethyl Pyridino-1,4-η-2-methoxycyclohexa-1,3-Diene Iron Tricarbonyl Complexes. *Asian Journal of Research in Chemistry* Vol. 5, No.1, 146-153.
- 16. Adejoro, I. A., Ogunyemi, B. T., and Semire, B. (2012). Theoretical Study on the Structural and Electronic Properties of New Materials based on Benzothiodiazole and Pyrrole derivatives. *Der Pharma Chemica*, Vol.4, No.6, 2214-2221

17. Adejoro, I. A., Oyeneyin, O. E., Adeboye, O. O. and Obaleye, J. A. (2012). PM3 Semi-empirical Quantum Mechanical Calculations on a Novel Dichlobis (N-{4-[2pyrimidinyl-kN-amino) sulfonyl} acetamide] copper (II) Containing a Metabolite Nacetyl sulfadiazine. *Journal of Computational Methods in Molecular Design*, Vol.2, No.4, 142-148

18. Adejoro, I. A., Oyeneyin, O. E., Adeboye, O. O. and Obaleye, J. A. (2013). Characterization of a novel polymeric Zinc (II) complex containing the anti-malarial Quinine as ligand: A Theoretical approach (Semi-empirical and DFT methods). *American Journal of Science and Industrial Research*, Vol. 4, No. 1, 111-122.

- 19. Adejoro, I. A., Ibeji, C. U., and Aigbe, A. E. (2013). Theoretical Studies on Substituent effect on the Properties of Benzofused thieno [3, 2-b] Furan and its Isomeric Form. *Nature and Science*. Vol.11, No. 1, 74-82.
- Adejoro, I. A., and Adeboye, O. O. (2013). Quantum Mechanical Studies of the Kinetics, Mechanisms and Thermodynamics of the Gas-phase Thermal Decomposition of Ethyl Vinyl Ether. *Southern Brazilian Journal of Chemistry* Vol. 21, No 21, 41-60.
- Adejoro, I. A., Adeboye, O. O. and Esan, T. (2013). ab-initio and DFT Studies of the Kinetics, Mechanisms and Thermodynamics of the Gas-phase Pyrolysis of Ethyl Bromide. *African Journal of Pure and Applied Chemistry*. Vol. 7, No. 6, 231-241
- 22. Adejoro, I. A. and Ibeji, C. U. (2013). A Theoretical Study on the effect of Substituent properties of pyrrole and thiophene. *New York Science Journal*, Vol. 6, No. 7, 99-105.
- 23. Adejoro, I. A. and Ogunyemi, B. T. (2013). Theoretical Investigation on the Structural and Electronic Properties of Conjugated Organophosphorus Compounds. *Journal of Chemical and Pharmaceutical Research*, Vol. 5, No. 9, 27-33.
- Adejoro, I. A., T.I. Odiaka and Akinyele, O.F., (2013). Structure and Electronic Properties of Aminopyridino-1-4-η-2-Methoxycyclohexa-1,3-diene iron tricarbonyl Complexes - A Semi-Empirical PM3 Approach. Asian Journal of Research in Chemistry, Vol. 6, No 11, 1034-1039.
- Adekunle, F. A. O., Adejoro, I. A., Akinyele, O. F. and Odunola, O. A. (2013). Synthesis and Quantum Mechanical Studies of [2, 6-Diacetylpyridine bis-(benzoichydrazone)]. *International Journal of Research in Engineering and Applied Sciences*, Vol. 3, No. 6, 18-27
- 26. Adekunle, F. A. O., Adejoro, I. A. and Akinyele, O. F. and Odunola, O. A. (2013). Synthesis, Spectroscopy and Theoretical Studies of Alkyl and Aryl Substituted Acid Hydrazide. *International Journal of Basic and Applied Chemical Sciences* Vol. 3, No. 2, 10-22
- 27. Adejoro, I. A., Odiaka, T. I. and Akinyele, O.F., (2014). Density Functional Theory and Reactivity Parameters of Dimethylpyridino-1-4-η-Cyclohexa-1, 3-diene iron tricarbonyl Complexes. *Journal of Natural Sciences Research*, vol. 4, No 1, 38-45.
- Adejoro, I. A., Adeboye, O.O., B. Akintoye, and Akinyele, O. F. (2014). Quantum Mechanical Characterization of Mixed-Ligand Complex of Co (II) Dimethylglyoxime. *Trends in Molecular Sciences*, Vol. 6 No. 1, 13-21
- 29. Adejoro, I. A., Akintemi, E.O, Adeboye, O.O. and Ibeji, C.U. (2014). Quantum Mechanical studies of the Structure-Activity Relationship and Electronic Vibration of some Dietary Flavonoids. *Asian Journal of Applied Sciences*, Vol. 7 No. 3, 117-128.

