

Advanced Computational Modelling of Materials

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Presentations



science & innovation

Department:
Science and Innovation
REPUBLIC OF SOUTH AFRICA



Dr Obodo Onyebuchi Kingsley



Prof Tjaart Kruger



Dr Aniekan M. Ukpong



Overarching aim



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Can we have sustainable energy development !!!

- Considering Social contract
- Energy independence
- Economic freedom
- Environment and Climate

- Indigenous people
- Country centric solutions



Prof Tjaart Kruger (UP)

DFT on Terpolymers

Optimized Geometries



BDTTEH



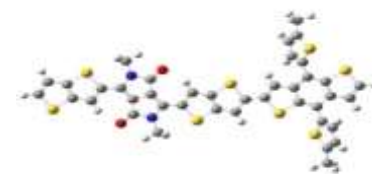
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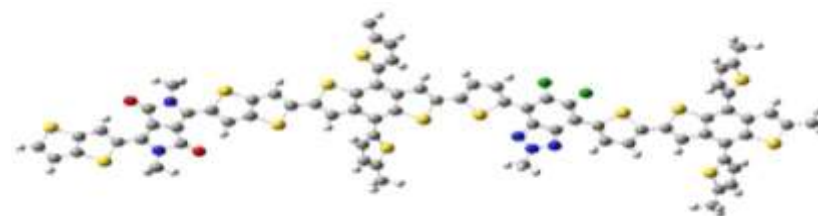
ZG23



ZGP_X



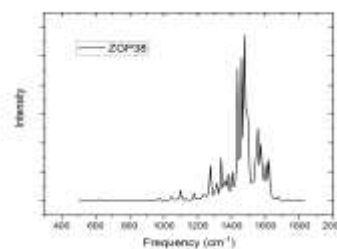
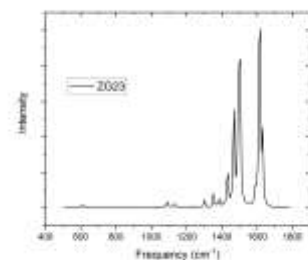
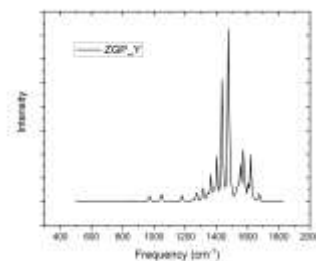
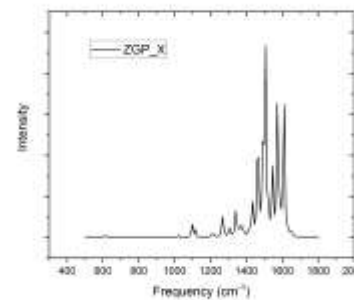
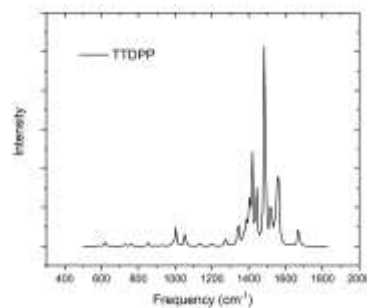
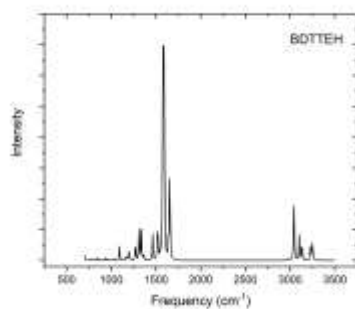
ZGP_Y



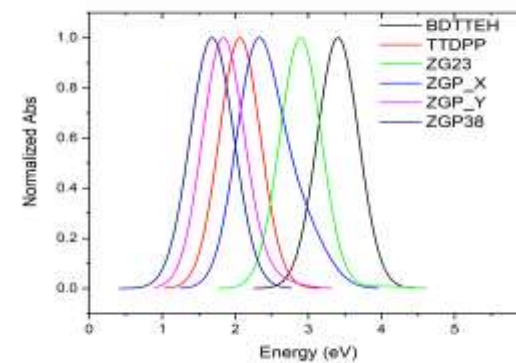
ZGP38

Calculated spectra

Raman



Absorption



Calculations to determine aggregation types of a benzodithiophene-isoindigo copolymer

