

Publications

- 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.
- 2 Akande, A. A., Obi-Egbedi, N. O. and **Ojo, N. D.** (2019). Effects of Solvents on the Electronic and Molecular Properties of 4-((2-methyl-4-nitrophenyl)iminomethyl)phenol. *International Journal of Advances in Scientific Research and Engineering* Vol. 5 No. 8: 102–108.
- 3 **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.
- 4 **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.
- 5 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.
- 6 Oyeneyin O., Ipinloju N., **Ojo N. D.** and Akerele D. D. (2021). Structural modification of ibuprofen as new NSAIDs via DFT, molecular docking and pharmacokinetics studies. *International Journal of Advances in Engineering and Pure Sciences* Vol. 33 No. 4: 614-626.
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- 8 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.
- 9 Akinyele, O. F., Adekunle, A. S., Olayanju, D. S., Oyeneyin, O. E., Durodola, S. S., **Ojo, N. D.**, Akinmuyisitan, A. A., Ajayeoba, T. A. and Olasunkanmi, L. O. (2022). Synthesis and Corrosion Inhibition Studies of (E)-3-(2-(4-chloro-2-nitrophenyl)diazenyl)-1-nitronaphthalen-2-ol on Mild Steel dissolution in 0.5 M HCl Solution- Experimental, DFT and Monte Carlo Simulations. *Journal of Molecular Structure*, Vol. 1268: 1-14.
- 10 Oyeneyin, O. E., **Ojo, N. D.** and Ipinloju, N., Agbaffa, E. B. and Emmanuel, A. V. (2022). Investigation of the corrosion inhibition potentials of some 2-(4-(substituted)arylidene)-1H-indene-1,3-dione derivatives: density functional theory and molecular dynamics

- simulation. *Beni-Suef University Journal of Basic and Applied Sciences*, Vol. 11 No. 1: 1-14.
- 11 Ramalingam, A., Kuppusamy, M., Sambandam, S., Medimagh, M., Oyenehin, 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.
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 - 13 Oladipo, S. D., Obi-Egbedi, N. O., Adeoye, M. D., **Ojo, N. D.** and Badeji, A. A. (2023). Studies on the effect of solvents on the electronic absorption spectra of 4-phenylmorpholine and 1-phenylpyrrole. *Scientia Africana*, Vol 22 No. 1: 243–254.
 - 14 Oluwafemi, K. A., Oyenehin, O. E., **Ojo, N. D.** and Aigbogun, J. A. (2023). Alkyne-Allene Transformation: Density Functional and in silico Studies of 5-bromo-1-(Propargyl)-7-azabenzimidazole and its 1,2-propadiene Analogue. *Chemistry Africa*, Vol. 6 No. 2: 1117–1123.
 - 15 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.
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 - 17 **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*.