



Nelson Yaw Dzade

Assistant Professor of Energy and Mineral Engineering

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PERSONAL PROFILE

Dr Nelson Dzade is a passionate educator and an interdisciplinary research scientist. He leads the Materials and Minerals Theory Group, which specializes in developing and applying advanced theoretical methods to unravel structure-property-performance relationships in solid-state materials. Often taking place in close collaboration with experiments, Dzade's current research emphasizes the development and use of ab initio methods to understand (i) complex catalytic reaction mechanisms at surfaces, (ii) unravel complex interface structures in heterojunction materials. An important context for his research has been renewable energy (solar cells, batteries, and electro(photo)catalysts), where novel materials, sulfides, oxides, perovskites, organics, and interfaces feature prominently. Dr. Dzade is a skilled writer and an effective communicator with an interactive teaching style that promotes effective participation and enthusiasm while facilitating learning. He is highly organized and can effectively prioritize and coordinate multiple tasks to accomplish projects creatively and enthusiastically.

EDUCATION AND TRAINING

2010–2014	Ph.D. Computational Materials Science (Date Awarded: October 28 th , 2014) University College London (UCL), London, United Kingdom
2009–2010	Postgraduate Diploma (PGDip) Materials Science (Date Awarded: May 21 st , 2010) Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India
2008–2009	MSc Materials Science (Distinction) (Date Awarded: December 19 th , 2010) African University of Science and Technology, Abuja, Nigeria
2003–2007	BSc Mathematical Science (Statistics option) 1st Class Honors (Awarded: July 31 st , 2007) University for Development Studies, Tamale, Ghana

RESEARCH AND PROFESSIONAL EXPERIENCE

2025-present	Co-Chair (Organizing Committee) of the Critical Minerals and Materials Session The 2026 U.S.-Africa Frontiers program of the National Academies of Sciences, Engineering, and Medicine (NASEM).
2024-Present	Chair of the Undergraduate Energy Engineering Program John and Willie Leone Family Department of Energy and Mineral Engineering The Pennsylvania State University (PSU), USA
2024-Present	Co-Director of Alliance for Education, Science, Engineering, and Design with Africa (AESEDA) , College of Earth & Mineral Sciences, The Pennsylvania State University, USA
2021-Present	Assistant Professor of Energy and Mineral Engineering John and Willie Leone Family Department of Energy and Mineral Engineering The Pennsylvania State University, USA

2022-Present	Exploitation Advisory Board Member For the European Innovation Council (EIC) Pathfinder SOLARUP project “Advanced Strategies for Development of Sustainable Semiconductors for Scalable Solar Cell Applications - SOLARUP”.
2022-Present	Advisory Board Member Centre for Climate Change Adaptation and Mitigation Studies (C3AMS), African University of Science and Technology (AUST), Abuja, Nigeria.
2018 – 2021	EPSRC (Engineering & Physical Sciences Research Council) Innovation Fellow and Independent Group Leader School of Chemistry, Cardiff University, UK.
2018-Present	Visiting Professor of Materials Science and Engineering African University of Science and Technology (AUST), Abuja-FCT, Nigeria
2014-2017	Postdoctoral Training in Materials Design and Heterogeneous Catalysis) Utrecht University, The Netherlands
2015 – 2022	Co-investigator/Trainer on Chem4Energy Africa Research Consortium “New Materials for a Sustainable Energy Future” is funded by the UK Department for International Development to strengthen research and training capacity in Kwame Nkrumah University of Science and Technology (KNUST), Ghana, and the University of Namibia and the University of Botswana.
2012-2013	Research Associate, British Petroleum (BP), UK University College London, Research project: “Computer Simulations of the Effect of Fuel Additives on Metal Oxide Surfaces”, an important problem in chemical fouling of fuel pipelines in car engines.

AWARDS, SCHOLARSHIPS & RECONGNITIONS

2025	U.S.-Africa Frontiers Fellowship Award Awarded by the National Academies of Sciences, Engineering, and Medicine to build high-impact research collaboration and strengthen capacity building with two African scientists.
2025	G. Montgomery and Marion Mitchell Award for Innovative Teaching This award is given in recognition of Penn State College of Earth and Mineral Sciences faculty who use innovative teaching techniques in their courses.
2024	DOE Early Career Research Awards, Penn State, USA Awarded by the Department of Energy. This five-year prestigious award is given to the nation's outstanding early-career research scientists who are helping to tackle the toughest challenges that will secure the economic competitiveness of the United States.
2020–2021	DUO-India Professor Fellowship Award, Cardiff University, UK DUO-India Fellowship Programme, which funds the exchange of professors between India and European countries.
2018–2021	EPSRC Innovation Research Fellowship Award, Cardiff University, UK Awarded by UK Research and Innovation to innovative individuals in the early stages of their research career, whose research can help to achieve the aims of the UK’s Industrial Strategy.
2010–2014	Overseas Research Scholarship University College London, UK. Awarded to exceptional international students with strong academic achievements.
2010–2014	Faculty of Mathematical and Physical Sciences Studentship University College London, UK. Awarded to doctoral students who demonstrate outstanding scholarship and evidence of community service.

2008–2009	World Bank Scholarship African University of Science and Technology, Nigeria. Awarded to postgraduate students who demonstrate strong academic achievements and a commitment to their home country's development.
2009–2010	Department of Science and Technology (DST), Government of India scholarship International Centre for Material Science (ICMS), Bangalore, India.
2006–2007	Ghana Education Trust Fund (GETFund) Scholarship University for Development Studies, Ghana. Awarded to brilliant but needy students.
Dec. 19, 2009	Gold Medallist, best graduating MSc. Materials Science student African University of Science and Technology, Abuja, Nigeria
Dec. 15, 2007	Overall best-graduating student and valedictorian (2006/20017) University for Development Studies, Tamale, Ghana.

RESEARCH GRANTS & FUNDING

- **Co-PI (50%):** U.S.-Africa Frontiers Fellowships “*Advancing Novel Energy Materials through a Synergistic Computational-Experimental Modelling and Simulation Approach*”. **Investigator(s):** Nelson Y. Dzade, Linda Nyamen, and Lahoucine Atourki. **Sponsor:** National Academies of Sciences, Engineering, and Medicine. **Amount:** \$10,000; **Date Awarded:** 04/21/2025; **Start Date:** 05/01/2025; **End Date:** 12/31/2025.
- **PI (80% credit):** “*Rational Design of Ecofriendly Collectors for Efficient and Selective Flotation of Critical Minerals*”. **Investigator(s):** Nelson Y. Dzade, Adri van Duin, Olumide Ogunmodimu. **Sponsor:** Materials Research Institute (MRI) 2025 Interdisciplinary Seed Grants and Transdisciplinary Teaming Initiative awards. **Amount:** \$50,000; **Date Awarded:** 03/17/2025; **Start Date:** 04/01/2025; **End Date:** 06/30/2026.
- **PI (100% credit):** “*Multiscale Modeling of Heteroepitaxial Interfaces for Scalable Thin-Film Solar Cell Applications*”. **Investigator(s):** Nelson Y. Dzade. **Sponsor:** Department of Energy (DOE) Early Career Research Awards. **Amount:** \$875,000. **Start Date:** 07/01/2024; **End Date:** 07/31/2029.
- **Co-PI (30%):** “*Quantitative Study on the Search for Sulfur-bearing Molecular Ice Signatures*”. **Investigators:** Nelson Y. Dzade, Danna N. Qasim. **Sponsor:** The Space Telescope Science Institute, STScI. **Reference No:** JWST-AR-04810.015-A, **Amount:** \$55,325, **Start Date:** 08/01/2024, **End Date:** 07/31/2026.
- **PI (80% credit):** “*Rational Design of Bio-inspired and Earth-abundant Catalysts for Carbon Dioxide Reduction into Fuels and Fine Chemicals*”. **Investigator(s):** Nelson Y. Dzade and Ismaila Dabo. **Sponsor:** Penn State Institutes of Energy and the Environment – IEE ICDS Seed Grant Program. **Amount:** \$15,000. **Date Awarded:** 03/02/2023; **Start Date:** 05/01/2023, **End Date:** 12/31/2024.
- **PI (80% credit):** “*Toward the Rational Design of Chalcogenide Perovskites Heterojunction Photovoltaics*”. **Investigator(s):** Nelson Y. Dzade, Ismaila Dabo, Adri van Dui. **Sponsor:** Penn State Institute for Computational and Data Sciences (ICDS) Seed Grant. **Amount:** \$50,000. **Date Awarded:** 03/30/2022; **Start Date:** 5/1/2022; **End Date:** 12/30/2023.
- **Co-PI:** “*Addressing the Energy Transition Puzzle Through Combined Experimental and Computational Efforts*”. **Investigators:** Nutifafa Y. Doumon, Nelson Y. Dzade, Olumide Ogunmodimu, Thandazile Moyo, and Ivy Asuo. **Sponsor:** Penn State Inter-Institutional Partnerships for Diversifying Research (IPDR) Funded by the Institutes of Energy and the Environment. **Amount:** \$30,000. **Date Awarded:** 03/30/2022; **Start Date:** 09/01/2023; **End Date:** 08/31/2024.
- **Co-PI (20% credit):** “*SOLARUP -Advanced Strategies for Development of Sustainable Semiconductors for Scalable Solar Cell Applications*”. **Sponsor:** European Innovation Council (EIC) Pathfinder Grant. **Amount:** €2,450,878 (\$2,682,657.53). **Start Date:** 10/01/2022; **End Date:** 09/31/2026.
- **PI (50% credit):** DUO-India Professor Fellowship Award “*Rationally Design of Novel ABO₃ Compounds and their Nano-Hetero-Architectures for Catalytic PEC Water Splitting Applications*”. **Investigators:** Nelson Yaw Dzade and Rupesh Devan. **Sponsor:** DUO-India Fellowship Programme. **Amount:** £6,000 (\$7,846.50). **Start Date:** 01/15/2020; **End Date:** 01/14/2021.

