UNIVERSITÀ DEGLI STUDI DI MILANO

TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B post-doc fellowship

[Emmanuel Igumbor]

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Igumbor
Name	Emmanuel
Date of birth	[04, 11, 1980]

PRESENT OCCUPATION

Appointment	Structure
2018	PostDoctoral Fellow

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degree	Physics	University of Pretoria	2017
Specialization	Theoretical and Computational Physics	University of Pretoria	
PhD	Physics	University of Pretoria	2017
Master	Theoretical Physics	Africa Univeristy of Science and Technology	2009
Degree of medical specialization			
Degree of European specialization			
Other			

REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of registration	Association	City
2015	Member South Africa Institute of Physics	Pretoria

Università degli Studi di Milano - Divisione Stipendi e Carriere del Personale
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
Assegni.postdoc@unimi.it

2013	Professional member Material Science and Technology Society of Nigeria	Abuja

FOREIGN LANGUAGES

Languages	level of knowledge
English	Excellent

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2017	Faculty of Natural and Agricultural Sciences PhD Exceptional Achievers award
2014	University of Pretoria Post graduate bursary
2008.	African University of Science and Technology World Bank assisted scholarship
2005	Department of mathematics statistics and computer best graduating student
2001	Delta state of Nigeria government undergraduate scholarship

TRAINING OR RESEARCH ACTIVITY

description of activity

I am a computational physics PhD holder (completed December 2016 and awarded January 2017) from the University of Pretoria. Sequel to this, I have completed my MSc and BSc in theoretical physics and mathematics/statistics, respectively. The mathematical and theoretical skills I acquired during my BSc, MSc and PhD made it possible for me to combine both computational and mathematical skills in my postdoctoral fellowship research work since February 2017 at then Physics Department University of Pretoria, and now High-performance Unit, School of Science, Engineering and Technology University of South Africa.

For the past ten years I have been performing density functional theory, MBPT and molecular dynamics calculations with focus on predicting the intrinsic properties of materials, which includes charge defects and exciton in semiconductors and low-dimensional TMDs, optical properties of graphene, boronitride, and new functional materials. My research activities over the period have yielded several articles published in rated journals. The published articles as listed in the last part of my CV (Publication list) are mainly results from the modelling and characterization of defects in semiconductors implementation of different algorithms used to characterize strongly correlated materials, surface properties and catalytic activities of metal oxide materials mostly on 2D and 3D bulk and hybrid materials. I have excellent command and usage of several computational advanced materials science software, data crystal virtualizing (Materials Studio, CASTEP ASAP, GaussView, Xcryden, GDIS Quantum Espresso, VASP and MedeAVASP), a good programming experience of python and FORTRAN and advance experience in DFT, DFT+U, hybrid+DFT, TDDFT GW-Bethe-Salpeter equation and molecular dynamics. My research activities is not only limited to theory, but as well as experiment with the mind-set of engaging in multi-disciplinary research areas.

The following trainings have been completed

- 18th International workshop on computational physics and materials science: Total energy and force methods. Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste Italy 8-1th January 2019 This is a training that focused on computational physics and materials science with application in quantumesspresson as it is applied to density funtional theory, molecular dynamices and other computational codes.
- Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste Italy 14-18th January 2019.

This training invovles the used of USPEC for data predictions.

- 18th International workshop on computational physics and materials science: Total energy and force methods. Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste Italy This is a training that focused or computational physics and materials science with application in quantumesspresson as it is applied to density funtional theory, molecular dynamices and other computational codes
- Advanced school and workshop on bre optics: Light in action from science to technology. University of Fort Hare Alice, Eastern Cape, South Africa, 28th September-1st October 2015. This training focused on the light and its operations.
- Summer school on electronic structure and quantum transport method calculation at ICTP/SAIFR-Brazil, 13-24th October 2014. This training is based on the introdcution to eletronic structures prediction using quantum esspresoo and SIESTA. The advance stateg of eletronic prediction using several codes were demostrated.
- CHPC winter school on high performance computing. University of Cape-Town South Africa, 30th June-5th July 2014. This worsjop is focused on high performance computing, using MPI open MPI, working in high performance enviroement and data manipulations.
- Samuel Adegboyega workshop on teaching skills, teaching methods and class room behaviour and management Edo State Nigeria, May 16th, 2012. This trianing is focused on classroom management as a teacher.