- 30. Adejoro, I. A. and Ogunyemi, B. T. (2014). Pi-Conjugated Phosphole Derivatives: Promising Building Blocks for  $\pi$ -Conjugated Organic Materials. *Chemistry and Material Research*, Vol. 6, No. 5, 48-54.
- Adejoro, I. A., Ogede, R. O., Ibeji, C. U. and Adeboye, O. O. (2014). The Free Radical Bromination of Ethyl Pyridazines: Theoretical Studies. *Southern Brazilian Journal of Chemistry*, Vol. 22, No. 22, 53-60.
- Adejoro, I. A., Ojo, F. K. and Obafemi, S. K. (2014). Corrosion Inhibition Potentials and Ampicillin for mild steel in hydrochloric acid solution. *ScienceDirect- Journal of Taibah University for Science*, Vol. 9, No.2, 196-202
- 33. Olalekan, T. E., Adejoro, I. A., VanBrecht, B. and Watkins, G. M. (2015). Crystal structures, spectroscopic and theoretical study of novel Schiff bases of 2-(methylthiomethyl) amines. *Spectrochimica Acta Part A: Molecular and Bimolecular*, Vol. 139, 385-395
- 34. Adejoro, I. A., Orodepo, G. O. and Ibeji, C. U. (2015). Theoretical Study on the Molecular Structure and Optoelectronic Properties of Benzoxazole-based Alternating Donor-Acceptor Conjugated Polymers. *Research and Reviews: Journal of Chemistry*, Vol. 4, No. 1, 1-10
- 35. Adejoro, I. A., Akintoye, B., Adeboye, O. O. and Akinyele, O. F. (2015) Theoretical Study of the Characterization of Mixed-Ligand Complexes of Ni (II) Dimethylglyoxime. *Ife Journal of Science*, Vol. 17, No.3, 533-541.
- 36. Adejoro, I. A., Oyeneyin, O. E. and Ogunyemi, B, T. (2015). Computational Investigation on Substituent and Solvent Effects on the Electronic, Geometric and Spectroscopic Properties of Azobenzene and some Substituent Derivatives. *International Journal of Computational and Theoretical Chemistry*, Vol. 3, No 6, 50 -57.
- Ibeji, C. U., Adejoro I. A. and Adeleke, B. B. (2015). A Benchmark Study on the Properties of Unsubstituted and Substituted Polypyrole. *Journal of Physical Chemistry* and Biophysics, Vol. 5, No. 6, 1-11
- Ibeji, C. U., Adegboye, T. S., Adejoro, I. A. and Adeleke, B. B. (2015). Computational investigation of some Isomeric forms of 3-Ethyl Pyrrole. *New York Science Journal*, Vol. 8 No. 12, 9-15.
- Sobola, A. O., Watkins, G. M., VanBrecht, B. and Adejoro, I. A. (2016). Synthesis, Structure and Theoretical Studies of bis(pentacoordinated) μ-o-[CuL2]2: Predicting Distortion towards Trigonality. *Journal of Coordination Chemistry*, Vol. 69, No. 1, 81-89