- **PI (100% credit):** “Computer-Aided Design of Zinc Phosphide Heterojunctions for Efficient Solar Energy Conversion”. **Reference Number:** EP/S001395/1. **Investigator:** Nelson Yaw Dzade. **Sponsor:** UK Engineering and Physical Sciences Research Council (EPSRC) Innovation Research Fellowship Grant. **Amount:** £525,254 (\$686,900.92); **Start Date:** 06/29/2018; **End Date:** 09/14/2021.
- **Co-PI (25% credit):** “Earth-abundant materials for the sustainable catalysis of CO₂ to fuels and chemicals: Linking computation to experiment”. **Investigators:** Nora de Leeuw, Nelson Y. Dzade, Mariette Wolthers, Helen E. King. **Sponsor:** Netherlands Organization for Scientific Research ECHO grant. **Amount:** €250,000 (\$280,637.50); **Funded Period** Dec 2018 - Dec 2021.
- **Co-PI (25% credit):** “International Innovation Project on the Computer-aided High Throughput Development and Upscaling of Tailored Zeolites as Wastewater Filters in Ghana”. **Reference Number:** NE/R009376/1. **Investigators:** Nora de Leeuw, Alexander O'Malley, and Nelson Yaw Dzade. **Sponsor:** The Natural Environment Research Council (NERC) Research. **Amount:** £107,175 (\$140,158.11); **Start Date:** 11/01/2017; **End Date:** 04/30/2020.

LIST OF PEER-REVIEWED PUBLICATIONS (*Corresponding Author)

Citation: 3869, **h-index** =38, and **i10-index**=93, Google Scholar, Date May 28, 2025.

Publications at Penn State

1. Patrick M. Bacirhonde, Devendra Shrestha, Kyoungin Kang, Esensil M. Hia, Nikhil Komalla (**Graduate Student**), **Nelson Y. Dzade***, Merve Buldu-Akturk, Michelle P. Browne, Milan Babu Poudel, Dong J. Yoo, Eun-Suk Jeong, Ahmed Y. Mohamed, Byoung G. Han, Deok-Yong Cho, Matthew T. Curnan, Geun H. Gu, Jeong W. Han, Chan H. Park* “Understanding the Metal-Center Mediated Adsorption and Redox Mechanisms in a FeMn(NbTa)₂O₆ Columbite Material for Anion Exchange Membrane Water Electrolyzers”. *Advanced Energy Materials* (2025) 2404479. [DOI](#)
2. **Henry I. Eya** (**Graduate Student**), and **Nelson Y. Dzade***. “First-Principles Investigation of Oxygen and Water Adsorption on (010), (100), and (111) Surfaces of BaZrS₃ Chalcogenide Perovskite”. *J. Phys. Chem. C* (2024), 128, 18409–18421. [DOI](#)
3. Ganesh K. Rahane, Balpartap Singh, Anurag Roy, Nilesh G. Saykar, Animesh Mandal, Dikshant Afria, Yogesh A. Jadhav, Sawanta S. Mali, **Nelson Y. Dzade***, Sachin R. Rondiya. “Tailoring Interface via Tuning the Phase and Morphology of TiO₂ for Efficient Mesoporous Perovskite Solar Cells”. *Langmuir* 2024, 40, 22526–22539. [DOI](#)
4. Ricardo Amaral (**Graduate Student**), and **Nelson Y. Dzade***. “DFT Insights into the Adsorption Mechanisms of Lithium Polysulfides on Ni₂P (0001) Surface for Lithium-Sulfur Batteries”. *Applied Surface Science* (2024), 659, 159847. [DOI](#)
5. Y. A. Jadhav, G. K. Rahane, T. Goswami, K. Jagadish, K. Chordiya, A. Roy, T. Debnath, S. B. Jathar, R. Devan, M. U. Kahaly, S. R. Rondiya, H. N. Ghosh, and **N. Y. Dzade***. “Novel Au/Cu₂NiSnS₄ Nano-Heterostructure: Synthesis, Structure, Heterojunction Band Offset and Alignment, and Interfacial Charge Transfer Dynamics”. *ACS Appl. Mater. Interfaces* (2024), 16, 21746–21756. [DOI](#)
6. T. L. L. Doan, D. C. Nguyen, N. Komalla (**Graduate Student**), N. V. Hieu, L. Nguyen-Dinh, **N. Y. Dzade**, C. S. Kim, C. H. Park. “Molybdenum oxide/nickel molybdenum oxide heterostructures hybridized active platinum co-catalyst toward superb-efficiency water splitting catalysis”. *Journal of Colloid and Interface Science* (2024), 670, 12–27. [DOI](#)
7. O. F. Awe (**Graduate Student**), H. I. Eya (**Graduate Student**), R. Amaral (**Graduate Student**), N. Komalla (**Graduate Student**), P. Nbelayim, and **N. Y. Dzade***. “Unraveling the origin of the high photocatalytic properties of earth-abundant TiO₂/FeS₂ heterojunctions: insights from first-principles density functional theory” *Phys. Chem. Chem. Phys.*, (2024) 26, 12869–12879. [DOI](#)
8. Marietjie J. Ungerer, Evans Adei, Theopolina Amakali, Cecil H. Botchway, Likius S. Daniel, James Darkwa, **Nelson Y. Dzade**, Foster Mbaiwa, Mary Mensah, Maipelo Nyepetsi, Banothile Makhubela, Claire E. Mitchell, Oluwasegun Emmanuel Olaoye, Olayinka A. Oyetunji, Meenakshisundaram Sankar, Fortunate P. Sejie, Jacobina Sheehama, Richard Tia, Veikko Uahengo, Aleksandar Živković and Nora H. De Leeuw. “Chem4Energy: a consortium of the Royal Society Africa Capacity-Building Initiative”. *Interface Focus* (2024), 14 (4), 20240001. [DOI](#).

