CURRICULUM VITAE

Ι	 (a) <u>Name</u>: (underline surname) (b) <u>Department:</u> (c) <u>Faculty</u>: 	Nathanael Damilare <u>OJ</u> Chemistry Science	<u>IO</u>
II	 (a) <u>First Academic Appointment</u>: (b) <u>Present Post (with date)</u>: (c) <u>Date of Last Promotion (with date)</u>: 	Assistant Lecturer (5 Fo Lecturer I (1 October, 2 1 October, 2021	• • • • •
III	<u>University Education (with dates)</u> University of Ibadan, Ibadan University of Ibadan, Ibadan University of Ibadan, Ibadan	20	04 - 2008 011 - 2012 014 - 2019
IV	Academic Qualifications (with dates and granting bo B.Ed. Chemistry/Physics (Ibadan) M.Sc. Physical Chemistry (Ibadan) Ph.D. Physical Chemistry (Ibadan)	20 20	008 112 119
V	Professional Qualifications and Diplomas (with dates	<u>s):</u> Ni	1
VI	 <u>Scholarships, Fellowships and Prizes (with dates)</u> <u>in Respect of Undergraduate and Postgraduate Work</u> (a) Stephen Oluwole Foundation for Best Graduating Science Education Student (b) Tertiary Education Trust Fund grant 	20	08 16-2017
VII	<u>Honours, Distinctions and Membership of Learned S</u> (a) Associate Member, Royal Society of Chemistry ((b) Member, Chemical Society of Nigeria (CSN)	(AMRSC) 20	017 018
VIII	<u>Details of Teaching/Work Experience:</u> (a) Work experience (i) Assistant Lecturer, Department of Chemistry, University (ii) Lecturer II, Department of Chemistry, University		014 – 2018 018 to date
	 (b) Teaching Experience <u>Undergraduate courses :</u> CHE 156: Physical Chemistry I (17%) CHE 195: Practical Chemistry (15%) CHE 251: Electrochemistry I (22%) CHE 256: Physical Chemistry II (56%) CHE 256: Physical Chemistry- Practical (50%) CHE 259: Physical Chemistry for Life Sciences CHE 351: Electrochemistry II (50%) CHE 356: Physical Chemistry III (25%) CHE 452: Molecular Spectroscopy (33%) CHE 458: Symmetry and Group Theory (33%) CHE 481: Seminar Topic (All Lecturers) ICH 399: Industrial Attachment II (All Lecturer) 	20 20 20 20 20 20 20 20 20 20 20 20 20 2	914 - 2021 914 to date 918 - 2020 914 to date 915 - 2016 914 - 2020 918 - 2019 921 to date 921 to date 921 to date 914 to d

Postgraduate courses:

CHE 744 – Symmetry and Group Theory (33%)2021 to dateCHE 851 – Recent advances in Physical Chemistry (17%)2021 to dateCHE 852 – Experimental techniques in Physical Chemistry (17%)2021 to date

Research Supervision:

Completed:	
B.Sc.	18 students
M.Sc.	4 students
Ongoing:	
B.Sc.	2 students
M.Sc.	1 student

(c) Administration Responsibilities:

` ´		2014 / 1 /
	(i) Member, Departmental registration committee	2014 to date
	(ii) Member, Examination Committee	2018 to date
	(iii) Member, Coordination Committee for Demonstrators	2018 to date
	(iv) Member, University of Ibadan Senate	2020 to date
	(v) Member, Emergency Remote Teaching (ERT) Committee	2021 to date
	(vi) Member, Departmental Finance Committee	2021 to date
	(vii) Member, Faculty of Science Website and Conference	2021 to date
4)	Community Somico	
u)	Community Service	
	(i) Reviewer, Egyptian Journal of Chemistry	2020 to date
	(ii) Reviewer, Journal of the Nigerian Society of Physical Sciences	2021 to date
	(iii) Reviewer, Spectrochimica Acta A, Elsevier	2023 to date

- (iv) Reviewer, Scientific Reports, Springer Nature 2023 to date
- (v) Reviewer, Structural Chemistry, Springer Nature 2023 to date

