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RESEARCH

Interests	Computational Materials Chemistry · DFT · TDDFT · Heterogeneous Catalysis · Electrochemistry
Areas	Materials Chemistry · Organic Chemistry · Renewable Energy, Sustainability and the Environment · Catalysis · Electrical and Electronic Engineering · Electronic, Optical and Magnetic Materials

RESEARCH SUMMARY

32	146	6	5	0.26	0%
Publications	Citations	h-index	i10-index	Field-weighted impact	World top 10%

Counted from the 32 publications listed below, 2016–2026. Field-weighted impact is the mean over the 31 works scored for it; 1.00 is the world average for works of the same field, type and year. 0 of the 31 papers scored for it are among the world's most cited tenth for their field, type and year.

PUBLICATIONS

Journal articles 31

1. Di Girolamo, Camilla, Fleming, Patricia C., **Kwawu, Caroline R.**, Guimarães, Amanda R., Muldoon, Jimmy, Bruno-Colmenarez, Julia, Ortin, Yannick, Probert, Michael R., Fantuzzi, Felipe, Palma, Aniello (2026). Cyclo-Proline: Chameleonic All-Peptide Macrocycles with Induced-Fit Host-Guest Recognition. *Kent Academic Repository (University of Kent)*.
2. Camilla Di Girolamo, Patricia C. Fleming, **Caroline R. Kwawu**, Amanda R. Guimarães, Jimmy Muldoon, Julia Bruno-Colmenarez, Yannick Ortin, Michael R. Probert, Felipe Fantuzzi, Aniello Palma (2026). Cyclo-Polyproline: Chameleonic All-Peptide Macrocycles With Induced-Fit Host-Guest Recognition. *Angewandte Chemie International Edition*. https://doi.org/10.1002/anie.8698780
3. Badou Sarr, Ndeye Maty Ndiaye, Ibrahima Ngom, Makha Ndao, **Caroline Rosemyya Kwawu**, Ahmed Subrati, Eduart Gutierrez-Pineda, Sergio E. Moya, Balla Diop Ngom (2026). Developing nanocomposite materials based on zinc cobaltite and activated carbon derived from rice straw extracts for supercapacitor electrode applications. *MRS Advances*. https://doi.org/10.1557/s43580-026-01552-4
4. Papa Alpha Ndiaye, El Hadji Mamour Sakho, Ndeye Maty Ndiaye, Makha Ndao, **Caroline Rosemyya Kwawu**, Ahmed Subrati, Eduart Gutierrez-Pineda, Sergio E. Moya, Balla Diop Ngom (2026). Synthesis and electrochemical performance of MnFe2O4@BC@AC composites from rice straw for supercapacitor application. *MRS Advances*. https://doi.org/10.1557/s43580-026-01633-4
5. Bernard Konadu Amoah, **CR Kwawu**, FD Wireko-Manu (2025). Experimental and Theoretical Investigation of a Naphthyl-Based Saline Compound as a Multi-Anion Chemosensor. *Materials International*. https://materials.international/wp-content/uploads/2025/12/Materials74.040.pdf
6. 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
7. Seynabou Mbodj, El Hadji Mamour Sakho, Makha Ndao, Ndeye Maty Ndiaye, Astou Seck, Ncholu

Manyala, Abdoulaye Djire, Abdou Karim Diallo, **Caroline Rosemyya Kwawu**, Balla Diop Ngom (2025). Size-dependent electrochemical behavior of green synthesized MnCo2O4@g-C3N4/BC nanocomposites for supercapacitor applications. *MRS Advances*. https://doi.org/10.1557/s43580-025-01386-6