PROJECT ACTIVITY

Year	Project
2014	Point defects study in Ge using hybrid funtional theory
2017	Predicting the electrically active induced energy levels and metastability of defects in 4H SiC
2018	Ab initio study of intrinsic defect and their electronic, optical, electrical and transport properties of BN, MoS2, CrS22 and TiS3.
2020	Stability of dopant and vacancy complexes in semiconductor materials (Si and Ge) using hybrid functional.
2021	Defects engineering of MoS2 and CrS2

PATENTS

Patent

CONGRESSES AND SEMINARS

Date	Title	Place
28 Jan-1 Feb 2019	2nd African Synchrotron Light Source Conference AfLS2-2019	Accra, Ghana,
, 24-29 June 2018.	21st International Conference on Ion Beam Modication of Materials (IBMM-2018),	San Antonio, Texas, USA
	International conference on defects in semiconductor, Matsue Shimane Japan.	Matsue Shimane Japan.

Università degli Studi di Milano - Divisione Stipendi e Carriere del Personale
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
Assegni.postdoc@unimi.it

3rd 7th July 2017	62nd South African Institute of Physics Conference.	Stellenbosch University, Stellenbosch South Africa.
27th 31st March 2017	7th South African Conference on Photonic Materials (SACPM2017).	Amanzi Game Reserve central Free State Province South Africa.
19th 21st January 2017	5th International conference on Nano material science.	San Diego California, USA.
5 9th Dec 2016	CHPC national meeting and conference	International conference centre, East London South Africa.
30th Oct - 4th Nov. 2016	20th International conference on ion beam modication of materials	Wellington New Zealand
25th - 30th July. 2016	9th International conference on superlattices, nanostructures and nanodevices	City University of Hong Kong,
19th-25th September, 2015	Gettering and Defect Engineering in Semiconductor Technology GADEST.	Badstaesltein Germany
23rd-31st July 2015.	International conference on defects in semiconductor.	Aalto university, Espoo Finland.
24th August -5th September 2014	Summer school on computational modern science.	University of Oldenburg, Oldenburg Germany
8-1th January 2019.	18th International workshop on computational physics and materials science: Total energy and force methods.	Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste Italy
28th Sep-1st Oct 2015	Advanced school and workshop on bre optics: Light in action from science to technology.	University of Fort Hare Alice, Eastern Cape, South Africa,
13-24th Oct 2014	Summer school on electronic structure and quantum transport method calculation	ICTP/SAIFR-Brazil,
30th Jun-5th July 2014	CHPC winter school on high performance computing.	University of Cape-Town South Africa,
8-13th May 2011	Advance oxide interfaces.	The Abdus Salam International centre for Theoretical Physics Trieste Italy,
Dec 2009	First principle study of adsorption of molecular hydrogen sulphide on gold clusters.	AUST-Abuja Nigeria,

PUBLICATIONS

Books
1. Tuning the electronic structure and thermodynamic properties of hybrid graphene-hexagonal boron nitride monolayer. FlatChem, 24 100194, 2020

Università degli Studi di Milano - Divisione Stipendi e Carriere del Personale
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
Assegni.postdoc@unimi.it