9. S. N. Rahane, G. K. Rahane, A. Mandal, Y. Jadhav, A. Godha, A. Rokade, S. Shah, Y. Hase, A. Waghmare, N. G. Saykar, A. Roy, K. N. Salgaonkar, D. Dubal, S. K. Makineni, **N. Y. Dzade***, S. R. Jadkar*, and S. R. Rondiya*. "Lead-Free $\text{Cs}_2\text{AgBiCl}_6$ Double Perovskite: Experimental and Theoretical Insights into the Self-Trapping for Optoelectronic Applications". *ACS Phys. Chem Au* (2024), [DOI](#)
10. A. Eskanolou, B. J. Arnold, Y. Foucaud, M. Badawi, and **N. Y. Dzade**. "Optimizing flotation separation of fluorapatite from Florida waste clay using a multiscale approach" *Applied Surface Science* (2024) 662 16006. [DOI](#)
11. A. Rokade, G. K. Rahane, A. Živković, S. N. Rahane, H. S. Tarkas, K. Hareesh, N. H. de Leeuw, S. D. Sartale, **N. Y. Dzade**, S. R. Jadkar, and S. R. Rondiya. "Fabrication of ZnO Scaffolded CdS Nanostructured Photoanodes with Enhanced Photoelectrochemical Water Splitting Activity under Visible Light". *Langmuir* (2024), 40, 13, 6884. [DOI](#)
12. Amaral, R. (**Graduate Student**), and **Dzade, N.Y.*** "Mechanistic insights into the adsorption and dissociation of nitrogen oxides on nickel phosphide (Ni_2P) catalysts." *Materials Today Comm.* (2024) 38, 107824. [DOI](#)
13. Patil, J.V., Mali, S.S., Rondiya, S.R., **Dzade, N.Y.**, Hong, C.K. "Bilayered graded phase homojunction $\text{FA}_{0.15}\text{MA}_{0.85}\text{PbI}_3$ -based organic-inorganic hybrid perovskite solar cells crossing 22 % efficiency." *Progress in Solid State Chemistry* (2024). [DOI](#)
14. Barma, S.V., Jathar, S.B., Huang, Y.-T., Jadhav, Y.A., Rahane, G.K., Rokade, A.V., Nasane, M.P., Rahane, S.N., Cross, R.W., Suryawanshi, M.P., Jo, S.B., Hoyer, R.L.Z., Jadkar, S.R., **Dzade, N.Y.***, Rondiya, S.R.* "Synthesis and Interface Engineering in Heterojunctions of Tin-Selenide-Based Nanostructures for Photoelectrochemical Water Splitting" *ACS Appl. Nano Mater.* (2024), 7, 1986–1999. [DOI](#)
15. Offia-Kalu, N.E., Nwanonyi, S.C., Abdulhakeem, B., **Dzade, N.Y.**, Onwalu, P.A. "Theoretical investigation of electronic, energetic, and mechanical properties of polyvinyl alcohol/cellulose composite hydrogel electrolyte." *J. Mol. Graph. Model.* (2024) 127, 108667. [DOI](#)
16. Eya, H.I. (**Graduate Student**) and **Dzade, N.Y.*** "Density Functional Theory Insights into the Structural, Electronic, Optical, Surface and Band Alignment Properties of BaZrS_3 Chalcogenide Perovskite for Photovoltaics". *ACS Appl. Energy Mater.* (2023), 6, 5729–5738. [DOI](#)
17. T.L.L. Doan, D.C. Nguyen, K. Kang, A. Ponnusamy, H.I. Eya (**Graduate Student**), **N.Y. Dzade***, C.S. Kim, C.H. Park*. "Heterojunction of Semi-conductive MoS_2 Nanoparticles/Metallic CoS_2 Nanotubes as an Efficient Multifunctional Catalyst for Urea-Water Electrolysis". *Applied Catalysis B: Environmental*, (2023), 123295. [DOI](#)
18. S.R. Rondiya, S.S. Mali, A. Roy, G.K. Inwati, G.K. Rahane, Y.A. Jadhav, S. Suresh, T. Debnath, C.K. Hong, **N.Y. Dzade***. "Interfacial Band Offset Engineering with Barium-doping Towards Enhanced Performance of All-Inorganic CsPbI_2Br Perovskite Solar Cells". *Phys. Chem. Chem. Phys.*, (2023), 25, 29050-29060. [DOI](#)
19. S. S. Mali, J. V. Patil, J.-Y. Shao, Y.-W. Zhong, S. R. Rondiya, **N. Y. Dzade**, and C. K. Hong, "Phase-heterojunction all-inorganic perovskite solar cells surpassing 21.5% efficiency". *Nature Energy* (2023) 1-13. [DOI](#)
20. P.M. Bacirhonde, A.Y. Mohamed, B. Han, D.-Y. Cho, S. Devendra, J.-W. Choi, C.-R. Lim, E.O. Afranie, K.-H. Baik, K. Kang, S. Lee, E.-S. Jeong, N. Komalla (**Graduate Student**), **N. Y. Dzade**, C.H. Park, C.S. Kim "Ruthenium Engineered $\text{A}_2\text{B}_2\text{O}_6$ -Hybrid Columbite Ferrite for Bifunctional pH-Universal Water Splitting", *Advanced Energy Materials*, 2023, 2300174. [DOI](#)
21. Narasimharao Kitchamsetti, Manopriya Samtham, Diwaka Singh, Ekta Choudhary, Sachin R. Rondiya, Yuan-Ron Ma, Russell W. Cross (**Graduate Student**), **Nelson Y. Dzade**, Rupesh S. Devan. "Hierarchical 2D MnO_2 @1D mesoporous NiTiO_3 core-shell hybrid structures for high-performance supercapattery electrodes: Theoretical and experimental investigations". *Journal of Electroanalytical Chemistry* (2023) 936,11735. [DOI](#)
22. Rohini Udavant, Sachin Thawarkar, Sachin Rondiya, Ankita Shelke, Rahul Aher, Thalasseril G. Ajithkumar, Russell W. Cross (**Graduate Student**), **Nelson Y. Dzade**, Sandesh Jadkar. "Lead-Free Solid State Mechanochemical Synthesis of $\text{Cs}_2\text{NaBi}_{1-x}\text{Fe}_x\text{Cl}_6$ Double Perovskite: Reduces Band Gap and Enhances Optical Properties". *Inorg. Chem.* (2023), 62, 4861–4871. [DOI](#)
23. Mustapha Shehu, Tolani T. Oladipo, Farouk U. Baffa, Tahir Abdullahi, Chibuike K. Ugwu, Amina M. Tanimu, Jide Adegboyega, Gideon K. Korir, Isyaku A. Odoguje, and **Nelson Y. Dzade***, "First-principles insights into sulfur oxides (SO_2 and SO_3) adsorption and dissociation on layered iron sulfide (FeS) catalyst". *Materials Today Communications* (2023), 34, 105452. [DOI](#)