IX <u>Research:</u>

- (a) <u>Completed:</u>
- (i) Synthesis and characterisation of some Schiff bases and perimidines with electronic and nonlinear optical properties. The research was completed in 2019.
- (b) <u>In Progress:</u>
- Investigation of photoluminescent properties of some Schiff bases and perimidines is currently on-going using Ultraviolet-Visible and fluorescence spectrophotometry. This research started in 2014 and is aimed at exploring absorption and fluorescence properties of some synthesised Schiff bases and perimidines. This research will be completed in 2030.
- (ii) Computational investigation of optical, electronic, corrosion inhibition and drug-like properties of some aromatic organic compounds. This work started in 2018 and is aimed at designing, modifying and studying optoelectronic, anti-corrosion and druglike properties of functional aromatic compounds. This research will be completed in 2030.
- (c) <u>Project, Dissertation and Thesis:</u>
- (i) Ojo, N. D. (2012). Computational Studies of Corrosion Inhibition Potentials of 1Himidazo[4,5-F][1,10]phenanthroline Derivatives Using Density Functional Theory. M.Sc. project, Department of Chemistry, University of Ibadan. 93pp.
- (ii) Ojo, N. D. (2019). Synthesis and Investigation of Electronic and Nonlinear Optical Properties of Some Schiff Bases and Perimidines. Ph.D. thesis, Department of Chemistry, University of Ibadan. 197pp.

X <u>Major Conferences and Workshops Attended with Papers Read (in the last five years):</u>

- International Conference on Science Technology and Management (ICSTM-21), Accra, Ghana. June 7-8, 2021.
 Paper read – Oral – Ojo N. D. and Obi-Egbedi N. O. Optoelectronic, photophysical and nonlinear optical properties of N-(1H-benzo[d]imidazol-2-yl)-1-(3substitutedphenyl)methanimines: spectroscopic and computational approaches.
- 54th Annual (Hybrid) Conference and 60th Anniversary Celebration of the Science Association of Nigeria, "OLUYOLE 2021", Faculty of Science, University of Ibadan, Ibadan, Nigeria. June 20-24, 2021
 Paper read Oral Ojo N. D. and Obi-Egbedi N. O. Benzimidazole Schiff bases as optoelectronic and nonlinear optical materials: spectroscopic and computational approach.
- 4th Commonwealth Chemistry Conference, October 4-5, 2023.
 Paper read Oral Ojo N. D., Adekusibe O. D. and Obi-Egbedi N. O. N-(1H-benzo[d]imidazol-2-yl)-1-(3-substituted phenyl) methanimines as optoelectronic and nonlinear optical materials: spectroscopic and computational approach

XI Ten Best Publications that Reflect the Totality of my Contributions to Scholarship