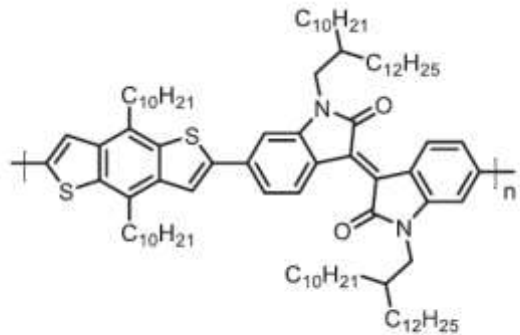


FIG. 1. Chemical structure of PBBDT-DT, R = 2-decyltetradecyl.

TABLE I. Four most probable excited states of the BDTI trimer with the corresponding dominantly contributing transitions.

Excited state	Excitation energy (eV)	Oscillator (a.u.)	Transition strength	Contribution per band (%)
S ₁	2.413	3.858	HOMO → LUMO	67
			HOMO - 3 → LUMO	11
			HOMO - 2 → LUMO + 3	9.6
S ₃	2.695	0.304	HOMO - 1 → LUMO + 2	31.4
			HOMO → LUMO + 2	31.1
			HOMO - 3 → LUMO + 1	18.6
S ₇	3.280	1.509	HOMO → LUMO	27
			HOMO - 3 → LUMO + 2	15
			HOMO - 3 → LUMO + 1	14.3
			HOMO - 2 → LUMO + 3	12
			HOMO - 2 → LUMO	10
S ₉	3.412	0.286	HOMO - 2 → LUMO	33.2
			HOMO - 2 → LUMO + 1	22.8
			HOMO - 1 → LUMO + 1	22.7

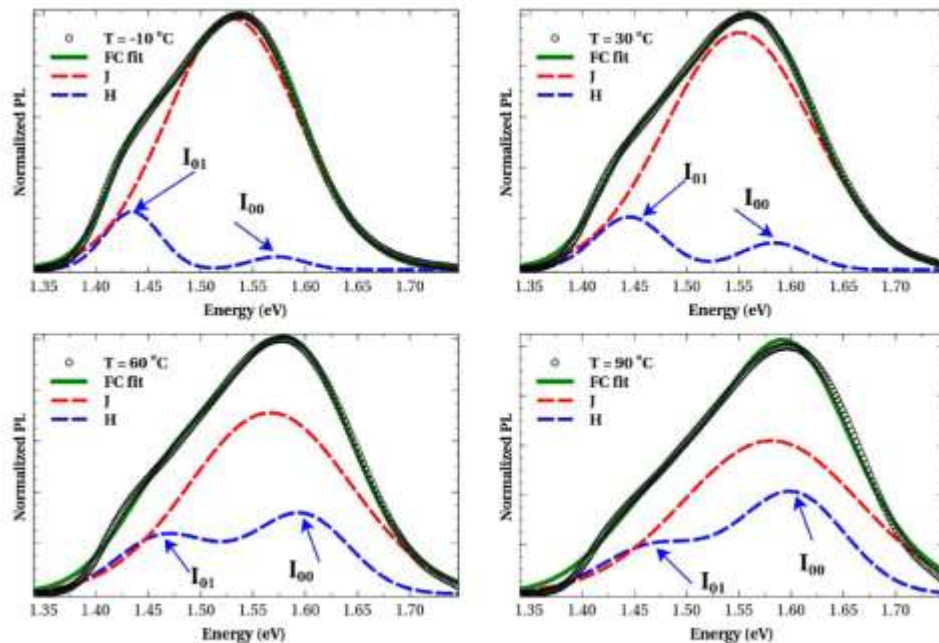


FIG. 9. FC fit of PBBDT-DT in solution at selected temperatures for both J- and H-progressions.

Main conclusion:

J- and H-aggregates are present, with the latter being dominant.

