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KINGSLEY ONYEBUCHI OBODO (Ph. D)

PERSONAL DATA

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Google scholar:

https://scholar.google.com/citations?hl=en&user=KQrC_6IAAAAJ&view_op=list_works

PROFESSIONAL PROFILE

A computational condensed matter scientist with vast expertise in computational condensed matter physics, *ab initio* modeling, general computing, high performance computing (HPC), holistic and heuristic thought process applicable in both the business and academic sector. A fast learner, ambitious, intelligent, eloquent, and a responsible person looking forward to further broaden my horizons and skills base in any given sector.

RESEARCH & OTHER INTERESTS

- *Ab initio* modeling of materials properties for catalytic applications.
- Understanding the kinetics for liquid organic hydrogen carriers (LOHC) dehydrogenation.
- Quantum mechanical studies of solid-state systems as well as magnetic and thermal properties of materials.
- Defects, surfaces, semiconductors, interface, hard and ultra-hard materials.
- Electronic properties of energy-relevant materials and catalysis.
- Computational high through put screening, high-performance computing.
- Innovative technologies, Project management, curriculum development.
- Sustainable business research solutions in new frontiers

TEACHING AND MENTORING EXPERIENCE

- [2016 to 2019] First year physics courses- Tutor at Turning point tutors, Pretoria
- [2011 to 2014] First year introductory physics – Lecturer at the University of Pretoria
- [2011 to 2014] First year laboratory experiment – Demonstrator at the University of Pretoria
- Electronic structure school 2012 (ASESMA) – Mentor/Tutor in Kenya.
- [2011 to 2013] Electrodynamics, Quantum and Statistical mechanics, and Solid-State physics for third - Tutor at the University of Pretoria

EDUCATION

Ph.D., Physics, University of Pretoria (UP), Pretoria

2011 - 2014

Concentrations: Computational Condensed Matter Physics, Materials Science

Dissertation: Quantum Mechanical Studies of Early Actinide Compounds

Dissertation Advisors: Prof Nithaya Chetty Ph.D

**M. Sc., Materials science, African University of Science and Technology AUST), Abuja
2008 - 2009**

Concentrations: Materials science and engineering

Thesis: Variation of the constraint factor with respect to temperature using indentation techniques

Thesis Advisor: Prof. U. Ramamurty Ph. D.

**B. Tech., (Physics and electronics technology) Nnamdi Azikiwe University, Awka
2002 - 2007**

Concentrations: Physics and electronics Second class upper with honours (4.41 out of 5)

Project: Computerised Digital Poultry Incubator

Project Advisor: Prof SO Ezeonu Ph.D.

Most Recent Employment

Postdoctoral Researcher, Hydrogen South Africa (HySA - Infrastructure) CoC, North-West University, (NWU) Potchefstroom

Jan 2019 - to date

Achievements

- Modelled the de-hydrogenation of liquid organic hydrogen carriers (LOHC), activity of transition metal catalysts, hydrogen evolution reaction and oxygen evolution reaction using density functional theory.
- Published in high impact factor peer-reviewed journals and gave conference presentations.
- Co-supervision of PhD student supervision.
- Consulted on other projects, wrote reports, and participated in grants/funding applications.

Postdoctoral Researcher, University of South Africa, (UNISA) Pretoria

June 2016 – Dec 2018

Achievements

- Established key understanding of magnetism in alkali systems.
- Showed catalytic and magneto-optical property in 2D systems.
- Part of the organizers of finite element workshop at UNISA and symposium at the CHPC national conference.
- PhD student supervision published in high impact factor peer-reviewed journals and give invited conference presentations as well as oral presentations.

Research Scientist, Johnson Matthey Research South Africa, (JM RSA) Pretoria

July 2014 – Mar 2016

Achievements

- Developed computational solutions on the partial methane oxidation.
- Determined active Pt alloys configurations for HER and developed solution in catalysis.
- Investigated potentially new materials for thermo-chromic and thermoelectric materials
- Presentations of scientific findings, monthly documentation of research progress and findings

