

## **EZEKIEL OYENIYI, Ph.D.**

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**Current address:** Department of Physics, University of Ibadan, Nigeria

### **Research Interest:**

Electronic structure and spectroscopy of bulk, molecular and nano systems.

### **Education:**

- Postgraduate:
  - University of Ibadan, NIGERIA (2021) - Ph.D., Physics
  - University of Ibadan, NIGERIA (2011) - M.Sc. Physics
- Undergraduate:
  - Ladoke Akintola University of Technology, NIGERIA (2008) - B.Tech. Physics

### **Professional Membership:**

- Member, African Physical Society (AFPS)
- Member, Collaborative Research in Atomistic/Molecular Modeling
- Member, American Physical Society (APS)

### **Professional experience:**

- 2015 – To Date- Lecturer, Department of Physics, University of Ibadan, NIGERIA.
- 2010- 2015 – Lecturer, Department of Applied Science, Kaduna Polytechnic, Kaduna, NIGERIA.

### **Publications:**

- **E. Oyenyi, O. Akin-Ojo, and O. O. Popoola (2023).** oeINDO: Efficient Determination of Excitation Energies and UV-Vis Absorption Spectra of nano-sized Zn, Cd, S and their complexes. *Computational and Theoretical Chemistry*, 1223, 114096.
- **E. Oyenyi.** (2022). Electronic and optical properties of Mg<sub>3</sub>XN (X = P, As, Sb, Bi) antiperovskites: The GW/BSE approach. *Solid State Communications*, 114927.
- **E. Oyenyi and O. Akin-Ojo.** (2019). Efficient determination of excitation energies and absorption spectra for quantum dots and large systems from ab initio data, *Chem. Phys. Lett.* 721 12.
- **A. A. Ajayi, E. Oyenyi and O.M. Oshakuade (2022)** Bulk and surface properties of liquid Ag-Cu, Ag-Sb and Cu-Sb. *Pramana*, 97(2), 72.

**Presentations:**

- Efficient determination of excitation energies and absorption spectra of large atomic clusters and nanoclusters. Poster presentation at the On-line Workshop on Excited Charge Dynamics in Semiconductors organized by ICTP, Trieste, Italy, September 2020.
- Bash scripting training at Collaborative Research in Atomistic/Molecular Modeling online workshop. 26-27 December, 2021. Facilitator
- Electronic and optical properties of antiperovskites: The GW/BSE approach. Poster presentation at ASESMA, 2023 in Kigali, Rwanda.
- UV-Vis absorption spectra using semi-empirical Hamiltonian plus a machine learning model presented at APS March Meeting, 2024 virtually.

**Current Research:**

- The study of antiperovskites as materials for photocatalytic water splitting
- Machine learning + semi-empirical Hamiltonian model approach for obtaining excitation energies and absorption spectra of nano-clusters.
- In collaboration with Alex Urban (Columbia University) group, we are working on an active learning project: Optimal data sets for construction of machine learning data sets.
- A collaborative research with Prof. Michele Pavanello Group (Rutgers University-Newark) on efficient pseudopotentials for orbital free DFT.

**Experience in using:**

- DFT implemented in QUANTUM-ESPRESSO (Condensed matter code)
- GW/BSE (YAMBO code)
- DFT, TDDFT and Post-Hartree Fork methods implemented in ORCA and GAUSSIAN (quantum chemistry codes)
- DFTpy and qepy
- Atomistic Simulation Environment (ASE)
- UNIX/LINUX operating systems
- High Performance Computer
- Microsoft operating system.

**Skills:**

- Python scripting (e.g I wrote machine learning codes for obtaining excitation and spectra of molecules and active learning.)
- Bash scripting (e.g For optimization of semi-empirical Hartree Fork Hamiltonian for accurate prediction of excitation energies and spectra of nanoclusters.)

### **Grants/Research Visit**

- Research visit to ICTP-EAIFR, Kigali for a collaborative research with Dr Omololu Akin-Ojo (Former Director, ICTP-EAIFR) (2018).

### **Workshops/conferences attended:**

- African School on Electronic Structure Methods and Applications (ASESMA-2016), in Ghana.
- On-line Workshop on Excited Charge Dynamics in Semiconductors, organized by ICTP in 2020
- African Physical Society (AfPS) International Conference, 2020
- 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, 2021
- Ab-initio Many-Body Methods and Simulations with the Yambo Code, 2022
- Machine Learning in Electronic Structure and Molecular Dynamics organized by ICTP-EAIFR, 2022
- Young Researchers' Workshop on Machine Learning for Materials organized by ICTP, 2022.
- African School on Electronic Structure Methods and Applications (ASESMA), 2023 in Kigali, Rwanda
- APS March meeting, 2024.

### **Research Supervision Experience:**

- Undergraduate physics students' project at the University of Ibadan, Nigeria (2016- To date)
- M.Sc Physics students' project at the University of Ibadan, Nigeria (2024)

### **Teaching Experience:**

- Undergraduate: Mathematical Methods of Physics II (2016 – to date) at the University of Ibadan, NIGERIA
- Undergraduate: Thermal and Statistical Physics (2016 – to date) at the University of Ibadan, NIGERIA

### **Collaborators/Referees:**

- Dr Omololu Akin-Ojo (Former Director ICTP-EAIFR, Kigali), Department of Physics, University of Ibadan, Nigeria.  
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