Omololu AKIN-OJO, Ph.D.

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Name: Omololu AKIN-OJO

Current address: ICTP East African Institute for Fundamental Research, University of Rwanda, KIST2 Building Nyarugenge Campus, Kigali, RWANDA

Education:

- Postgraduate:
  - University of Delaware, U.S.A. (2006) – Ph.D., Physics
  - University of Ibadan, NIGERIA (1998) – M.Sc. Physics
- College:
  University of Ibadan, NIGERIA (1995) – B.Sc. Physics, First Class Honors

Professional Membership:

- Member, American Physical Society (APS)
- Member, American Chemical Society (ACS)
- Member, Materials Research Society (MRS)

Professional experience:

- September, 2017 – Present: Interim Director, ICTP East African Institute for Fundamental Research, Kigali Rwanda
- July, 2015 – Present: Senior Lecturer, Department of Physics, University of Ibadan, NIGERIA
- July, 2015 – August, 2017: Assistant Professor (Part-time) in the Theoretical and Applied Physics Department, African University of Science and Technology (AUST), Abuja, NIGERIA
- 2014 – Present: Regular Associate, International Centre for Theoretical Physics (ICTP), Trieste Italy
- July, 2015 – Present: Assistant Professor (Part-time) in the
- July, 2012 – July, 2015: Assistant Professor in the Theoretical Physics Department, African University of Science and Technology (AUST), Abuja, NIGERIA
- February – April 2015: Visiting Scholar in the Department of Physics and Astronomy, University of Delaware
- January/February 2014: Visiting Scientist in the Finite Systems Group at the Max Planck Institute for Complex Systems, Dresden, GERMANY
- December 2013: Visiting Scientist in the Condensed Matter and Statistical Physics Group at the International Centre for Theoretical Physics, Trieste, ITALY
- April – July, 2012: Senior Lecturer in the Physics Department, Covenant University, Ota Ogun state, NIGERIA
- March, 2012: Visiting Assistant Professor at the African University of Science and Technology, Abuja, NIGERIA
- 2011 – 2012: (Short-term) Postdoctoral fellow at the Department of Physics and Astronomy, University of Delaware, USA

- 2009 – 2011: Postdoctoral fellow at the International Centre for Theoretical Physics, Trieste, ITALY
- 2006 – 2009: Research associate at the Chemistry Department, Boston University, USA
- 1998 – 2006: Graduate Teaching and Research Assistant at the Department of Physics and Astronomy, University of Delaware, USA

Publications:

1. *Efficient determination of excitation energies and absorption spectra for quantum dots and large systems from ab initio data*, E. Oyeniyi and O. Akin-Ojo, Chem. Phys. Lett. **721** 12 (2019).
2. *Does a pair of methane molecules aggregate in water?*, O. Akin-Ojo and K. Szalewicz, J. Chem. Phys. **150** 084501 (2019).
3. *First Principles Prediction of the Electronic Structure and Carrier Mobilities of Biaxially Strained Molybdenum Trioxide (MoO_3),* B. S. Dandogbessi and O. Akin-Ojo, J. Appl. Phys. **120** 055105 (2016).
4. *First Principles Predictions of Superconductivity in Doped Stanene,* Y. Shaidu and O. Akin-Ojo, Comput. Mater. Sci., **118** 11 (2016).
5. *Ab Initio Water Pair Potential with Flexible Monomers,* P. Jankowski, G. Murdachaew, R. Bukowski, O. Akin-Ojo, C. Leforestier, and K. Szalewicz, J. Phys. Chem. A **119** 2940 (2015).
6. *Controlling current reversals in chaotic ratchet transport,* B.S. Dandogbessi, O. Akin-Ojo, and A. Kenfack, Physica Scripta **90** 055206 (2015).
7. *How well can polarization models of pairwise nonadditive forces describe liquid water?*, O. Akin-Ojo and K. Szalewicz, J. Chem. Phys., **138** 024316 (2013).
8. *Effects of the dispersion interaction in liquid water*, O. Akin-Ojo and F. Wang, Chem. Phys. Lett., **513** 59 (2011).
9. *The quest for the best non-polarizable water model from the adaptive force matching method*, O. Akin-Ojo and F. Wang, J. Comput. Chem. **32** 453 (2011)
10. *Correcting for dispersion interaction and beyond in density functional theory through force matching*, Y. Song, O. Akin-Ojo, and F. Wang, J. Chem. Phys. **133**, 174115 (2010).