Publications in the past year

On organic polymers

Published

The Journal of Chemical Physics

ARTICLE

pubs.aip.org/jcp

Investigation into aggregation types in a benzodithiophene–isoindigo copolymer

Cite as: J. Chem. Phys. 159: 034901 (2023); doi: 10.1063/5.0151318
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Published Online: 17 July 2023

Eninges Asmare,¹ Fekadu Gashaw Hone,¹ Wendimagegn Mammo,¹ Tjaart P. J. Krüger,^{1,2}
and Newayemedhin A. Tegegne^{1,3}

IOP Publishing

Journal of Physics D: Applied Physics

J. Phys. D: Appl. Phys. 56 (2023) 044007 (Ipp)

<https://doi.org/10.1088/1361-6483/acd987>

Benzodithiophene unit copolymerization to improve the stability of thiophene-based organic solar cells

Hiroki Saito¹, Takayuki Uchiyama¹, Yoshiko Okada-Shudo¹, Wendimagegne Mammo²,
Tjaart P J Krüger^{3,5}, Varun Vohra¹ and Newayemedhin A Tegegne^{1,4}

Submitted

L.T. Nchinda, N.A. Tegegne, W. Mammo, Z. Genene, T.P.J. Krüger, “Unveiling the Thermal Stability of Diketopyrrolopyrrole-Based Terpolymers: A Key Element for Enhanced Efficiency and Stability of Organic Solar Cells” *submitted to New Journal of Chemistry*

Ready for Submission: 4 manuscripts

Conference presentations

- 16 international conference presentations
- 4 national conference presentations

Research visits & training

- Ugandan collaborator to UP
- Ethiopian PhD student to UP
- UP PhD student to USA
- UP PhD student to Germany

Highlights

- NRF's Research Excellence Award For Next Generation Researchers awarded to one of the PhD students
- 2 conference oral presentation student awards
- The PI received an NRF C1 rating
- The PI was promoted to a Senior Editor of the *Journal of Physics Chemistry Letters*
- 1 conference was organized
- 7 invited international conference presentations
- 1 invited national conference presentation
- 1 public lecture given to primary school children



Dr Aniekan M. Ukpong

Field-theoretic computations for facile energy interconversion using condensed matter models

Peer- Reviewed Research Articles

Lucas Squillante, Luciano S. Ricco, Aniekan Magnus Ukpong, Roberto E. Lagos-Monaco, Antonio C. Seridonio, and Mariano de Souza, Grüneisen parameter as an entanglement compass and the breakdown of the Hellmann-Feynman theorem, *Physical Review B* (IF 3.7), Vol. 108, 06 October 2023, pp. L140403. <https://doi.org/10.1103/PhysRevB.108.L140403>

Obada, S.A. Abolade, R. S. Kumare, A.M. Ukpong, A. Akande, Ab initio calculations of the properties of defective CsSnCl₃: The role of anion-cation pair defect, *Solid State Ionics* (IF 3.2), Vol. 399, 01 October 2023, pp. 116262. <https://doi.org/10.1016/j.ssi.2023.116262>

D. O. Obada, E. Okafor, S.A. Abolade, A.M. Ukpong, D. Doodoo-Arhin, A. Akande, Explainable machine learning for predicting the band gaps of ABX₃ perovskites. *Materials Science in Semiconductor Processing* (IF 4.1). 01 July 2023, Vol. 161, pp. 107427. <https://doi.org/10.1016/j.mssp.2023.107427>

Michael Tsamparlis, Linearization of Second-Order Non-Linear Ordinary Differential

Equations: A Geometric Approach, *Symmetry* (IF 2.7), 2023, 15, 2082. <https://doi.org/10.3390/sym15112082>.

Conference Presentations

David Olubiyi Obada, A. M. Ukpog, Simeon Akindele Abolade, Akinlolu Akande, Properties of Pristine and Defective RbGeX₃(Cl, Br, I) Perovskites: An Ab initio Study, In-person Oral presentation at the 4th International Computational Science and Engineering Conference ICSEC23, 16 - 17 October 2023, Texas A&M University, Qatar's Advanced Scientific Computing Center, Education City, Doha, Qatar.