2. Stability, electronic and defect levels induced by substitution of Al and P pair in 4H-SiC. Journal of Physics and Chemistry of Solids, 109448 2020
3. Determination of capture barrier energy of the E-center in palladium Schottky barrier diodes of antimony-doped germanium by varying the pulse width. Materials Research Express 7 025901 2020.
4. Electronic properties of vacancies in bilayer graphane. Physica B: Condensed Matter 573, 67-71 2019
5. Barrier height inhomogeneities on Pd/n-4H-SiC Schottky diodes in a wide temperature range. Materials Science and Engineering: B, 247, 114370
6. First principles prediction of the solar cell eefficiency of chalcopyrite materials AgMX2 (M= In, Al; X= S, Se, Te). Computational Condensed Matter 21,00391 2019
7. Electronic properties and defect levels induced by group III substitution-interstitial complexes in Ge. Journal of Materials Science, 54(15),10798-10808 2019.
8. Ab-initio study of the optical properties of beryllium-sulphur co-doped graphene. AIP Advances, 9(2), 025221. 2019
9. The study of low temperature irradiation induced defects in p-Si using deep-level transient spectroscopy. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 442, 28-30 2019
10. Defect levels induced by double substitution of B and N in 4H-SiC. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 442, 41-46 2019.
11. Induced defect levels of P and Al vacancy-complexes in 4H-SiC: A hybrid functional study.Materials Science in Semiconductor Processing 89 77-84. 2019
12. The influence of thermal annealing on the characteristics of Au/Ni Schottky contacts on n-type 4H-SiC. Applied Physics A 124 1-7 2018
13. Electrical characterization of deep level defects created by bombarding the n-type 4H-SiC with 1.8 MeV protons. Surface and Coatings Technology 355:15, 2-6 2018
14. Electrically active induced energy levels and metastability of B and N vacancy-complexes in 4H-SiC. Journal of Physics: Condensed Matter 30.18 2018
15. A systematic study of the stability, electronic and optical properties of beryllium and nitrogen co-doped graphene. CARBON 129, 207-227, 2018
16. Electrically active defects in p-type silicon after alpha-particle irradiation Physica B: Condensed Matter 535, 99-101 2017
17. Electronic properties of B and Al doped graphane: A hybrid density functional study Physica B: Condensed Matter Volume 535, 287-292:2017
18. Density functional theory calculation of monolayer WTe2 transition metal dichalcogenides doped with H, Li and Be. Physica B: Condensed Matter 535, 167-170: 2017
19. Thermal stability of defects introduced by electron beam deposition in p-type silicon. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 409 46-49 2017
20. Rare earth interstitial-complexes in Ge: Hybrid density functional studies. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 409 9-13. 2017
21. Rare earth substitutional impurities in germanium: a hybrid density functional theory study. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 409 31-35 2017
22. The effects of high-energy proton irradiation on the electrical characteristics of Au/Ni/4H-SiC Schottky barrier diodes. Nuclear Instruments and Methods in Physics Research Section B: Beam

Università degli Studi di Milano - Divisione Stipendi e Carriere del Personale
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
Assegni.postdoc@unimi.it

Interactions with Materials and Atoms 409 241-245. 2017
23. Electrical characterization of defects induced by electron beam exposure in low doped n-GaAs. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 409 36-40. 2017
24. Rare earth interstitials in Ge: a hybrid density functional theory study. Journal of Electronic Material 46 (2) 1022-1029. 2017
25. Ab initio study of aluminium impurity and interstitial substitutional complexes in Ge using a hybrid functional (HSE). Journal of Electronic Materials, 46(7) 2017
26. A first-principle hybrid functional calculation of Tm3+Ge-VGe defect complexes in germanium. Computational Condensed Matter 8 31 2016
27. A hybrid functional calculation of Tm^{3+} defects in germanium (Ge). Materials Science in Semiconductor Processing 43 129-133. 2016
28. Ab initio study of germanium di-interstitial using a hybrid functional (HSE). Physica B: Condensed Matter 480 191-195, 2016
29. Silicene and transition metal-based materials: prediction of a two-dimensional piezomagnet. Journal of Physics: Condensed Matter, 22(37), 37550. 2010

Articles in reviews
1. Visibility and Research Growth Analysis of Publishing in Density Functional Theory in African Institutions, between 1989 and 2019. Data in brief (2020)
2. Systematic study of stability and electronic properties of vacancy, antisite and defect-complexes in monolayer CrS2, MoS2 and WS 2. Physical Review B (2021)
3. The origin of halogen and nonmetals defects induced n- and p-type conductivity and excitonic behaviour in monolayer MoS2. ACS nano (2021)

Congress proceedings
1. Electrical characterization of electron beam exposure induced defects in epitaxially grown n-type silicon. In AIP Conference Proceedings USA 080003, 2019.
2. Predicting the Mo dopant induced electrical levels in Ge. Journal of Physics conference proceedings South Africa Institute of Physics (SAIP) South Africa 2018.
3. Ab-initio studies of self-interstitial (Mgi and Te i) in MgTe,A Wide Band Gap Semiconductor Nano Hybrids and Composites (NHC) vol. 16, Trans Tech Publications Switzerland, 47-51,2017.
4. A hybrid density functional study of silicon and phosphorus doped hexagonal boron nitride monolayer. Journal of Physics: Conference Series USA. 759 (2016):
5. Ab initio Study of MgSe Self-Interstitial (Mgi and Sei) Solid State Phenomena. Vol. 242. Trans Tech Publications Switzerland, (2015).