Research Supervision experience:

- Ph.D. supervision

  * Topic – Transport phenomena in model and real systems: Bruno DANDOGBESSI (2012– 2016, Graduated from the African University of Science and Technology, AUST Abuja Nigeria, co-supervised with Prof. A. Kenfack)

  * Topic – Calculation of the excitation energies and absorption spectra of large clusters and quantum dots using a semi-empirical method: E. Oyeniyi (2016 – 2021, University of Ibadan)

* Topic – Hubbard U and V in density functional theory for strongly-correlated systems: S. Irambona (2020 – Present, University of Rwanda)

* Topic – Density functional theory for catalysis: S. Ogenyi (2021 – Present, University of Rwanda)

* Topic – Topological Insulators for Dissipationless Electronics and Quantum Computing R. Kouemo (2021 – Present, University of Rwanda)

- M.Sc. supervision of students at the University of Rwanda

  * Machine Learning Techniques for Predicting the Supertconducting Critical Temperatures of Metals: Mr. Firas SHUAIB, 2019/2020

  * Effect of the Hubbard U parameter in DFT+U on the effective mass of materials. Mr. Paul Byaruhanga 2020/2021

  * Effect of the Hubbard U parameter in DFT+U on the magnetizatio of materials. Mr. Thacien Habamahoro 2020/2021

- M.Sc. supervision of students at the University of Ibadan

  * Towards an Orbital Free Kinetic Energy Density Functional for the water molecule: Mr. Doyin SHITTU, 2015/16

  * Mechanical stability of possible environmentally benign Methylammonium lead iodide Perovskites for solar cell application: ONOJAFE Emmanuel Obaroene 2015/16

  * A computational numerical analysis, simulation, and modelling of a solar cell: AKINPELU Akinwumi 2015/16

  * Ab initio calculation of phonon dispersion and phonon density of Methlyammonium Germanium Iodide [$CH_3NH_3GeI_3$] Perovskite for solar cell applications: BORIWAYE Temitope Oluwaseun 2016/17

  * Design and construction of an electrodeposition system and application to CdZnSeS thin-films: MUSILIYU Kazeem Adeleke 2016/17

  * Characterization of some factors controlling the absorption spectra of organic semiconductors: ZHIYA Wumani Victor 2016/17

  * Simulation of a supercapcitor with a new electrolyte aqueous BeF_2: ONI Oluwatobi Lekan J 2016/17

  * Formulation of a new exchange-correlation functional for better band gaps: AYOOLA Adeolu Olusola 2016/17

  * Optical Absorption Spectra of $(CdZnTeSe)_n$, (n= 1, 2, 3) for Applications in Quantum Dot Solar Cells: AKINOLA Naheem Alabi 2016/17

  * Fabrication of $Cd_2ZnSe_xS_{1-x}$ thin film and its optical properties at different pH, thickness, and Selenium-Sulphur concentrations: OLANIRAN Sikiru Adesina 2016/17

  * Determination of an optimal solar cell via numerical modeling: AGBER Joseph 2017/18

  * Theoretical and experimental investigation of several dyes for dye-sensitized solar cells application: OGBU Ben 2017/18

- M.Sc. theses of students at the African University of Science and Technology (AUST), Abuja, NIGERIA, 2014

  * Molecular Dynamics Simulation of Transport of Encapsulated Drug Through a Lipid Bilayer: Mr. Ibrahim Buba GARBA, 2014

  * Development of a Correction Term for the Kinetic Energy Density Functional: UDOKA Nwankwo, 2014

  * Superconductivity of White Tin and Doped Stanene: Mr. Yusuf SHAIDU, 2014

  * Limiting Efficiency of Perovskite Solar Cells, 2014

  * Performance Optimization of Tin Halide Perovskite Solar Cells, 2014

* Simulation-based Thermal Ablation of Prostrate Cancer: Mr. Mas-ud Ayodeji ABDULKAREEM, 2014

Teaching experience:

- **Postgraduate: Mathematical Methods for Physics (2019)** at the East African Institute for Fundamental Research (EAIFR) Kigali, Rwanda
- **Postgraduate: Advanced Electromagnetism (2019)** at the East African Institute for Fundamental Research (EAIFR) Kigali, Rwanda
- **Postgraduate: Electromagnetic Theory (2017)** at the University of Ibadan, NIGERIA
- **Postgraduate: Thermodynamics (2017)** at the University of Ibadan, NIGERIA
- **Postgraduate: Manifest Properties of Matter (2015, 2016)** at the University of Ibadan, NIGERIA
- **Postgraduate: Classical Mechanics (2014)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Statistical Mechanics (2014)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Electrodynamics (2013,2015,2016)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Computational Modeling (2013,2014,2016)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Computational Physics (2013,2014,2015)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Modelling and Simulations (2012,2014)** at the African University of Science and Technology (AUST), Abuja, NIGERIA
- **Postgraduate: Solid-State Physics (2012)** at the African University of Science and Technology (AUST), Abuja, NIGERIA
- **Postgraduate: Electrodynamics (2012)** at Covenant University, Ota, Ogun State, NIGERIA
- **Postgraduate: Mathematical Methods (2012)** at Covenant University, Ota, Ogun State, NIGERIA
- **Postgraduate: Computational Physics (2012,2013,2014)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Postgraduate: Quantum Mechanics I (2012, 2013)** at the African University of Science and Technology (AUST) Abuja, NIGERIA
- **Undergraduate: Mathematical Methods of Physics II (2015,2016)** at the University of Ibadan, NIGERIA
- **Undergraduate: Principles of Quantum Physics (2016,2017)** at the University of Ibadan, NIGERIA
- **Undergraduate: Solid State Physics II (2016,2017)** at the University of Ibadan, NIGERIA
- **Undergraduate: Mechanics and Properties of Matter (2016,2017)** at the University of Ibadan, NIGERIA

- **SCEN102 (Science for Non-science majors)** (Summer 2002) at the University of Delaware, USA:

  prepared and taught lectures;

  prepared exams, quizzes, labs; graded exams;

  coordinated lab and discussion teaching assistants

- **Teaching assistant for "Science for Non-science majors" (SCEN101)** at the University of Delaware, USA:

  Labs – Fall 1998, Winter 1999, Summer 1999;

  Discussion sections – Winter 2002, Spring 2003.

- **Teaching assistant for "Science for Non-science majors" (SCEN102)** Discussions and Labs: Spring 2000.

- **Teaching assistant for "Introductory physics" (PHYS201)** Discussions and Labs at the University of Delaware: Fall 2001: facilitated discussion and lab sections, graded homework and exams, set up office hours.

Presentations:

1. *Machine Learning the Superconducting Critical Temperatures of Metals*, by O. Akin-Ojo and F. Shuaib. A talk given at the US Africa Initiative on Electronic Structure Workshop: https://usafricainitiative.org/JuneWorkshop2021/ (June 16, 2021)

2. *Modeling Excitation Energies of Quantum Dots based on First Principles Data*, O.Akin-Ojo and E. Oyeniyi, March meeting of the American Physical Society held in Boston (USA), March 2019

3. *A second-principles approach for efficient determination of excitation energies and absorption spectra of quantum dots and large systems from* ab initio *data*, Atomic, Molecular and Optical (AMO) Physics seminar, University of Delaware (USA), 26 November 2019

4. *A new dissociative water model*, O. Akin-Ojo, Spring meeting of the American Chemical Society held in San Francisco (USA), April 2017

5. *Towards a new kinetic energy density functional for the water molecule*, O. Akin-Ojo and D. S. Shittu, March meeting of the American Physical Society held in New Orleans (USA), March 2017

6. *Elucidating the degradation of methylammonium lead iodide perovskite ($CH_3NH_3PbI_3$) at high temperatures and humid conditions via molecular dynamics simulations with ab initio force fields*, O. Akin-Ojo, March meeting of the American Physical Society held in San Antonio, Texas (USA), March 2015

7. *The effects of three-body non-additive exchange and induction forces in liquid water*, O. Akin-Ojo and K. Szalewicz, March meeting of the American Chemical Society held in Denver, Colorado (USA), March 2015

8. *How well can the properties of liquid water be described without the inclusion of many-body exchange forces?*, O. Akin-Ojo and K. Szalewicz, contributed talk at the 2014 March meeting of the American Chemical Society, held in Dallas, Texas (USA), March 2014.