Human Capital Development

Students trained: ##UG, #Honours, #MScs, #PhDs, #postdocs



Dr Obodo Onyebuchi
Kingsley



Outline



science & innovation

Department:
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- Overview of HySA
- Where I am From
- Student Supervision
- Current Research/Collaborative research
- Book Chapters
- Articles
- Conference presentations
- Highlights of the Year and Research Alignment to national interest



Overview HySA



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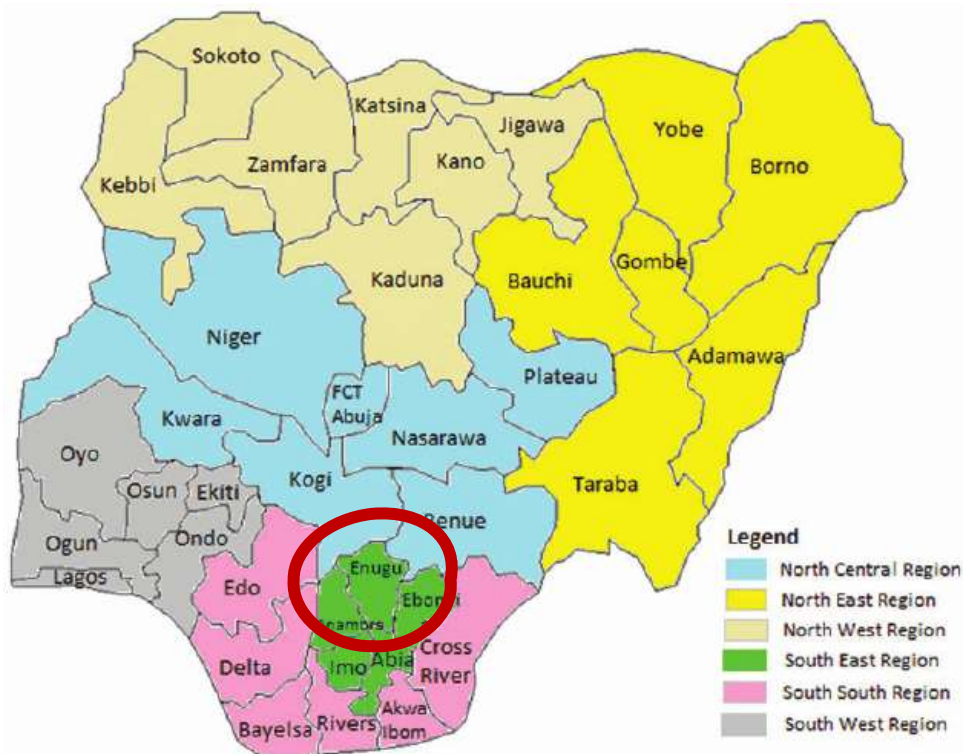


Where Am I From?



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- Amandim Olo
- Ezeagu Local government area
- Enugu state
- Nigeria