OTHER INFORMATION

Job Experience

- Postdoctoral fellow: (July 2018-till date) School of Interdisciplinary Research and Graduate Studies, University of South Africa. Pretoria South Africa.
  Responsibilities:
  Research on defects in 2D materials.
  Supervision of post graduate students.

Teaching postgraduate computational physics.
Examination moderator for rst year physics students

- Postdoctoral fellow: (February 2017-Jan 2018) Department of Physics, University of Pretoria. South Africa.
  Responsibilities:
  Research on defects in 3D and 2D materials.
  Supervision of postgraduate (MSc and PhD) students.
  Teaching undergraduate physics and Postgraduate computational physics.
  Examination moderator for rst year physics students
- Assistant lecturer: (2016) Faculty of Engineering, ENGAGE programme, University of Pretoria. South Africa.
  Responsibilities:
  Teaching second year engineering students material science for engineers.
  Conducting laboratory exercises for second year engineering students.
  Examination moderator for second year engineering students
- Teaching and research assistant: (2014-2016) Department of Physics, University of Pretoria. South Africa.
  Responsibilities:
  Teaching and conducting experiment for rst year physics PHY114 (First semester physics), PHY124 (Second semester physics), FSK 116 (First semester engineering physics)
  Conducting laboratory exercises for second year engineering students.
  Research in solid state materials and computational physics.
  Mentoring undergraduate physics students.
  Examination moderator for second year engineering students

Other Occupational Input

- CACTUS Editage freelancer member (2019 till date)
- Statistical analyses and interpretation of data for Department of Optometry University of KwaZulu-Nata postgraduate (MSc) student thesis. (2016-2017)
- Statistical analyses and interpretation of data for Department of Economics University of Nigeria: Postgraduate (MSc and PhD) student thesis. (2012)

Skills

- Excellent computational, English communication and writing skills.
- Team player and self motivation. Can work under pressure and also independently.
- Integrity, honesty, ethical values, professional conduct and soberness of character
- Ability to collaborate both local and internationally
- Advanced Materials Science Software, Data and crystal structure virtualizing (Materials Studio, CASTEP, VESTA, Xcryden, QuantumEspresso, VASP and MedeAVASP).
- Linux and Microsoft Oce Prociency (Vim, Vi, Gedit, Word, Access, Excel, Adobe-Page Maker, Word-Pad, Power-Point, Publisher).
- Programming Language Prociency: Fortran, High performance computing.
- Statistical Software Packages (Latex, Minitab and SPSS).
- Computer hardware installation / assemble, trouble shooting and basic designing for high performance computing clusters

Visit as a Researcher to University or Research Institution

- April 2011, Research visit to Theoretical Physics 11 Universitat Augsburg Germany.
- September-November 2009, Research visit to the Abdus Salam International Centre for Theoretical Physics Trieste Italy.

Student Supervision

1Udoa Benjamin MSc, Theoretical Physics Department. African Univerasity of Science and Technology Abuja. Modelling and predicting the electronic properties of defects in alloy (August 2019)

Referees

Università degli Studi di Milano - Divisione Stipendi e Carriere del Personale
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
Assegni.postdoc@unimi.it

- Prof. Walter E. Meyer Department of Physics University of Pretoria Hateld, Pretoria South Africa. wmeyer@up.ac.za,+277827858432.
- Dr Barry Iyare Department of Mathematical and Physical Sciences, Samuel Adegboyega University Ogwa Edo Nigeria. barryiyare@yahoo.com, +2348080838824, +2348037268511
- Dr. AT Raji Research and Academic Computing (HPC), College of Science Engineering and Technology, University of South Africa, Preller Street, Muckleneuk Ridge. tuderaji@gmail.com rajiat1@unisa.ac.za,+27 12 429 4201.
- Dr Ezekiel Omotoso Department of Physics, Obafemi Awolowo University, Ife, Nigeria omotoeze@gmail.com; omotoeze@yahoo.co.uk, +27842911287

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: __Warri__Delta State, ____26-07-2021_

SIGNATURE

_____