- 40. Adejoro I. A, Tolufashe, F. G. and Ibeji, C. U. (2016). Density Funtional Theory (DFT) Study of a New 4-[(Z)-{Phenyldiazenyl]- 2H- Chromen-2-one Dye for Its Use as Sensitiser in Molecular Photovoltaics. *Researcher*, Vol. 8, No. 3, 83- 89
- 41. Adejoro I. A, Waheed, S. O. and Adeboye, O. O. (2016). Molecular Docking Studies of Lonchocarpus Cyanescens Triterpenoids as Inhibitor for Malaria. *Journal of Physical Chemistry and Biophysics*, Vol. 6, No. 2, 1-4
- 42. **Adejoro, I. A**. and Adeboye, O. O. (2016). Computational Studies on the α- and βpathways for the Kinetics and Thermodynamics of the Gas-phase Pyrolysis of Allyl Formates. *Nature and Science*. Vol. 14, No. 4, 74 – 82.
- 43. Adejoro, I. A., Ojo, F. K. and Akinyele, O. F. (2016). Theoretical Studies on the Efficiencies of some Triazolopyrimidine Derivatives on Corrosion Inhibitors of Mild Steel in Acidic Medium Using AM1 and DFT Approach. *International Research Journal of Pure and Applied Chemistry*, Vol. 12, No.4, 1-9
- 44. Akinyele, O. F., Odiaka, T. I. and Adejoro, I. A. (2016). Molecular Simulation of Tricarbonyl (1-4-η-5-exo-NX, X-dimethylpyridino-cyclohexa-1, 3-diene) Iron Complexes:- A Semi Empirical PM6 Approach American Chemical Science Journal Vol.16, No.4, 1-8
- 45. Ibeji C. U., Okpala E. O., Adejoro, I. A., Onyia, K. K. (2016). Theoretical Investigation of New Organic Electroluminescent Materials Based on 4-Azaindole Groups and Oligopyrrole. *Journal of Applied Computational Mathematics* Vol. 5, No. 35, 1-4
- 46. **Adejoro, I. A.**, Onyia, K. K. and Akintemi, E.O. (2016). Theoretical Studies of the Effects of  $\alpha$ -methylation and  $\beta$ -methylation on the Gas-phase Kinetics of Thermal Decomposition of Allyl formates. *Journal of Science Research*, Vol. 6, No. 21, 16-21
- Adejoro, I. A., Akintayo, D. C. and Ibeji, C. U. (2016). The efficiency of Chloroquine as Corrosion Inhibitor for Aluminium in 1M HCl Solution: Experimental and DFT Study. *Jordan Journal of Chemistry*, Vol. 11 No. 1, 38-49
- 48. Adejoro, I. A., Ojo, F. K. and Lori, J. A. (2016). Theoretical Study of the Efficiency of Some NitroBenzenamine Derivatives in Acidic Medium to Serve as Excellent Organic Corrosion Inhibitors of Mild Steel. *International Research Journal of Pure & Applied Chemistry* Vol. 10, No. 1, 1-10.
- 49. Ibeji, C. U, Tolufashe, G. F. and **Adejoro, I. A**. (2017). Synthesis, solvent effects and computational study of new 4-methyl-5, 5-diphenyl-2(5H)-furanone. *Journal of Research in Science* Vol. 3, 31-36.
- 50. Adejoro, I. A., Esan, T. O., Adeboye, O. O. And Adeleke, B. B. (2016). Quantum mechanical studies of the kinetics, mechanisms and thermodynamics of gas-phase

thermal decomposition of ethyl dithiocarbonate (Xanthate) *ScienceDirect-Journal of Taibah University of Science*, Vol. 11, 700-709

- Adejoro, I. A., Waheed, S.O., Adeboye, O. O. and Akhigbe, F.U. (2017). Molecular Docking of the Inhibitory Activities of Triterpenoids of *Lonchocarpus cyanecens* against Ulcer. *Journal of Biophysical Chemistry*, Vol. 8, 1-11.
- 52. Ibeji, C. U., Adejoro, I. A., Fayoyiwa, A. D., Ochonogor, A. E., and Onoabedje, E. A. (2017). Theoretical study on the molecular structure of Quinoline and its derivatives as an anti- malaria drug *International Journal of Pharmaceutical Research & Allied Sciences*. Vol. 6 No.1, 52 -74
- Adejoro, I. A., Ibeji, C. U. and Akintayo, D. C. (2017). Quantum Descriptors and Corrosion Inhibition Potentials of Amodaquine and Nivaquine. *Chemical Sciences Journal*. Vol. 8, No. 1, 1-6
- 54.Adejoro, I. A., Orodepo, O. G., Adeboye, O. O. and Akhigbe, U. F. (2017). Theoretical Study of the Properties of Isatin (1H-indole-2, 3-Dione) Based Alternating Donoracceptor Type conjugated Oligomers. *Physical Science International Journal*, Vol. 15, No. 4, 1-6.
- 55. Esan, O. T., Adejoro, I. A., Ogunyemi, B. T. and Oyeneyin, O. E. (2017). Quantum Mechanical Study on the Kinetics and Thermodynamics of O-Alkyl S-Methyl Dithiocarbonates through α- and β- Elimination Pathways. *Leonardo Journal of Sciences Volume 6, Issue 31, 1-20*
- 56. Latona, D. F. and Adejoro, I. A. (2018). Kinetics of Acidic Mn (VII) Oxidation of Acetaldehyde in Aqueous and 5% Ethanol-Water Solvent. *American Journal of Chemical Research, Volume 2, No. 6, 1-8*
- 57. Ojo, F. K., Adejoro, I. A., Akpomie, K.G., Ogunyemi, B. T. and Oyeka, E.E. (2018). Effect of iodide ions on the inhibitive performance of o-, m-, p-Nitroaniline on Mild Steel in Hydrochloric Acid Solution. *Journal of Applied Science and Environmental Management, Volume 22, No. 5, 775-782*
- 58. Oyeneyin, O. E., Adejoro, I. A., Ogunyemi, B. T and Esan, T. O. (2018). Structural and Solvent Dependence on the Molecular and Nonlinear Optical Properties of 10-Octyl Thiophene-based Phenothiazine and Substituted Derivatives-A Theoretical Approach. *Journal of Taibah University of Science (Taylor and Francis) Volume 12, No.4, 483-493.*
- 59. Oyebamiji, A. K., Oyedeji, F. O., **Adejoro, I. A**. and Adeleke, B. B. (2018). Antifungal Activities of 2, 4-Dinitrophenyl Hydrazones Derivatives: Dft and Docking Approaches, *Academic Arena, Volume 10, No. 6: 12-16*