- 1. Obi-Egbedi, N. O. and **Ojo, N. D.** (2015). Computational Studies of the Corrosion Inhibition Potentials of some Derivatives of 1H-imidazo[4,5-F][1,10]phenanthroline. *Journal of Science Research* Vol. 14: 50-56.
- Ojo, N. D., Krause, R. W. and Obi-Egbedi, N. O. (2020). Electronic and Nonlinear Optical Properties of 2-(((5-aminonaphthalen-1-yl)Imino)Methyl)Phenol: Experimental and Time-Dependent Density Functional Studies. *Journal of Molecular Liquids* Vol. 319: 1–8. https://doi.org/10.1016/j.molliq.2020.114157.
- 3. **Ojo, N. D.**, Krause, R. W. and Obi-Egbedi, N. O. (2020). Electronic and Nonlinear Optical Properties of 3-(((2-Substituted-4-Nitrophenyl)Imino)Methyl)Phenol. *Computational and Theoretical Chemistry* Vol. 1192: 1–8. https://doi.org/10.1016/j.comptc.2020.113050.
- Oyeneyin, O., Akerele, D., Ojo, N. D. and Oderinlo, O. (2021). Corrosion Inhibitive Potentials of Some 2H-1-Benzopyran-2-One Derivatives- DFT Calculations. *Biointerface Research in Applied Chemistry* Vol. 11 No.6: 13968–13981. https://doi.org/10.33263/BRIAC116.1396813981.
- 5. Obi-Egbedi, N.O. and **Ojo, N.D.** (2021) Synthesis, Light Harvesting Efficiency, Photophysical and Nonlinear Optical Properties of 3-(5-(4-hydroxybenzylideneamino)naphthalen-1-yliminomethyl)phenol: Spectroscopic and Quantum chemical approach. *Research on Chemical Intermediates* Vol. 47: 5249-5266. https://doi.org/10.1007/s11164-021-04579-4.
- 6. Oyeneyin, O.E., **Ojo, N.D.,** Ipinloju, N., James C.A. and Agbaffa, E.B. (2022) Investigation of Corrosion Inhibition of Some Aminopyridine Schiff Bases Using Density Functional Theory and Monte Carlo Simulation. *Chemistry Africa* Vol. 5: 319–332. https://doi.org/10.1007/s42250-021-00304-1.
- Ramalingam, A., Kuppusamy, M., Sambandam, S., Medimagh, M., Oyeneyin, O. E., Shanmugasundaram, A., Issaoui, N. and Ojo, N. D. (2022). Synthesis, spectroscopic, topological, hirshfeld surface analysis, and anti-covid-19 molecular docking investigation of isopropyl 1-benzoyl-4-(benzoyloxy)-2,6-diphenyl-1,2,5,6-tetrahydropyridine-3-carboxylate. *Heliyon*, Vol. 8 No. 10: 1-14. https://doi.org/10.1016/j.heliyon.2022.e10831.
- Olawale, M. D., Akintemi, E. O., Ojo, N. D., Isaac, A. Y., Su, H. and Obaleye, J. A. (2023). Synthesis, Characterization, Density Functional Theory, Monte Carlo, and Molecular Dynamics Simulations of [Ni (II)(TPY)₂] Metal Organic Framework and Congo Red Dye Application. *Journal of Computational Biophysics and Chemistry*, Vol. 22 No. 7: 845–862. https://doi.org/10.1142/S2737416523500448.
- Oyeneyin, O. E., Ibrahim, A., Ipinloju, N., Ademoyegun, A. J. and Ojo, N. D. (2023). Insight into the corrosion inhibiting potential and anticancer activity of 1-(4-methoxyphenyl)-5methyl-N'-(2-oxoindolin-3-ylidene)-1H-1,2,3-triazole-4-carbohydrazide via computational approaches. *Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2023.2260491.
- 10. **Ojo, N. D.**, Adekusibe, O. D., Odozi N. W., Obi-Egbedi, N. O. (2024) N-(1H-Benzo[d]imidazol-2-yl)-1-(3-substituted phenyl) methanimines as optoelectronic and nonlinear optical materials: spectroscopic and computational approaches. *Chemical Papers*. https://doi.org/10.1007/s11696-024-03625-w.

RESEARCH FOCUS

My research is focused on spectroscopic and computational aspects of Physical Chemistry. Application of molecular spectroscopic (Ultraviolet-Visible and fluorescence) techniques in studying optical and electronic properties of some synthesised organic compounds (especially Schiff bases and perimidines) has been adopted in unravelling effectiveness of imine and perimidine compounds as semiconducting and photoluminescent materials. So far, compounds with benzimidazole, hydroxyl and amine functional groups have been observed to possess good fluorescence properties. Effects of solvent perturbation on electronic properties of these compounds have also been studied to understand the sensitivity of the reactivity and stability of the compounds in different media.

Also, computational techniques (mainly density functional, molecular docking and molecular dynamics approaches) have been utilised in investigating molecular and optical properties of some aromatic compounds with a view to exploring their corrosion inhibition, electronic, nonlinear optical, photovoltaic and drug-like properties. These techniques are essentially important in modelling, predicting and elucidating applicability of useful organic systems in materials science, optoelectronics and design of drug candidates.