24. H.J. Yashwanth, Sachin R. Rondiya, Henry I. Eya (**Graduate Student**), **Nelson Y. Dzade**, Deodatta M. Phase, Sanjay D. Dhole, K. Hareesh. "Synergy between nitrogen, phosphorus co-doped carbon quantum dots and ZnO nanorods for enhanced hydrogen production". *Journal of Alloys and Compounds*, (2023), 937, 168397. [DOI](#).
25. Sejie, F.P., Oyetunji, O.A., Darkwa, J., Beas, I.N., Makhubela, B.C.E., **Dzade, N.Y.**, de Leeuw, N.H. "The Transfer Hydrogenation of Cinnamaldehyde Using Homogeneous Cobalt(II) and Nickel(II) (E)-1-(Pyridin-2-yl)-N-(3-(triethoxysilyl)propyl)methanimine and the Complexes Anchored on Fe₃O₄ Support as Pre-Catalysts: An Experimental and In Silico Approach". *Molecules* (2023), 28, 659. [DOI](#).
26. Kigozi, M. (**Graduate Student**), Koech, R. K., Orisekeh, K., Kali, R., Kamoga, O. L., and **Dzade, N. Y.** "Porous carbon derived from Zea mays cobs as excellent electrodes for supercapacitor applications". *Open Journal of Analytical and Bioanalytical Chemistry* 2023, 7(1), 10. [DOI](#).
27. Bidhan Pandit, Sachin R. Rondiya, Shoyebmohamad F. Shaikh, Mohd Ubaidullah, Ricardo Amaral (**Graduate Student**), **Nelson Y. Dzade**, Emad S. Goda, Abu H. S. Rana, Harjot Singh Gill, Tokeer Ahmad. "Regulated electrochemical performance of manganese oxide cathode for potassium-ion batteries: A combined experimental and first-principles density functional theory (DFT) investigation". *Journal of Colloid and Interface Science*, (2023), 633 886–896. [DOI](#).
28. Patrick M. Bacirhonde, **Nelson Y. Dzade**, Henry I. Eya (**Graduate Student**), Cheol Sang Kim, and Chan Hee Park. "A Potential Peanut Shell Feedstock Pyrolyzed Biochar and Iron-Modified Peanut Shell Biochars for Heavy Metal Fixation in Acid Mine Drainage". *ACS Earth Space Chem.* (2022), 6, 11, 2651–2665. [DOI](#).
29. Dario Campisi, Thanja Lamberts, **Nelson Y. Dzade**, Rocco Martinazzo, Inge Loes ten Kate, and Alexander G. G. M. Tielens. "Adsorption of Polycyclic Aromatic Hydrocarbons and C60 onto Forsterite: C–H Bond Activation by the Schottky Vacancy". *ACS Earth Space Chem.* (2022), 6, 2009–2023, [DOI](#).
30. H. J. Yashwanth, Sachin R. Rondiya (**Postdoc**), **Nelson Y. Dzade**, Robert L. Z. Hoye, Ram J. Choudhary, Deodatta M. Phase, Sanjay D. Dhole; K. Hareesh "Improved photocatalytic activity of TiO₂ nanoparticles through nitrogen and phosphorus co-doped carbon quantum dots: an experimental and theoretical study". *Phys. Chem. Chem. Phys.*, (2022), 24, 15271–15279, [DOI](#). Editor's Choice 2022 PCCP HOT Articles
31. Kumar, S.A.; Jarvin, M.; Inbanathan, S.S.R.; Umar, A.; Lalla, N.P.; **Dzade, N.Y.**; Algadi, H.; Rahman, Q.I.; Baskoutas, S. "Facile Green Synthesis of Magnesium Oxide Nanoparticles using Tea (Camellia sinensis) Extract for Efficient Photocatalytic Degradation of Methylene Blue Dye". *Environmental Technology & Innovation* (2022), 28, 102746, [DOI](#).
32. Amakali, T., Živković, A., Warwick, M. E., Jones, D. R., Dunnill, C. W., Daniel, L. S., Uahengo, V., Mitchell, C. E., **Dzade, N. Y.**, and de Leeuw, N. H. "Photocatalytic degradation of rhodamine B dye and hydrogen evolution by hydrothermally synthesized NaBH₄-spiked ZnS nanostructures". *Frontiers in Chemistry* (2022), 10, 835832. [DOI](#).
33. Sawanta S. Mali, Jyoti V. Patil, Sachin R. Rondiya (**Postdoc**), **Nelson Y. Dzade**, Mohammad Khaja Nazeeruddin, Pramod S. Patil, Chang Kook Hong. "Terbium-Doped and Dual-Passivated γ -CsPb(I_{1-x}Br_x)₃ Inorganic Perovskite Solar Cells with Improved Air Thermal Stability and High Efficiency". *Advanced Materials* (2022), 2203204, 1-12, [DOI](#).
34. Thi Luu Luyen Doan, Dinh Chuong Nguyen, Patrick M. Bacirhonde, Ahmed S. Yasin, Abdelrahman I. Rezk, **Nelson Y. Dzade**, Cheol Sang Kim, Chan Hee Park. "Atomic Dispersion of Rh on Interconnected Mo₂C Nanosheet Network Intimately Embedded in 3D Ni_xMoO_y Nanorod Arrays for pH-Universal Hydrogen Evolution". *Energy & Environmental Materials*, (2022), 0,1–15. [DOI](#).
35. Patrick M. Bacirhonde, **Nelson Y. Dzade***, Carmen Chalony, Jeessoo Park, Emmanuel O. Afranie, Sunny Lee, Do-Hwan Kim, Chan Hee Park*, Cheol Sang Kim*. "Reduction of Transition-Metal Columbite-Tantalite as a Highly Efficient Electrocatalyst for Water Splitting". *ACS Appl. Mater. Interfaces* (2022), 14, 13, 15090–15102, [DOI](#).
36. Bidhan Pandit; Sachin R. Rondiya; Russell W. Cross (**Graduate Student**); **Nelson Y. Dzade**, Babasaheb R. Sankapal. "Vanadium Telluride Nanoparticles on MWCNTs Prepared by Successive Ionic Layer Adsorption and Reaction for Solid-state Supercapacitor". *Chemical Engineering Journal* 429 (2022) 132505, [DOI](#).
37. Barbara Farkaš, Aleksandar Živković, Veikko Uahengo, **Nelson Y. Dzade*** and Nora H. de Leeuw. "First-Principles DFT Insights into the Stabilization of Zinc Diphosphide (ZnP₂) Nanocrystals via Surface Functionalization by 4-Aminothiophenol for Photovoltaic Applications". *ACS Appl. Energy Mater.* (2022), 5, 2, 2318–2328, [DOI](#).

38. Deepak Parmar, Cecil H. Botchway (**Graduate Student**), **Nelson Y. Dzade**, Kavitha Kumari, Sanjeev Maken, Manju Rani, Naveen Kumar. "Volumetric, Acoustic and IR Properties of Binary Mixtures (1, 2-Diaminopropane + methyl-, ethyl-, n-propyl- and n-butyl acetates: A Combined Experimental and First-principles Investigation". *Journal of Molecular Liquids* (2022), 347, 118279, [DOI](#).

Publications Prior to Penn State

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113. Boateng, I. W.; Tia, R.; Adei, E.; **Dzade, N. Y.***; Catlow, C. R. A.; and de Leeuw, N. H. "A DFT+U Investigation of Hydrogen Adsorption on the $LaFeO_3(010)$ Surface". *Phys. Chem. Chem. Phys.* (2017), 19, 7399-7409, [DOI](#).
114. Kwawu, C. R.; Tia, R.; Adei, E.; **Dzade, N. Y.***; Catlow, C. R. A.; and de Leeuw, N. H. "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* (2017), 400 293–303, [DOI](#).
115. Wu, L.; **Dzade, N. Y.**; Gao, L.; Scanlon, D. O.; Öztürk, Z.; Hollingsworth, N.; Weckhuysen, B. M.; Hensen, E. J. M.; de Leeuw, N. H.; and Hofmann, J. P. "Enhanced Photoresponse of FeS₂ Films - The Role of Marcasite–Pyrite Phase Junctions". *Advanced Materials* (2016), 28, 9602–9607, [DOI](#). **Featured as Outside Back Cover, Photoelectrochemistry: Advanced Materials, Issue 28, 2016**
 116. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "Surface and Shape Modification of Mackinawite (FeS) Nanocrystals by Cysteine Adsorption - A first-Principles DFT-D2 Study". *Phys. Chem. Chem. Phys.* (2016), 18, 32007–32020, [DOI](#). **Featured as Outside Front Cover: PCCP, Issue 47, 2016.**
 117. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "DFT-D2 study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS)". *J. Phys. Chem. C* (2016), 120, 21441–21450, [DOI](#).
 118. Awuah, J. B.; **Dzade, N. Y.***; Tia, R.; Adei, E.; Kwakye-Awuah, B.; Catlow, C. R. A.; de Leeuw, N. H. "A Density Functional Theory Study of Arsenic Immobilization by the Al(III)-Modified Zeolite Clinoptilolite". *Phys. Chem. Chem. Phys.* (2016), 18, 11297–11305, [DOI](#).
 119. **Dzade, N. Y.***; Roldan, A.; and de Leeuw*, N. H. "DFT-D2 Simulations of Water Adsorption and Dissociation on the Low-Index Surfaces of Mackinawite (FeS)". *J. Chem. Phys.* (2016), 144, 174704, [DOI](#).
 120. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "Activation and Dissociation of CO₂ on the (001), (011), and (111) Surfaces of Mackinawite (FeS): A Dispersion-Corrected DFT Study". *J. Chem. Phys.* (2015), 143, 094703, [DOI](#).
 121. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "A density functional theory study of the adsorption of benzene on hematite (α -Fe₂O₃) surfaces." *Journal of Minerals*, (2014), 4, 89–115, [DOI](#).
 122. **Dzade, N. Y.**; Roldan, A.; and de Leeuw, N. H. "The Surface Chemistry of NO_x on Mackinawite (FeS) Surfaces: A DFT-D2 Study". *Phys. Chem. Chem. Phys.* (2014) 16, 15444–15456, [DOI](#).
 123. Tafreshi, S. S.; Roldan, A.; **Dzade, N. Y.**; and de Leeuw, N. H. "Adsorption of Hydrazine on the Perfect and Defective Copper (111) Surface: A Dispersion-Corrected DFT Study". *Surface Science* (2013), 622, 1–8, [DOI](#).
 124. **Dzade, N. Y.**; Roldan, A.; and de Leeuw, N. H. "Adsorption of methylamine on mackinawite (FeS): a density functional theory study" *J. Chem. Phys.* (2013), 139, 124708, [DOI](#).
 125. **Dzade, N. Y.**; Obodo, K. O.; Adjokatse, S. K.; Ashu, A. C.; Amankwah, E.; Atiso, C. D.; Bello, A. A.; Igumbor, E.; Nzabarinda, S. B.; Obodo, J. T.; Ogbuu, A. O.; Femi, O.; Udeigwe, J. O.; and Waghmare, U. V. "Silicene and Transition Metal-Based Materials: Prediction of a Two-Dimensional Piezomagnet". *J. Phys. Condens. Matter* (2010), 22, 375502. " *J. Phys. Condens. Matter* (2010), 22, 375502, [DOI](#).