GRANTS, AWARDS AND RECOGNITIONS

- North-West University postdoctoral fellowship, (Jan 2019 – Dec 2021)
- Knowledge Interchange & Collaboration (KIC) Mobility: African interaction (2018)
- Recipient of Unilever Science Communication Scholarship, (2014)
- Travel grant recipient from University of Pretoria and American Physical Society for research visit at Stanford Linear Accelerator Center (SLAC), Menlo Park, California, USA (July to October 2013).
- Recipient of the CHPC Best PhD Student Award (12 July 2013).
- Recipient of the University of Pretoria International Student Bursary (Jan 2011 – Dec 2013)
- Travel grants recipient from African University of Science and Technology, Abuja and Indian Institute of Science for master's Thesis Research at the Indian Institute of Science, Bangalore (2009-2010).
- Second best graduating student in Materials Stream at AUST (Dec 2009).
- Nelson Mandela Institute Scholarship for Masters in Material Science at the African University of Science and Technology - Abuja, Nigeria (June 2008)
- Third best student in a class of about 200 – Nnamdi Azikiwe University Awka (2007)
- Second best graduating student - Model International School (1996)

PUBLICATIONS (TOP 5 MOST CITED)

- 1) Dzade, Y. N.; **Obodo, O. K.**; *et al.* "Silicene and Transition Metal Based Materials: Prediction of a 2-dimensional Piezomagnet." *Journal of Physics: Condensed Matter*, 22(37), 375502, (2010).
- 2) **K.O. Obodo**; N. Chetty. "GGA + U studies of the early actinide mononitrides and dinitrides." *Journal of Nuclear Materials*, vol. 442(1-3), p. 235–244 (2013).
- 3) **K.O. Obodo**; N. Chetty. "First principles LDA + U and GGA + U study of protactinium and protactinium oxides: dependence on the effective U parameter". *Journal of Physics: Condensed Matter*, vol. 25, no. 14, p. 145603 (2013).
- 4) **K. O. Obodo**, C. N. M. Ouma, J. T. Obodo and Moritz Brauns: Influence of transition metal doping on the electronic and optical properties of ReS₂ and ReSe₂ mono-layers, *PCCP*, vol 19, p. 19050-19057, DOI: 10.1039/C7CP03455E (2017).
- 5) **K.O. Obodo**; R. Andrew; N. Chetty. "Modification of the band offset in boronitrene". *Physical Review B*. vol. 00, p. 005300 (2011).

PRESENTATIONS (RECENT 5)

- 1) 4th African conference/workshop on application of nanotechnology in energy, environment, agriculture, and health for the period 19th – 23rd July 2021.- As a plenary Speaker. Presentation titled: *Ti₃C₂ MXene monolayer as catalytic support for platinum towards the dehydrogenation of methylcyclohexane*
- 2) The 6th SA-UNESCO Engineering, Science and Technology Conference at North-West University, Mafikeng Campus, South Africa: 26th to 27th of September 2019 – As an invited Speaker: Presentation titled: *Ab initio modelling of 2D and 3D Materials: Materials prediction and characterization*
- 3) 3rd African conference/workshop on application of nanotechnology in energy, environment, agriculture and health for the period 15th – 21st July, 2018.- As an invited Speaker. "Presentation titled: *Density functional theory application to 2D systems and bulk materials*"

- 4) African Materials Research Society (AMRS) Conference at Gaborone Botswana: 9th to 14th of December 2017-Oral Presentation titled: *Single and multisite transition metals dopant ions in MoS₂: a first principle study*
- 5) 9th International Conference on Materials for Advanced Technologies at Suntec Singapore: 18th to 23rd June 2017-Oral presentation titled: *Influence of transition metal doping on the electronic and optical properties of ReS₂ and ReSe₂ mono-layers.*
- 6) 1st Africa Energy Materials (AEM-2017) conference at the CSIR International Convention Centre, Pretoria, South Africa: 28 - 31 March 2017 - Oral presentation titled: *Influence of transition metal doping on the electronic and optical properties of ReS₂ and ReSe₂ mono-layers.*

PROFESSIONAL MEMBERSHIPS

- South African Institute of Physics (SAIP)

REFERENCES

- 1) Prof. Bachir Bouhafs (Bbouhafs@gmail.com)
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Université DJILLALI Liabès de Sidi Bel-Abbès
Telephone: +213771182147
- 2) Prof Moritz Braun (moritz.braun@gmail.com)
Department of Physics,
University of South Africa
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- 3) Dr. Garu Gebreyesus (garu.gebreyesus@yahoo.com)
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