- 60. Oyeneyin, O. E., Adejoro, I. A. and Esan, T. O. (2018). Substituent Effects on the Structural and Non-linear Optical Properties of 1-{4-({(E)[4-(methylsulfanyl)phenyl]methylidene}amino)phenyl]ethanoate and some of its substituted derivatives- a Theoretical Method. *Physical Chemistry Research, Volume* 6, No. 3, 667-683
- 61. LT Ogundele, Adejoro, I. A., PO Ayeku (2019). Health risk assessment of heavy metals in soil samples from an abandoned industrial waste dumpsite in Ibadan, Nigeria *Environmental monitoring and Assessment 191 (5), 1-10*

62. BT Ogunyemi, DF Latona, **Adejoro, I. A.** Molecular modeling and quantitative structure–property relationships (QSPRs) of purine derivatives as corrosion inhibitor in acid medium *Scientific African 8, e00336* 

63. LT Ogundele, PO Ayeku, AS Adebayo, AP Olufemi, **Adejoro, I. A.** (2020)Pollution Indices and Potential Ecological Risks of Heavy Metals in the Soil: A Case Study of Municipal Wastes Site in Ondo State, Southwestern, Nigeria *Polytechnica, 1-9* 

64. BT Ogunyemi, DF Latona, AA Ayinde, **Adejoro, I. A.** (2020). Theoretical Investigation to Corrosion Inhibition Efficiency of Some Chloroquine Derivatives Using Density Functional Theory. *Advanced Journal of Chemistry-Section A 3 (4)*, 485-492

65. BT Ogunyemi, OE Oyeneyin, OT Esan, **Adejoro, I. A.** (2020).Computational modelling and characterisation of phosphole adopted in triphenyl amine photosensitisers for solar cell applications. *Results in Chemistry 2, 100069* 

66. OO Adeboye, **Adejoro, I. A.**, AM Olatunde (2020). Computational Modelling of the Kinetics and Thermodynamics of Diels-Alder reaction: 1, 3-cyclohexadiene and substituted ethene. *Leonardo Electronic Journal of Practices and Technologies 33*, 207-21867.

67. **Adejoro, I. A.**, Babatunde, D. D. and Tolufashe, G. F. (2020), Molecular docking and dynamic simulations of some medicinal plants compounds against SARS-CoV-2: an insilico study. Journal of Taibah University for science, volume 14, issue 1, 1563-1570

68. OE Oyeneyin, **Adejoro, I. A.**, BS Obadawo, JS Amoko, IO Kayode (2021). Investigation into the Molecular Properties of 3-(4-Hydroxyphenyl) Prop-2-en-1one 4-Phenyl Schiff Base and Some of Its Derivatives-DFT and Molecular Docking Studies *Science Letters 9 (1), 4-11* 

# (f) Books, Chapters in Books and Articles already accepted for publication:

# (g) Technical Reports and Monographs:

\*Publications that have appeared/ been accepted since last promotion.

## XI <u>Major Conferences Attended with Papers Read (in the last 5 years)</u>

- 2<sup>nd</sup> International Conference on Scientific Research and Innovation held by Faculty of Science, University of Ibadan, Nigeria Adejoro, I. A., Akintemi, E. O., Ezekwe, C. C. and Adewole, F. S. (2015). Computational Study of the Gas-phase Substitution of Phenoxy in 2, 4-Dinitrodiphenylether with Dimethylamine.
- 2. AFRE International Conference on Communication Engineering, Data Mining, Information Technology & Applied Science (CDITA), held at Ibis Styles Accra Airport Hotel, Ghana on July 25-26, 2018,

**Adejoro, I. A.** and Sulaimon, R. (2018). Molecular Docking of the Inhibitory Activity of Chromone Rhamnoside of Mimosa Pigra Linn., and its Methoxyl Derivative Against Tuberculosis

Sign: -----

Date: -----

Nil