BOOK CHAPTER PUBLICATIONS

1. Deshmukh, T., **Dzade, N.Y.**, "Spray Pyrolysis: Thin Film Coating" In: Sankapal, B.R., Ennaoui, A., Gupta, R.B., Lokhande, C.D. (eds) Simple Chemical Methods for Thin Film Deposition. (2023) Springer, Singapore. [DOI](#)
2. Sachin R. Rondiya (**Postdoc**), Anurag Roy, Ganesh K. Rahane, Ashok Jadhavar, Mahesh M. Kamble, Puneeth Kumar P., Hareesh K., Mahesh P. Suryawanshi, **Nelson Y. Dzade**, Sandesh R. Jadkar. "Physical Methods for Synthesis and Thin Film Deposition" Chapter 4 In Applications of Nanomaterials for Energy Storage Devices. 1st ed.; Amit Saxena, Bhaskar Bhattacharya, Felipe Caballero-Briones., Eds.; Routledge and CRC Press, (2022), ISBN 9781032106311, [DOI](#).
3. Moses Kigozi (**Graduate Student**), Blessing N. Ezealigo, Azikiwe Peter Onwualu & **Nelson Y. Dzade** "Hydrothermal Synthesis of Metal Oxide Composite Cathode Materials for High Energy Application" In Chemically Deposited Nanocrystalline Metal Oxide Thin Films: Synthesis, Characterizations, and Applications, 1st ed.; Ezema, F.I., Lokhande, C.D., Rajan, J., Eds.; Springer International Publishing: Cham, Switzerland, (2021); pp. 489–508, [DOI](#).

SEMINARS AND INVITED TALKS

- **Invited Speaker:** (May 21, 2025) "*Rational Design of Advanced Materials for Next-Generation Energy Conversion and Storage Devices*". IndustryXchange 2025: Technologies for the Future of Energy, at the Nittany Lion Inn.
- **Invited Speaker:** (May 20, 2025) "*Powering the Future: Pathways to a Just Energy Transition*". Next Level Conversations, Penn State Climate Solutions Symposium, at The Penn Stater Hotel & Conference Center.
- **Keynote Lecture:** (April 9, 2025) "*Rational Design of Advanced Materials for Next-Generation Energy Conversion and Storage Devices*" at the EI student-led symposium on Energy Innovations. Energy Institute (EI) - Inter-Institutional Program for Driving Research (IPDR) Symposium, University Park, Penn State.
- **Keynote Address:** "*From Gold Coast to Global Coast: Navigating Career Success as a Ghanaian in the Diaspora*", Ghanaians at Penn State: 68th Ghana's Independence Anniversary Celebration, March 7th, 2025
- **Invited Speaker:** (February 18-20, 2025), "*Accelerating Advanced Energy Materials Design and Mineral Separation*". Third U.S.-Africa Frontiers of Science, Engineering, and Medicine Symposium, Kigali, Rwanda.
- **Invited Speaker:** (January 23, 2025), "*Making a Materials Difference to Green Energy Solutions via a Synergistic Computational-Experimental Approach*". Invited "Semiconductor Talk Series" at the Department of Materials Engineering, Indian Institute of Science, Bangalore, India.
- **Invited Speaker:** (January 20-22, 2025), "*Computational Modeling of Energy Band Alignment at Semiconductor Heterojunctions*". Invited pedagogical lecture at the Biennial School on Modelling and Simulation of Materials, at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India.
- **Invited Speaker:** (December 14-15, 2024), "*Making a Materials Difference to Green Energy Solutions via Computer-Accelerated Design and Optimization*". 12th International Conference of the African Materials Research Society (AMRS2024), Kigali, Rwanda.
- **Invited Pre-Conference Workshop Organizer and Instructor:** (December 14-15, 2024), "*Introduction to Computational Materials Science*", 12th International Conference of the African Materials Research Society (AMRS2024), Kigali, Rwanda.
- **Invited Speaker:** (November 11-12, 2024). "*Atomistic Modeling and Simulation of Energy Materials and Minerals Systems*". Mintek@90 Conference, Sandton Convention Centre, Johannesburg, South Africa.
- **Invited Speaker:** (October 31, 2024). "*Atomistic Modeling and Simulation of Energy Materials and Minerals Systems*". African University of Science and Technology Webinars, Abuja, Nigeria.
- **Invited Panel Member:** (October 30, 2024). "*Critical Minerals: Exploring AI Applications, Mechanisms of Occurrence, Health Implications, Sustainability and Socio-Political Considerations*". 2024 Penn State Materials Day, University Park, PA, USA.
- **Invited Panel Member:** (September 15, 2024). "*Study Abroad Fair – How to Prepare a Strong Graduate School Application*". Organized by the Graduate Students Association of Ghanaian Students in the USA (GRASAG-USA), attended by 160 prospective students.
- **Invited Lecture:** "*Rational Design and Optimization of Advanced Energy Materials*" at the IPDR Mini-Symposium on "Meeting the Renewable Energy Needs for a Sustainable Future" at Morgan State University on September 26th, 2024, Maryland, USA.
- **Invited Speaker:** "*Making a Materials Difference to Green Energy Solutions via Computer-Accelerated Design and Optimization*" Sustainable, Clean & Emerging Energy Technologies Conference (SCEETC 2024), University of Nigeria, Nsukka, 21 – 26 July 2024.
- **Invited Speaker:** "*Computer-Aided Understanding of Interfacial Phenomena in Thin Film Solar Cells*" 2024 Spring Meeting of the European Materials Research Society (E-MRS), Convention & Exhibition Centre of Strasbourg (France), May 27 to 31, 2024.
- **Panel Member:** "*The power of Storytelling - How to Effectively Persuade, Engage, and Connect with your Audience*" PAN-APA 7th Annual Conference, 13 April 2024, Pasquerilla Center, Penn State.
- **Invited Lecture:** "*Computer-Accelerated Energy Materials Discovery, Design, and Optimization*" at the IPDR Mini-Symposium on "Meeting the Renewable Energy Needs for a Sustainable Future" at Howard University on March 14, 2024.