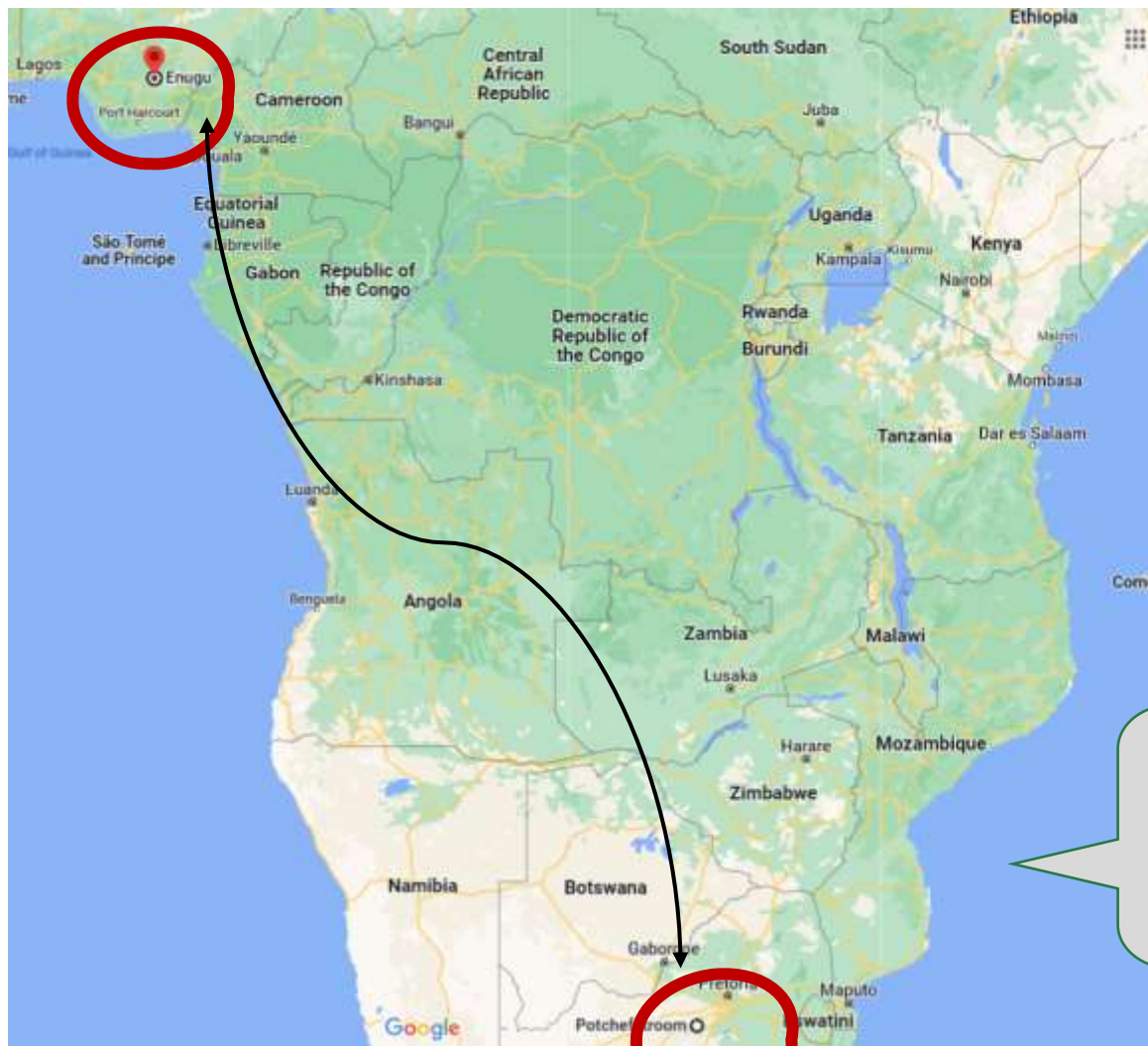


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- Enugu state
- Nigeria
- Potchefstroom
- South Africa

