

CURRICULUM VITAE - CAROLINE ROSEMYA KWAWU, PhD.

Personal Details: Nationality: Ghanaian

Employment: Lecturer, Kwame Nkrumah University of Science and Technology (KNUST), Ghana

Date of Birth: 29th August, 1988

Email address: kwawucaroline@gmail.com, kwawucaroline@knust.edu.gh

Phone number: +233(0)501375345, +233 555354614

Address: Computational Chemistry Lab, Department of Chemistry, UPO, Kumasi, Ghana

Interests/ skills: Theoretical/ Computational Materials Chemistry, Renewable Energy Materials, Electrochemistry, Photochemistry.

Education:

2012 – 2017

Ph.D. Computational Chemistry

Kwame Nkrumah University of Science and Technology (KNUST), Kumasi, A/R, Ghana

Title: Computational studies on transition metal catalysts for CO₂ conversion into hydrocarbon fuels

Supervisors: Prof. Evans Adei (KNUST), Dr. Richard Tia (KNUST), Prof. Nora de Leeuw (UCL, London) and Prof. C. Richard A. Catlow (UCL, London)

2007 – 2011

B.Sc. Chemistry (First Class Division)

KNUST, Kumasi, A/R, Ghana

Title: The characterisation and antimicrobial activity of the alkaloidal constituents of the Morinda lucida leaves

Teaching:

- Jan 2018 - Present **Lecturer**
Department of Chemistry, KNUST
Courses Taught: Undergraduate and Postgraduate Physical Chemistry (Thermodynamics, Chemical Kinetics, electrochemistry, materials chemistry, Surface chemistry and catalysis, photochemistry, computational materials science, quantum chemistry)
- Nov 2015 - Dec 2015 **Visiting Researcher**
UCL, London, UK.
Duties: Laboratory demonstrator
- Sep 2013 - June 2015 **Graduate Assistant**
KNUST, Kumasi, Ghana.
Duties: Laboratory demonstrator
- Oct 2011 - July 2012 **Teaching and Research Assistant**
KNUST, Kumasi, Ghana.
Duties: Taught inorganic and physical chemistry courses.

Research:

- **Areas**
 - i. Heterogeneous reaction mechanisms
 - ii. Adsorption and Charge Transfer Processes
 - iii. Photoabsorbers and Sensitizers
 - iv. Properties of Materials

- **Grants**

Date	Award	Amount
2018	2018 TWAS Research Grant award (18-032 RG/CHE/AF/AC_I)	USD 14,000
2018	Royal Society Leverhulme Africa Postdoctoral Fellowships (LAF\R1\180013)	£ 17,800 Equivalent (USD 24,764)

- **Publications: 6; Total citations: 8 H-index: 2**
PhD Publications (2)

1. Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study, CR Kwawu, R Tia, E Adei, NY Dzade, CRA Catlow, NH De Leeuw, Applied Surface Science 400, 293-303, 2017
2. CO₂ activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study, CR Kwawu, R Tia, E Adei, NY Dzade, CRA Catlow, NH de Leeuw, Physical Chemistry Chemical Physics 19 (29), 19478-19486

Post-PhD Publications (5)

1. Mechanisms of CO₂ reduction into CO and formic acid on Fe (100): a DFT study, CR Kwawu, A Aniagyei, D Konadu, BY Antwi, Materials for Renewable and Sustainable Energy 10 (2), 1-8, 2021
2. Mechanism of Guaiacol Hydrodeoxygenation on Cu (111): Insights from Density Functional Theory Studies D Konadu, CR Kwawu, R Tia, E Adei, NH de Leeuw, Catalysts 11 (4), 523, 2021
3. Mechanisms of ethyne oxidation catalyzed by LMnO₃ (L= O⁻, Cl, NPH₃, CH₃, and Cp): a density functional theory study, A Aniagyei, C Kwawu, JJEK Harrison, R Kwakye, Journal of Molecular Modeling 26 (11), 1-10, 2020
4. Permanganyl chloride-mediated oxidation of tetramethylethylene: A density functional theory study, A Aniagyei, C Kwawu, R Tia, E Adei, Journal of Molecular Graphics and Modelling 98, 107616, 2020
5. A DFT investigation of the mechanisms of CO₂ and CO methanation on Fe (111), CR Kwawu, A Aniagyei, R Tia, E Adei, Materials for Renewable and Sustainable Energy 9 (1), 1-7, 2020

- **Collaborators:** Prof. Nora de Leeuw (UK), Ishanie Rangeeka Perera (Sri Lanka)
- **Research Supervision:** Undergraduates (30), Masters (1), PhD Students (-)
- **Journal Reviewer:** Food Chemistry
- **Mentors:** Prof. Evans Adei (KNUST, Ghana), Prof. Nora de Leeuw (Cardiff, UK), Prof. Nelson Dzade (Cardiff, UK)
- **Profiles:**
 - KNUST <https://webapps.knust.edu.gh/staff/dirsearch/profile/summary/0aff78562eb2.html>
 - Google scholar <https://scholar.google.com/citations?user=eVEMDeUAAAAJ&hl=en>
 - Researchgate <https://www.researchgate.net/profile/Caroline-Kwawu-3>
 - LinkedIn <https://www.linkedin.com/in/caroline-rosemyya-kwawu-6b1b8823/?originalSubdomain=gh>
 - Facebook <https://www.facebook.com/maya.kwawu.3>