- **Invited Lecture:** *"The Interface is Still the Device"* at the Millennium Café, organized by the Materials Research Institute, Penn State University, March 12, 2024.
- **Panel Member:** (October 27, 2023). *"Reducing dependence on critical minerals for energy storage systems through innovations in materials, reuse, and recycling"*. 2023 Penn State Materials Day, University Park, PA, USA.
- **Invited Speaker:** *"Strengthening Africa's Materials and Minerals Research and Training Capacity: Implications for Renewable Energy Generation and Storage"*. Minerals to Materials Symposium at University College London (UCL), UK, June 26th -27th, 2023.
- **Keynote Speaker:** *"Green hydrogen: A Viable Option for Transforming Africa's Energy Sector and Green Industrialization"*, Chem4Energy Annual Conference 2023 on Materials and Processes for a Sustainable Energy Future. North-West University Sports Village in Potchefstroom, South Africa. 30 March – 2 April 2023.
- **Keynote Speaker:** *"Making a Materials Difference to Green Hydrogen Production: Fuel of the Future"*. 1st International Conference on Green Hydrogen for Global Decarbonization (ICGHGD-2023), Pandit Deendayal Energy University, Gandhinagar, Gujarat, India. March 17-18, 2023.
- **Keynote Speaker:** *"Interface Engineering of Earth-abundant Materials for Renewable Energy Conversion"* Global Scientific Guild Conference: 6th Global Webinar on Materials Science and Engineering. March 09-10, 2023.
- **Invited Webinar:** *"The Role of Green Hydrogen in Decarbonizing the Transportation Sector: Opportunities for Africa"*. Centre for Climate Change Adaptation and Mitigation Studies (C3AMS) 3rd Decarbonization Pathway Series Seminar. Africa University of Science and Technology, Abuja, Nigeria.
- **Invited Lecture:** *"Computationally Driven Design of Earth-abundant Materials for Renewable Energy Conversion and Storage"*. The 11th International Conference of the African Materials Research Society (AMRS2022); 12-15 December 2022, Université Cheikh Anta Diop, Dakar, Senegal.
- **Invited Lecture:** *"The interface is still the device: engineering it for enhanced thin film solar cell performance."* Fall 2022 Earth and Environmental Systems Institute (EESI) EarthTalks series on Exploring the Multiple Dimensions of Solar Energy; 31 October 2022, at Penn State.
- **Invited Lecture:** *"Accelerating Advanced Energy Materials Design and Discovery via High-Performance Computing"*, Energy and Mineral Engineering Department Seminar. September 15, 2022 @ Penn State.
- **Invited Training Workshop (Online):** *"How to write a review paper and get it published"*, Organized by the Postgraduate Student Support of the Academic Development Unit of the Faculty of Engineering and the Built Environment, University of the Witwatersrand, Johannesburg, South Africa, May 4, 2023.
- **Invited talk:** *"Computer-aided Interface Engineering of Earth-abundant Materials for Renewable Energy Conversion and Storage"*, Global Energy Meet (GEM-2023) conference, March 06-08, 2023, at Boston, MA, USA
- **Keynote speaker:** *"Synergistic Computational-Experimental Approaches for Innovative Advanced Energy Conversion Materials"* International Conference on Advanced Materials Synthesis, Characterization and Applications (AMSCA-2022), Oct. 18-20, 2022, Savitribai Phule Pune University, Pune, India.
- **Invited Workshop (Online):** *"Literature Review - Learning the Basics of Research"*, Genius in Africa in collaboration with the African School of Fundamental Physics and Applications, August 5th, 2022.
- **Invited talk:** *"Accelerating Clean Energy Materials Discovery and Innovations through High-Performance Computing: Why Africa Can't Afford to Miss out on the New Paradigm"*, African Sustainability Resource Webinar, July 30th, 2022.
- **Faculty Research Spotlight Talk**, Department of Energy and Mineral Engineering, 2022 EME Research Showcase, *"Making a Materials Difference to Renewable Energy Transition: The Role of Advanced Modelling and Simulation"*. April 27th, 2022, at the HUB-Robeson Center, in the Flex Theater, Penn State University.
- **Conference chair:** 2nd International Conference on Materials & Manufacturing, jointly organized by Engineered Science Publisher, USA, in association with MVP's ASC College, India. February 26-28th 2022.
- **Invited lecture:** *"Computer-Accelerated Design of Next-Generation Materials for Solar Energy Conversion"*, Webinar: American Solar Energy Society, Penn State Chapter. October 7th, 2021.
- **Keynote speaker:** *"Computer-Accelerated Rational Design of Earth-abundant Materials for Renewable Energy Conversion"*. Engineered Science Symposium on Energy Conversion & Storage Devices", March 20th, 2021.

- **Invited speaker:** *"Zinc Phosphide (Zn_3P_2) Heterojunction Interface Engineering for Efficient Solar Energy Conversion"*. HPC Materials Chemistry Consortium Webinar, 28th July 2020.
- **Invited talk:** *"Computation and Experiment: A Powerful Combination to Rationally Design Functional Materials for Renewable Energy Applications"*. Invited Seminar, Swiss Federal Institute of Technology Lausanne (EPFL), February 17, 2020.
- **Keynote speaker:** *"Rational Design of Transition Metal Chalcogenide based Functional Materials for Renewable Energy Conversion"* International Chemistry Conference in Botswana, September 25–27, 2019, Botswana.
- **Invited speaker:** *"Bandgap and band-offset engineering of semiconductor heterostructures for photovoltaic and photocatalytic applications"*. 2nd Edition of Global Conference on Catalysis, Chemical Engineering & Technology (CAT 2018), September 13–15, 2018, in Rome, Italy.
- **Invited speaker:** *"Computer simulations of iron sulphide materials for photocatalytic applications"*. UK-Netherlands Bilateral International Meeting, Organised by the Royal Society and Royal Netherlands Academy of Arts and Sciences, February 21–22, 2018, Chicheley Hall, Milton Keynes.
- **Invited speaker:** *"Modelling band alignments and charge transfer in semiconductor heterostructures for photovoltaic and photocatalytic applications"*. Royal Society-DFID Africa Capacity Building Initiative semi-annual meeting/workshop, August 1–5, 2017, University of Namibia, Windhoek, Namibia.
- **Invited speaker:** *"Active sulfur vacancy sites for the activation and conversion of CO_2 on $FeS(001)$ surface"*. Computational Sciences for Future Energy conference, September 19–20, 2017, Eindhoven, The Netherlands.
- **Invited speaker:** *"Mixed pyrite-marcasite thin films for efficient solar energy conversion"*. Royal Society-DFID Africa Capacity Building Initiative semi-annual meeting, August 1–5, 2016, Kwame Nkrumah University of Science and Technology (KNUST), Kumasi, Ghana.
- **Invited speaker:** *"Unravelling the Role of Lithium in Enhancing the Hydrogen Evolution Activity of MoS_2 "* 10th Int. Conference of the African Material Research Society (AMRS), December 10–13, 2019, Arusha, Tanzania.
- **Contributed talk:** *"High Photoresponse of Marcasite–Pyrite Heterojunction and Its Origin: Insights from First-Principles DFT Calculation"*. European Materials Research Society (E-MRS) 2019 Fall Meeting, September 16 – 19, 2019. Warsaw University of Technology, Poland.
- **Contributed talk:** *"Organic Functionalization Zinc Phosphide (Zn_3P_2) Surfaces: Implications for PV Application"*. School of Chemistry Seminar, Cardiff University, August 15, 2018.
- **Contributed talk:** *"Characterization of the structures and properties of $As(OH)_3$ adsorption complexes at mackinawite water interfaces: A DFT-D2 study"*. Goldschmidt2017, August 13–18, 2017, Paris.
- **Contributed talk:** *"Surface and shape modification of FeS nanocrystals by cysteine adsorption for heterogeneous catalytic applications"*. Catalysis for Fuels Faraday Discussion, January 24–26, 2017, Cape Town, South Africa.
- **Contributed talk:** *"Nanostructuring of pyrite and marcasite FeS_2 surfaces/interfaces for photovoltaic applications"*. Computational Sciences for Future Energy 2016 conference, October 11, 2016, Media Plaza, Utrecht.
- **Contributed talk:** *"Mechanisms of thiophene adsorption and desulfurization of on layered FeS low-index Miller surfaces"*. Geochemistry Seminar, September 14, 2016, Utrecht University, The Netherlands.
- **Contributed talk:** *"Enhanced photo-response of FeS_2 films: the role of marcasite-pyrite phase junctions"*. Modelling of Advanced Functional Materials using Terascale Computing, Materials Chemistry Consortium Conference, April 6–8, 2016, Cardiff University, Wales, UK.
- **Invited speaker:** *"Bio-inspired layered iron sulfide nano-catalyst for CO_2 conversion"*. International conference on the Science behind CO_2 Capture and Conversion, June 24–28, 2015, Varadero, Cuba.
- **Keynote speaker:** *"Cysteine adsorption on the Low-Miller index surfaces of FeS : implications for nanocrystals shape modulation"*. The Centre for High Performance Computing (CHPC) National Conference, December 2–6 2013. Cape Town, South Africa.
- **Contributed talk:** *"Computational design of active and selective iron sulfide nano-catalyst for CO_2 activation and conversion"*. The 12th Int. Conference on Carbon Dioxide Utilization (ICCDU XII), June 23–27, 2013, Alexandria, Washington D.C., USA.
- **Contributed talk:** *"The surface chemistry of NO_x at mackinawite (FeS) surfaces"*. The Centre for High Performance Computing National Conference, December 2–6, 2012, Durban International Convention Centre, South Africa.