8. Mbaye Thiam, El Hadji Mamour Sakho, Makha Ndao, Ndeye Maty Ndiaye, **Caroline Rosemyya Kwawu**, Ahmed Subrati, Eduart Gutierrez-Pineda, Sergio E. Moya, Balla Diop Ngom (2025). Upcycling peanut shells into high-performance MgFe2O4–carbon nanocomposites for sustainable supercapacitors. *MRS Advances*. https://doi.org/10.1557/s43580-025-01442-1
9. 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
10. Emmanuel Komla Oyetey, **Caroline R. Kwawu**, Albert Aniagyei, Gabriel Amankwah, Richmond Arhin, Evans Adei (2024). A computational study into the mechanism and selectivities of the reaction of 1, 1-diaryl-2-isopropylidene-3-methylenecyclopropane (DIMCP) with C, N-diarylnitrone. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-024-03121-0
11. 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
12. Maame Tabitha Kuukua Osiban-Fordjour, **Caroline Rosemyya Kwawu**, Marian Asantewah Nkansah (2024). Evaluating metal levels and potential health risks of nail polish brands on the Ghanaian market. *International Journal of Environmental Health Research*. https://doi.org/10.1080/09603123.2024.2410457
13. 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
14. Gabriel Amankwah, Isaac Ofori, Joshua Atta-Kumi, **Caroline R. Kwawu**, Richard Tia, Evans Adei (2023). A quantum mechanistic insight into the chemo- and regio-selective [3 + 2]-cycloaddition reaction of aryl hetaryl thioketones with diazoalkanes and nitrile oxide derivatives. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2023.108418
15. **Caroline R. Kwawu**, Destiny Konadu, Paul Boamah, Kassim Fuwad Mohammed, Isaac Danso Boateng, Evans Adei (2023). Catalytic degradation and reforming pathways of guaiacol (lignin monomer) on Ru and Ni modified Cu (111). *MRS Advances*. https://doi.org/10.1557/s43580-023-00579-1
16. 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
17. 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
18. 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
19. 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
20. **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
21. **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

22. **Caroline Rosemyya Kwawu**, Albert Aniagyei (2021). A review on the computational studies of the reaction mechanisms of CO2 conversion on pure and bimetals of late 3d metals. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-021-04811-3
23. Destiny Konadu, **Caroline Rosemyya Kwawu**, Richard Tia, Evans Adei, Nora Henriette de Leeuw (2021). Mechanism of Guaiacol Hydrodeoxygenation on Cu (111): Insights from Density Functional Theory Studies. *Catalysts*. https://doi.org/10.3390/catal11040523
24. **Caroline R. Kwawu**, Albert Aniagyei, Destiny Konadu, Boniface Yeboah Antwi (2021). Mechanisms of CO2 reduction into CO and formic acid on Fe (100): a DFT study. *Materials for Renewable and Sustainable Energy*. https://doi.org/10.1007/s40243-021-00194-w
25. Albert Aniagyei, **Caroline Kwawu**, Ralph Kwakye, Boniface Yeboah Antwi, Jonathan Osei-Owusu (2021). Oxygen (O2) reduction reaction on Ba-doped LaMnO3 cathodes in solid oxide fuel cells: a density functional theory study. *Materials for Renewable and Sustainable Energy*. https://doi.org/10.1007/s40243-021-00200-1
26. A. B. Yeboah, J. K. Adu-Ntim, J. Koranteng, T. A. Tagbor, A. Aniagyei, **C. Kwawu** (2021). Perceptions of workers on the benefits of institutional source sorting: A case of the Council for Scientific and Industrial Research - Institute of Industrial Research (CSIR-IIR), Accra, Ghana. *Ghana Journal of Science*. https://doi.org/10.4314/gjs.v62i1.5
27. **Caroline R. Kwawu**, Albert Aniagyei, Richard Tia, Evans Adei (2020). A DFT investigation of the mechanisms of CO2 and CO methanation on Fe (111). *Materials for Renewable and Sustainable Energy*. https://doi.org/10.1007/s40243-020-0164-x
28. Albert Aniagyei, **Caroline Kwawu**, Jerry Joe E. K. Harrison, Ralph Kwakye (2020). Mechanisms of ethyne oxidation catalyzed by LMnO3 (L = O−, Cl, NPH3, CH3, and Cp): a density functional theory study. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-020-04569-0
29. Albert Aniagyei, **Caroline Kwawu**, Richard Tia, Evans Adei (2020). Permanganyl chloride-mediated oxidation of tetramethylethylene: A density functional theory study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2020.107616
30. **Caroline R. Kwawu**, Richard Tia, Evans Adei, Nelson Y. Dzade, C. Richard A. Catlow, Nora H. de Leeuw (2017). CO 2 activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. *Physical Chemistry Chemical Physics*. https://doi.org/10.1039/c7cp03466k
31. **Caroline R. Kwawu**, Richard Tia, Evans Adei, Nelson Y. Dzade, C. Richard A. Catlow, Nora H. de Leeuw (2016). Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study. *Applied Surface Science*. https://doi.org/10.1016/j.apsusc.2016.12.187

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