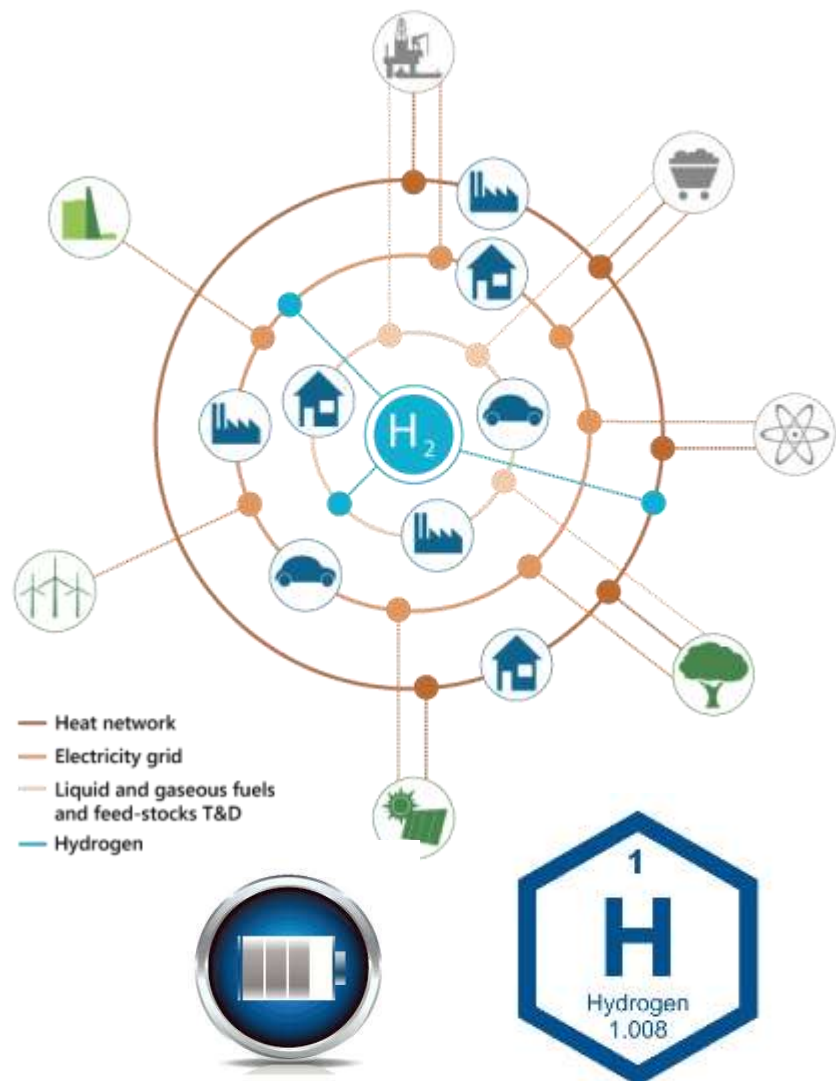


Student Supervision (Graduated)



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- Peter C. Obodo: (Graduated MSc); Quantum Mechanical Studies of Molybdenum Disulphide (MoS_2) and MXene-based Heterostructures for Photovoltaics and Water Splitting Applications) at Quantum Mechanical Studies of Molybdenum Disulphide (MoS_2) and MXene-based Heterostructures for Photovoltaics and Water Splitting Applications. University of Nigeria, Nsukka, Nigeria.
- Aseres Alula Arega: (Graduated MSc); First Principles Study Of $\text{TiS}_2/\text{Mo}_2\text{T}$ iC_2O_2 and $\text{TiS}_2/\text{T i}_3\text{C}_2\text{O}_2$ MXenes Heterostructure as Anode Material for Rechargeable Li-ion Batteries. Addis Ababa University, Ethiopia.
- Frew Gashaw Asefa: (Graduated MSc); Improved Photovoltaic Properties for Sn/Ge Substituting Pb Atoms in 2D $(3\text{AMP})_4\text{Pb}_4\text{I}_{16}$ Perovskite Using Density Functional Theory. Addis Ababa University, Ethiopia.
- Najib M. Sultan: (Graduated PhD) Universiti Teknologi PETRONAS (UTP), Bandar Seri Iskandar 32610, Perak, Malaysia.
- Houssam Eddine Hailouf: (Graduated PhD) University of Djelfa, 17000, Djelfa, Algeria.



Student Supervision



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Kassahun Desta (MSc)

Bereket Fekede (MSc)

Getachew Denbela Loko (PhD)

Jemal Mohamed (PhD)

Tsega Zemen (MSc)

Desalegn Nigatu (PhD)

Other students current based in Nigeria, Ghana, South Africa



Hydrogen economy via catalysis

- Sn-Pt based surfaces
- Pd/Pt alloys

2D Materials

- Photocatalysis
- Photovoltaics

Sorbent based technologies

- Water treatment

Modification of electronic and optical properties of 3D systems



Cost and environmental evaluations and comparisons of commonly used sorbents: K Obodo, UO Aigbe; Adsorption Applications for Environmental Sustainability, 14-1-14-13; 2023

Activated biosorbents for the removal of metals from aqueous solutionsUO Aigbe, KE Ukhurebor, RB Onyanha, B Okundaye, E Aigbe, K Obodo, ...; Adsorption Applications for Environmental Sustainability, 3-1-3-27; 2023

The types, characteristics, and management options (reusability/recyclability/final disposal) of commonly used adsorbents in environmental sustainability; K Obodo, UO Aigbe; Adsorption Applications for Environmental Sustainability, 2-1-2-25; 2023

Functionalized biosorbents for the sequestration of dye from aqueous solutions; UO Aigbe, KE Ukhurebor, RB Onyanha, B Okundaye, E Aigbe, K Obodo, ...; Adsorption Applications for Environmental Sustainability, 4-1-4-22; 2023

Utility of Magnetic Nanomaterials for Theranostic Nanomedicine; UO Aigbe, RB Onyanha, KE Ukhurebor, B Okundaye, E Aigbe, KO Obodo...; Magnetic Nanomaterials: Synthesis, Characterization and Applications, 47-86; 2023



Comprehensive theoretical studies of Sn and Ti doping induced modulation in electronic and optical properties of Na₂ZnP₂O₇ compounds using GGA+ U approach; HE Hailouf, KO Obodo, A Gueddin, L Gacem, B Bouhafs, K Reggab; Materials Science and Engineering: B 298, 116888; 2023.