- **Contributed talk:** “First-principles study of the structure and properties of silicene: A competitive 2D material”. Materials and Inorganic Chemistry Seminar, Nov. 13, 2012, University College London, UK.
- **Contributed talk:** “The reactivity of CO₂ with the low-index surfaces of FeS”. London Catalysis Winter Seminar, 19th January 2012, Imperial College London, UK.
- **Contributed talk:** “A DFT-D2 study of structure and properties of As(OH)₃ adsorption complexes on mackinawite (FeS)”. The Centre for High Performance Computing National Conference, December 7–9, 2011, Council of Scientific and Industrial Research (CSIR), International Convention Centre, Pretoria, South Africa.
- **Contributed talk:** “Bio-inspired (Fe, Ni)S nano-catalyst for CO₂ activation and reduction”. The World Association of Theoretical & Computational Chemists Congress, July 17–22, 2011, Santiago de Compostela, Spain.

RESEARCH MENTORING & ADVISING

Postdoctoral Scholar

- Sachin R. Rondiya, Postdoctoral Research Associate (2019-2021), Cardiff University. Project “Computer-Aided Design of Zinc Phosphide Heterojunctions for Efficient Solar Energy Conversion”. Now an Assistant Professor at the Department of Materials Engineering, Indian Institute of Science (IISc), Bangalore, India.

Ongoing Graduate (PhD and D.Eng.) Advising

- **Henry I. Eya (Advisor)**, Ph.D. Energy and Mineral Engineering, Penn State. Research: “Interface Engineering of Lead-free Chalcogenide Perovskite Thin-Film Solar Cells”. **Expected Graduation:** Fall 2025
- **Ricardo Amaral (Advisor)**, Ph.D. Energy & Mineral Engineering, Penn State. Research: “Interface Engineering of Nickel Phosphide-Based Heterostructures for Lithium-Sulfur Batteries”. **Expected Graduation:** Fall 2025.
- **Joy Atieno Adul (Primary Co-Advisor)**, Ph.D. Energy and Mineral Engineering, Penn State. Research: “Mechanistic Insights into the CO₂ Activation and Conversion on Calcium Copper Titanate (CaCu₃Ti₄O₁₂)”. **Expected Graduation Date:** Spring 2026.
- **Nikhil Komalla (Advisor)**, Ph.D. Energy & Mineral Engineering, Penn State. Research: “Rational Design of Transition Metal Chalcogenides Electrocatalysts for Green Hydrogen Production”. **Expected Graduation:** Fall 2026.
- **Tasseer Badri (Advisor)**, Doctor of Engineering in Engineering (D.Eng.), Penn State. Research “Economically sustainable refurbishment and redistribution of end-of-life solar photovoltaic (PV) panels, tailored to Indonesia’s unique market conditions and economic barriers.” **Expected Graduation:** Fall 2028.
- **Nishant Mishra (Advisor)**, Ph.D. Energy and Mineral Engineering, Penn State. Research: “Computational Modelling Interfacial Phenomena in Thin-Film Perovskite Solar Cells using First-principles and Machine Learning Approaches”. **Expected Graduation:** Fall 2029.

Completed Graduate (PhD and D.Eng.) Students

- **Russell W. Cross**, PhD Chemistry (2023), Cardiff University, U.K. Thesis “Computer-Aided Design of Transition Metal Phosphides Catalysts for Efficient Hydrogen Evolution Reaction (HER)”.
- **Cecil H. Botchway (Mentor & Co-Advisor)**, Ph.D. Chemistry (2022), KNUST, Ghana. Thesis “Understanding Methanol Diffusion and Framework Methylation Mechanism in Brønsted Acid and Alkaline Metal-Modified Zeolite Topologies: A Density Functional Theory and Molecular Dynamics Study”.
- **Moses Kigozi (Primary Co-Advisor)**, Ph.D. Materials Science & Engineering, 2021, African University of Science and Technology. Thesis “Activated Carbon & Graphene Oxide for Supercapacitor and Battery Application”.
- **Caroline Kwawu (Mentor & Co-Advisor)**, PhD Chemistry, (2017), Kwame Nkrumah University of Science and Technology (KNUST), Ghana, **Thesis:** “Computational studies on transition metal catalysts for CO₂ conversion into hydrocarbon fuels”.
- **Elliot S. Menkah (Mentor & Co-Advisor)**, PhD Chemistry, 2019, Kwame Nkrumah University of Science and Technology (KNUST), Ghana, **Thesis:** “Computational Design of Bimetallic Ni-Ru Catalysts for the Conversion of Syngas to Synthetic Fuels”.

Completed MSc/MChem Students

- **Adeline Weitknecht (Advisor)**, MSc. Energy and Mineral Engineering (Spring 2025), Penn State, Thesis *"Equitable Access to Community Solar: A Case Study of Kenya"*.
- **Oluwayomi F. Awe (Primary Co-Advisor)**, MSc. Energy and Mineral Engineering, (Spring 2024), Penn State, Thesis *"Unraveling the Origin of High Photocatalytic Properties of Earth-Abundant TiO₂/FeS₂ Heterojunction: Insights from First-Principles Density Functional Theory"*.
- **Sophie Colton (Advisor)**, Master of Chemistry (2020), Cardiff University. Thesis *"Computational Design of Chalcogenide Perovskites for Solar Energy Conversion Applications"*.
- **Eloise Lewis (Advisor)**, Master of Chemistry (2020), Cardiff University, Thesis *"First-Principles Mechanistic Insight into the Adsorption of Arsenic on Cobalt Ferrite (Fe₂CoO₄) Surfaces: Implications for Water Purification"*.
- **Abdulwaheed A. Bilau (Advisor)**, MSc Materials Science and Engineering, (2019), African University of Science and Technology, Abuja, Nigeria. Thesis: *"First-principles Density Functional Theory Study of the Structural and Electronic Properties of Prodigiosin as Cancer Drug"*.
- **Isyaku A. Odoguje (Advisor)**, MSc Theoretical Physics, (2019), African University of Science and Technology, Abuja, Nigeria, Thesis: *"Structural, electronic and optical properties of Cu₂SnS₃ solar absorber: a first-principles density functional theory investigation"*.
- **Tim Bögels (Advisor)**, MSc Earth Structure and Dynamics, (2019), Utrecht University Thesis *"Analyzing Hydrogen Evolution Reaction (HER) Catalytic Sites of Nickel Sulphides, A DFT Computational Study"*.
- **Isaac W. Boateng (Co-Advisor)**, MPhil Chemistry, (2016), KNUST, Ghana. Thesis *"Computational study of hydrogen adsorption on the (010) surface of Lanthanum ferrite (LaFeO₃)"*.