9. *Towards a dissociative potential for water*, O. Akin-Ojo, contributed talk at the 2014 March meeting of the American Physical Society, held in Denver, Colorado (USA), March 2014.

10. *Electron transport in ZnO nanostructures*, O. Akin-Ojo, invited talk presented at the 7th African-Materials Research Society Conference, Addis-Ababa, Ethiopia, December 2013

11. *Computational Modeling and Simulations at Different Length and Time Scales*, plenary talk presented at the 12th Nigerian Materials Congress, Abuja, Nigeria, November 2013

12. *The true role of many-body polarization forces in describing the properties of liquid water*, O. Akin-Ojo, poster presented at the 16th Total Energy Workshop in Trieste, Italy, January 2013.

13. *Ballistic electron transport in ZnO nanostructures*, O. Akin-Ojo, poster presented at the summer school "Computer Simulations on Nanotechnology for the Environment", Jacobs University Bremen, Germany, July 2011.

14. *Dispersion effects in liquid water*, O. Akin-Ojo and F. Wang, talk presented at the CMCSN meeting, Structure and Dynamics of Water and Aqueous Solutions (Dec., 2010) held at Princeton University, New Jersey, USA.

15. *Dispersion effects in liquid water*, O. Akin-Ojo and F. Wang, Poster presented at the Sanibel Symposium (2010) held at St. Simons Island, Georgia, USA.

16. *Adaptive force matching: a systematic method of generating high-quality force fields from QM/MM calculations*, O. Akin-Ojo and F. Wang, Poster presented at the Fall American Chemical Society (ACS) Meeting (2007), held at Boston.

17. *Simulations of the hydrophobic interaction between methane solutes in water: Effects of various force fields*, O. Akin-Ojo and K. Szalewicz, Talk presented at the Water Festival IV (Nov. 2005), held at the University of Delaware.

18. *Simulations of methane in liquid water using ab initio force fields*, O. Akin-Ojo and K. Szalewicz, Poster presented at the MARMACS Meeting 2005, held at Rutgers University.

19. *First-principles simulations of methane in liquid water*, O. Akin-Ojo and K. Szalewicz, Poster presented at the Sanibel Symposium (2005), held at St. Simon Island, Georgia.

20. *First-principles simulations of methane in water clathrates and liquid water*, O. Akin-Ojo and K. Szalewicz, Talk presented at the Water Festival III (2004), held at Princeton University.

21. *Can accurate properties of methane hydrates be obtained from molecular simulations using ab initio force fields?*, O. Akin-Ojo and K. Szalewicz, Poster presented at the ACS Meeting (2004), held at Philadelphia.

22. *NPT simulations of water using ab initio potentials*, O. Akin-Ojo and K. Szalewicz, Poster presented at the Winter School on Quantum Simulations of Complex Many-Body Systems: from theory to algorithms. Kerkrade, the Netherlands (2002).

23. *He–HCCCN intermolecular interaction*, O. Akin-Ojo and K. Szalewicz, Talk presented at the second PUUDEL conference. University of Delaware (2001).

24. *Intermolecular potential of He–HCCCN from ab initio calculations*, O. Akin-Ojo, Poster presented at the PET-CCM conference: Emerging Methods in Computational Chemistry and Material Science. Aberdeen, Maryland (2001).

Current research interests:

- Electronic structure theory and Molecular modeling with applications in

  * Energy Physics: Hydrogen for fuel cells via water splitting, Photovoltaics (Solar cells)

  * Biophysics: *ab initio* force field development for drug molecules, implicit solvent models from simulations with *ab initio* force fields

- Photovoltaic cells via solution of transport and Poisson equations

Skills:

- FORTRAN programming, MPI, and Perl and shell scripting.
- Experience in using:
  - molecular simulation programs: GROMACS, DLPOLY, and MOLDY
  - quantum chemistry packages: SAPT, MOLPRO, and GAUSSIAN
  - condensed matter codes: QUANTUM-ESPRESSO
  - UNIX/LINUX operating systems including writing shell scripts.
  - Microsoft operating system.

Collaborators:

1. Prof. K. SZALEWICZ, Department of Physics and Astronomy, University of Delaware, Newark DE 19716.
   email: szalewic@udel.edu