Ab Initio Study of Structural, Electronic, and Thermal Properties of Pt/Pd-Based Alloys; LM Botha, CNM Ouma, KO Obodo, DG Bessarabov, DL Sharypin, ...; Condensed Matter 8 (3), 76; 2023.

US Patent App. 18/119,589; 2023.

Hydrogenation of furfural-to-furfuryl alcohol over La-based inorganic perovskites: A study of oxygen vacancies as catalytic descriptors Y Nzuzo, S Ntshibongo, L Matsinha, A Adeyinka, KO Obodo, N Bingwa; Catalysis Communications, 106717 ([1](#)); 2023.

First principles-based approaches for catalytic activity on the dehydrogenation of liquid organic hydrogen carriers: A review DN Gemechu, AM Mohammed, M Redi, D Bessarabov, YS Mekonnen, KO Obodo; International Journal of Hydrogen Energy, [1](#); 2023.

Comparison of finite element density functional with NWChem results for 18 molecules; M Braun, KO Obodo; Indian Journal of Physics, 1-4; 2023.

Pt-like catalytic activity from an atomistically engineered carbonitride MXene for sustainable hydrogen production; E Uwadiunor, V Kotasthane, DK Yesudoss, H Nguyen, E Pranada, KO Obodo...; Chem Catalysis; [3](#); 2023.

Effect of Mn⁺² Doping and Vacancy on the Ferromagnetic Cubic 3C-SiC Structure Using First Principles Calculations; NM Sultan, TMB Albarody, KO Obodo, MB Baharom; Crystals 13 (2), 348; [1](#); 2023.



Comprehensive theoretical studies of Sn and Ti doping induced modulation in electronic and optical properties of Na₂ZnP₂O₇ compounds using GGA+ U approach; HE Hailouf, KO Obodo, A Gueddime, L Gacem, B Bouhafs, K Reggab; Materials Science and Engineering: B 298, 116888; 2023.

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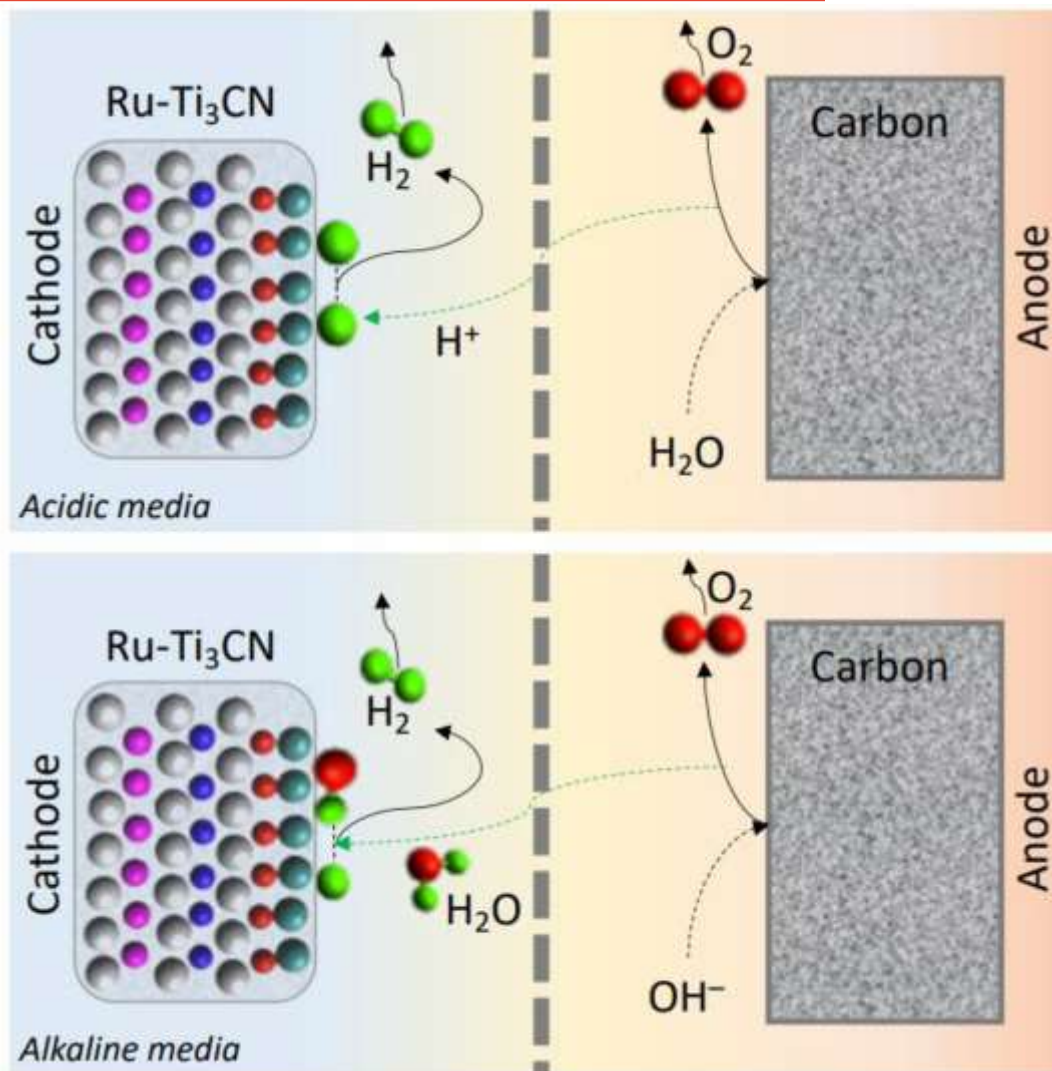
Comparison of finite element density functional with NWChem results for 18 molecules; M Braun, KO Obodo; Indian Journal of Physics, 1-4; 2023.

