Elliot Sarpong Menkah

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RESEARCH

Interests: Surface Catalysis & High Performance Computing · DFT · Electrochemistry · Molecular Mechanics · Physical Chemistry · HPC · Theoretical Chemistry

Areas: Organic Chemistry · Materials Chemistry · Renewable Energy, Sustainability and the Environment · Catalysis · Atomic and Molecular Physics, and Optics · Computational Theory and Mathematics

RESEARCH SUMMARY

15	75	4	2	0.49	8%
Publications	Citations	h-index	i10-index	Field-weighted impact	World top 10%

Counted from the 15 publications listed below, 2017–2026. Field-weighted impact is the mean over the 13 works scored for it; 1.00 is the world average for works of the same field, type and year. 1 of the 13 papers scored for it are among the world's most cited tenth for their field, type and year.

POSITIONS

Lecturer 2021–present
Chemistry, Kwame Nkrumah University of Science and Technology Department of Chemistry, Kumasi, Ghana

Postdoc 2019–2021
High-Performance Computing Section, National Institute for Mathematical Sciences, Kumasi, Ghana

EDUCATION AND QUALIFICATIONS

Master in High Performance Computing 2016–2018
High Performance Computing, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

PhD Physical Chemistry 2012–2018
Chemistry, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

BSc. Chemistry 2007–2011
Chemisty, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

PUBLICATIONS

Journal articles 13

1. **E Menkah** (2026). Cassava starch-based bioplastics reinforced with organic microparticles: Synthesis and characterization. *Next Materials*. https://www.sciencedirect.com/science/article/pii/S2949822826011202
2. Godfred Boakye Adusei, Albert Aniagyei, **Elliot Menkah**, Caroline R. Kwawu, Gabriel Amankwah, Richmond Arhin, Hawa Osman, Evans Adei (2025). Periselectivity, Chemoselectivity, and Regioselectivity of the Cycloaddition Reaction of Aza-Oxyallyl Cations With Cinnamaldehyde: A Density Functional Theory Study. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.70003

3. Komla Emmanuel Oyetey, Albert Aniagyei, **Elliot S. Menkah**, Caroline R. Kwawu, Collins Obuah, Hawa Osman, Evans Adei (2025). [3 + 2] cycloaddition reactions of C, N-diarylnitrone to arylallene and N-aryl-C-carbamoyl nitrones to methyl buta-2, 3-dienoate. A theoretical study of reactivity, site, and regio-selectivity. *Reaction Kinetics Mechanisms and Catalysis*. https://doi.org/10.1007/s11144-025-03027-3
4. Benjamin G. Akonor, Albert Aniagyei, Caroline R. Kwawu, Gabriel Amankwah, **Elliot S. Menkah**, Evans Adei (2024). A quantum mechanistic investigation into the unusual reactions of nitrilimine and nitrile oxide with 2,3,4,5-tetraphenylcyclopentadienone. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-024-06074-0
5. Muntaka Is-mail, Albert Aniagyei, Caroline R. Kwawu, Gabriel Amankwah, **Elliot Menkah**, Evans Adei (2024). Exploring the specific chemistries of the cycloaddition reactions of 5-benzoyl-3(2H)-isothiazolone and stable nitrile oxides: Insights from Density Functional Theory analysis. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4645
6. Ernest Dumba, Caroline R. Kwawu, Ama Konadu Agyemang, **Elliot Menkah**, Evans Adei (2023). DFT studies of the effect of sulfur impurities on the structural, electronic and magnetic properties of iron (100). *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-022-02945-y
7. Amos Afugu, Caroline R. Kwawu, **Elliot Menkah**, Richard Tia, Evans Adei (2023). Details of CO2 electrochemical reduction reaction (CO2ERR) on Mn–MoS2 monolayer: a DFT study. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-023-03001-z
8. Destiny Konadu, Caroline R. Kwawu, **Elliot S. Menkah**, Richard Tia, Evans Adei, Nora de Leeuw (2023). The catalytic hydrogenolysis of compounds derived from guaiacol on the Cu (111) surface: mechanisms from DFT studies. *Physical Chemistry Chemical Physics*. https://doi.org/10.1039/d2cp04352a
9. Gabriel Amankwah, Caroline R. Kwawu, **Elliot S. Menkah**, Evans Adei (2023). [3 + 2] Cycloaddition reaction of disubstituted-3-benzylidene succinimide with C, N-disubstituted nitrile imines for synthesizing spiro-heterocycles: A computational study. *Computational and Theoretical Chemistry*. https://doi.org/10.1016/j.comptc.2023.114138
10. Caroline R. Kwawu, Albert Aniagyei, Destiny Konadu, Kenneth Limbey, **Elliot Menkah**, Richard Tia, Evans Adei (2022). A DFT study of the oxygen reduction reaction mechanism on be doped graphene. *Chemical Papers*. https://doi.org/10.1007/s11696-022-02201-4
11. Jehoshaphat Oppong Mensah, Gilbert Boadu Ampomah, Edward Ntim Gasu, Abigail Kusiwaa Adomako, **Elliott Sarpong Menkah**, Lawrence Sheringham Borquaye (2022). Allosteric Modulation of the Main Protease (MPro) of SARS-CoV-2 by Casticin—Insights from Molecular Dynamics Simulations. *Chemistry Africa*. https://doi.org/10.1007/s42250-022-00411-7
12. Caroline R. Kwawu, Albert Aniagyei, Destiny Konadu, **Elliot Menkah**, Richard Tia (2022). First-principles DFT insights into the mechanisms of CO2 reduction to CO on Fe (100)-Ni bimetals. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-022-02879-5
13. **Elliot S. Menkah**, Nelson Y. Dzade, Richard Tia, Evans Adei, Nora H. de Leeuw (2019). Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study. *Applied Surface Science*. https://doi.org/10.1016/j.apsusc.2019.02.128

Book chapters 1

1. Amos Afugu, Caroline R. Kwawu, **Elliot Menkah**, Evans Adei (2023). Supported single-atom catalysts in carbon dioxide electrochemical activation and reduction. *Elsevier eBooks*. https://doi.org/10.1016/b978-0-323-99429-3.00010-2

Theses 1

1. **ES Menkah** (2017). Coupling of i-PI and ONETEP codes to enable large/petaScale simulations for first principles modeling of both electrons and nuclei for thousands of atoms. *SISSA*. https://iris.sissa.it/handle/20.500.11767/68046