Activities/ Professional Development

1. **Workshops/ Conferences**
 - **Organising Committee Member**

Conference/ Workshop	Date
8th GSA Research Seminar and Poster Presentations	May, 2019
Science Education Seminar Series for Females in First Cycle Institutions	July, 2018
DFID-RSC Materials for Renewable and Sustainable Energy: From Research to Development	June, 2019
7th GSA Research Seminar and Poster Presentations	July, 2018
WiSTEM Girl's Camp	August, 2018
WiSTEM Senior High School Visits	January, 2019
Females Supporting Females Girls Camp 2019	April, 2019

- **Participant**

Conference/ Workshop	Date	Presentation
Post-PhD		

Science Education Seminar Series for Females in First Cycle Institutions	July, 2018	Laboratory Demonstrator
IPO-WiSTEM Workshop for Young Female Academics KNUST	April, 2021	-
International Year of the Periodic Table Celebrations	Feb, 2019	Poster session coordinator
Women empowerment Programme themed, 'the female chemist, breaking through the glass ceiling'.	July, 2018	Resource Person
Innovation/ Entrepreneurship Training Workshop for Lecturers	May, 2018	-
Workshop on Research Leadership and Mentorship by BSU III and OGR	April, 2019	
Workshop on Research Leadership and Mentorship by BSU III and OGR	May, 2019	
8th Summer School KNUST on Improving Quality of Higher Education Through Effective Measurement and Evaluation	August, 2018	-
Connecting Minds Africa (CoMA) Kenya, Nairobi	Sept, 2019	Oral and panel member: Use of Aluminium
Materials for Renewable and Sustainable Energy: From Research to Development	June, 2019	
PhD		
International Conference on Materials Chemistry KNUST, Ghana	October, 2016	Oral: Computational Studies on Transition Metal Catalysts for CO ₂
Royal Society - DFID Conference on Catalysis and Crystallography KNUST, Ghana	August, 2016	Oral: Computational Studies on Transition Metal Catalysts for CO ₂ Conversion into Hydrocarbon Fuels
The 4th African School on Electronic Structure Methods and Applications (ASESMA) University of Ghana, Legon, Ghana.	June, 2016	-
Christmas Meeting on Solid State and Materials University of Kent, Canterbury	December, 2015	Poster: CO ₂ Activation and Dissociation Trends on the Low Miller Index Surfaces of Iron: A DFT Study
School in Computational Condensed Matter Physics: From Atomistic Simulation to Model Hamiltonians (ICTP), Trieste, Italy	September, 2015	Poster: CO ₂ Activation and Dissociation Trends on the Low Miller Index Surfaces of Iron: A DFT Study
16th Annual GSCS Conference University of Ghana, Legon, Ghana.	March, 2015	-
Workshop on Material Challenges in Devices for Fuel Solar Production and Employment ICTP, Trieste, Italy.	May, 2014	Poster: Effect of Nickel Deposition on the Structural and Electronic Properties of the Low Miller Indices of (bcc) Iron: A DFT Study
2nd CLIM-RUN School: Building Two-way Communication: A week of Climate Services ICTP, Trieste, Italy	December, 2013	-

2. Internal administrative

August 2019 – 2020	Seminar Coordinator - Department of Chemistry
August 2019 – 2020	Teaching Assistant Coordinator - Department of Chemistry
August 2019 - date	Graduate Programme's Coordinator - Department of Chemistry
August 2019 - date	Member - Tratech and Exhibition Committee
April 2018 - date	Member - Chemistry Departmental Board - IDL Committee
April 2018 - date	Member - KNUST - SCL Ambassadors Committee

3. External administrative

April 2018 - date **Member** - KNUST - SCL Ambassadors Committee

4. Affiliations

2018 till date	Fellow (Africa Hall)
2018 till date	Member/ LOC Member - Women in Sci. Tech. Eng. and Maths (WiSTEM. _{GH})
2018 to 2019	Member/ LOC member - Ghana Science Association
Jan 2019 - date	Member - Royal Society of Chemistry
Jan 2019 - date	Member - Ghana Science Association
Jun 2012 - date	Member - Ghana Chemical Society

Personal Statement

I am a Physical Chemist. In November 2017, I obtained a PhD in Computational Materials Chemistry from the Department of Chemistry, Kwame Nkrumah University of Science and Technology (KNUST), Ghana. In January 2018, I started my journey as an independent researcher and lecturer at the same department.

My research goal is to develop novel, low-cost, benign and efficient materials to aid sustainability. Thus for applications in solar cell fabrication and waste conversion (i.e. CO₂ and biomass valorization to fuels). This endeavour will contribute to addressing the issues of climate change, solid waste pollution and energy scarcity which are the current global challenges facing mankind.

I currently teach physical chemistry courses and conduct research in the areas of theoretical chemistry, quantum mechanics, electrochemistry and photoelectrochemistry. I was a Postdoctoral Fellow under the Royal Society-Leverhulme Africa Postdoctoral Fellowship Award Scheme (grant LAF\R1\180013), from 2018 - 2021. I was an awardee of The World Academy of Sciences (TWAS) individual research grant (grant 18-032RG/CHE/AF/AC_I), (from 2018 - 2021). I currently receive additional computing resource support from the Centre for High-Performance Computing (CHPC), South Africa.

As a young academic, I intend to build a vibrant research laboratory, and this requires acquiring more computing infrastructure locally. I am also building human capacity through the mentoring of young scientists, as well as improving my expertise in communication, leadership, networking and collaborative research.