Pt-like catalytic activity from an atomistically engineered carbonitride MXene for sustainable hydrogen production; E Uwadiunor, V Kotasthane, DK Yesudoss, H Nguyen, E Pranada, KO Obodo...; Chem Catalysis; [3](#); 2023.

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Conference presentations



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5th African Nano Conference/Workshop on Application of Nanotechnology to Energy, Environment, Agriculture and Health, University of Nigeria, Nsukka: 10th – 16th September 2023 – **Keynote Presentation titled:** “Computational Modelling using high performance computing for materials prediction and design”.

International Conference of Catalysis Society of South Africa 2023, Sun City, South Africa: 27 August - 01 September 2023 – **Poster Presentation titled:** “Multi-Scale Computational Modelling Techniques of Electrocatalysts for Oxygen Evolution Reaction”.

Application of Computational Modelling of Materials in Engineering, University of Nigeria, Nsukka: 16th – 20th January 2023 – **Speaker.**



• Highlights of the Year and Research Alignment to national interest



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C2 NRF Rating (2023 – 2027).

Invited Guest Speaker at University of Nigeria Nsukka (UNN) & Visiting Lecturer at UNN (Jan 2023).

Invited by AU high level panel on emerging technologies “3D printing technology”.

MSc and PhD Students graduated.

Organizing a Mini-school at CHPC national meeting (Dec 2023).

MSc and PhD Students invited to give presentations in Kenya & CHPC.

New Registered PhD student to be Supervised by Prof Tjaart Kruger, Prof Yedilfana Setarge and Dr Kingsley Obodo.

Possible collaboration with Prof. Catharine Esterhuysen (NITHeCS) and Dr Trisha Salagaram (UCT)

US Patent on Dehydrogenation reaction (2023).

Guest Lecture at University of Nigeria (Jan 2023).



Collaborators



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Some current collaborators

- Dr. Gebreyesus G. Hagoss (University of Ghana, Ghana)
- Prof. Luyanda Noto (University of South Africa, South Africa)
- Prof. Georgies Alene Asres (Addis Ababa University, Ethiopia)
- Prof. D. P. Rai (Pachhunga University College, Mizoram University, India)
- Prof. Bachir Bouhafs (University of Sidi Bel-Abbès, Algeria)
- Prof. Yedilfana Setarge Mekonnen (Addis Ababa University, Ethiopia)
- Prof. Victor S. Aigbodion (University of Nigeria, Nsukka, Nigeria)
- Prof. Fabian Ezema (University of Nigeria, Nsukka, Nigeria)



Acknowledgements