BSc. Students Project Supervision

Current

- Saif Almarzooqi, B.S Energy Engineering, Penn State, **Expected Graduation:** Spring 2026. *"First-Principles DFT Study of Structural, Electronic, and Optical Properties of CaHfS₃ and SrHfS₃ Chalcogenide Perovskites for Solar Cell Applications"*.
- Yuxiang Zhang, B.S Energy Engineering, Penn State, **Expected Graduation:** Fall 2026. *"Adsorption Mechanism of Lithium Polysulfides on NiCoP Host Material: Implications for Li-S Battery Applications"*.
- Al Khalil Al Hashemi, B.S Energy Engineering, Penn State, **Expected Graduation:** Fall 2026. *"DFT Mechanistic Insights into Water Adsorption and Dissociation of Ni₃P surface: Implications for Hydrogen Production"*

Completed

- Najd Alshamali, B.S Petroleum Engineering, (2025), Penn State. Schreyer Honors College Thesis *"Hydrogen Storage and Its Interaction with Subsurface Minerals"*.
- Fares Albishi, B.S Petroleum Engineering (Spring 2025), Penn State. Schreyer Honors College Thesis *"Floatovoltaics in Saudi Arabia: Feasibility, Impacts, and Case Studies"*.
- Olivia DiPrinzio, B.S Energy Engineering (Fall 2024), Penn State. Independent research student *"Bandgap Engineering of BaHfS₃ Chalcogenide Perovskite for Photovoltaic and Optoelectronic Applications"*.
- Sami Al Azri, B.S Energy Engineering (Fall 2024), PSU. Schreyer Honors College Thesis *"Investigating the Viability of Chalcogenide Perovskite as Next-Gen Solar Cell Technology - A Case Study of Sn-based CaSnS₃ Absorber Material"*.
- Gabriel K. Renninger, B.S Energy Engineering (Spring 2024), Penn State. Summer Internship research *"First-principles study of the structural, electronic, optical, surface, and interface properties of BaHfSe₃, and Earth-abundant and stable chalcogenide perovskite for solar cell applications"*.
- Ramakrishna Santrupth, B.S Energy Engineering (Spring 2024), Penn State. Summer Internship research *"Computational Study of the Optical properties of BaHfS₃ Chalcogenide Perovskite for Photovoltaic Applications"*.
- Lewis Old, BSc Chemistry, (2021), Cardiff University, Project *"Optoelectronic Properties of CaZrSe₃ Chalcogenide Perovskite Calculated from First-Principles Theory"*.

- Connor Duggan, BSc Chemistry, (2020), Cardiff University, Project “X-ray Photoelectron Spectroscopy-Based Valence Band Spectra of BaZrS₃: Insights from Density Functional Theory Calculations”.
- Jemima Moorcroft, BSc Chemistry, (2019), Cardiff University, Project “CO₂ Adsorption and Activation on Bimetallic Fe-Ni Catalysts: A Dispersion-Corrected DFT Analysis.”
- Jasper Huijsmans, BSc Earth Sciences, (2018), Utrecht University, Project “Computational Study of the Influence of Inorganic Solution Components on Lithium Carbonate Crystal Growth”.
- Manon Dierkx, BSc Earth Sciences, (2017), Utrecht University, Project Title “Computer Simulation of the Effects of pH on Phosphate Adsorption to Iron-oxides”.

Other Research Supervision (non-advisees)

MSc & Ph.D. Committee Member @ PSU

- Yanjun Guo, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Nelson Federico Colman Pedrozo, PhD, Mechanical Engineering, PSU. *Stage of Completion:* In Process.
- Alireza Sepehrinezhad, PhD, Mechanical Engineering, PSU. *Stage of Completion:* In Process.
- Praneetha Buddha, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Justin Lin, PhD, Materials Science and Engineering, PSU. *Stage of Completion:* In Process.
- Steven V. Chanci, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Do Hyun Lee, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Pathickal Abraham, PhD, Chemistry, PSU. *Stage of Completion:* In Process.
- Cyril Kumachang, PhD, Materials Science and Engineering, PSU. *Stage of Completion:* In Process
- Derek Rui Zhu, PhD, Chemical Engineering, PSU. *Stage of Completion:* In Process.
- Hanrui Zhang, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Rowfi Kha, PhD, Energy and Mineral Engineering, PSU. *Stage of Completion:* In Process.
- Sharmba, Tsunami, MSc Mineral Engineering, Penn State. *Completed:* October 21st, 2024.
- Lai, Jianwei, PhD, Energy and Mineral Engineering, PSU. *Completed:* February 20, 2025
- Sandra N. Ike, PhD, Energy and Mineral Engineering, PSU. *Completed:* January 29, 2025.
- Amir, Eskanolou, PhD, Mineral Engineering, Energy and Mineral Engineering, PSU. *Completed:* July 7, 2024.
- Afolayan, Emmanuel, PhD, Electrical Engineering, PSU. *Completed:* June 16, 2023.

Ph.D. Thesis Committee External Examiner (Based Abroad)

- Brian Ramogayana, PhD, Physics, University of Limpopo, South Africa. *Completed:* 2024. “Surface study of doped and coated Li-rich Mn-based cathode”.
- James B. Dankwah, PhD, Minerals & Resources Engineering, University of South Australia. *Completed:* 2023. “Improved Understanding of the Fundamentals of Coarse Particle Flotation”.
- Phala Wesley Masoga, PhD, in Physics, University of Limpopo, South Africa. *Completed:* 2023. “Evolutionary Algorithm Simulation Study of MnO₂ Nanoclusters”.
- Tshide Mogashoa, PhD, Physics, University of Limpopo, South Africa. *Completed:* 2023. “Atomistic Simulation Studies of Li₂MnO₃ Nanoarchitectures”.
- Bismark Kyeremeh, PhD, Minerals & Resources Eng., University of South Australia. *Completed:* 2022. “Sensing and Optimisation of Flotation Circuits and Integration with Grinding”.
- Jadhavar A. Arun, PhD, in Physics, Savitribai Phule Pune University, India. *Completed:* 2020. “Synthesis of intrinsic and doped nanocrystalline hydrogenated silicon (nc-Si:H) by using plasma enhanced chemical vapor deposition (PE-CVD) and evaluation of their optoelectronic properties for photovoltaic applications”.
- Subhash M. Pandharkar, PhD, in Physics, Savitribai Phule Pune University, India. *Completed:* 2021. “Synthesis and study of quaternary chalcogenide absorbers for solar cell applications”.
- Aher R. Ashokrao, Physics, Savitribai Phule Pune University, Ph.D. in Physics, *Completed:* 2021. “Synthesis of graphene analogous layered ternary topological insulators and their sensing, field emission and other applications”.

- Shruthi S. Nair, PhD, Physics, Savitribai Phule Pune University, India. Completed: 2021. *“Lead-free halide perovskite materials for photovoltaic applications: an experimental and theoretical approach”*.
- Ephraim M. Kiarri, PhD, Chemistry, University of Johannesburg. Completed: 2020. *“High Thermoelectric Performance and Electronic Structure of Traditional Thermoelectric/2D Hetero-Thermoelectric Materials for Efficient Energy Conversion: A first-Principles Study”*.
- Sharlene-Asia Naicker, PhD, Physics, University of KwaZulu-Natal, South Africa. Completed: 2020. *“A Computational Study of Corrosive Sulphur on Metal Surfaces”*.
- Ephraim F. Marondedze, PhD, Chemistry, University of Johannesburg, South Africa. Completed: 2019. *“In-Silico Design of a Novel Probe for The Potential Early Detection of Alzheimer’s Disease”*.
- Wahab Olaide Olalekan, PhD, Chemistry, University of Johannesburg, South Africa. Completed: 2019. *“Theoretical Prediction of Solubility, Reactivity and Degradation Pathways of Selected Azo Disperse Dyes”*.
- Francis Opoku, PhD, Chemistry, University of Johannesburg, South Africa. Completed: 2018. *“First-Principles Studies on The Development of Semiconductor-Based Photocatalyst Materials for Applications in Photocatalytic Water Splitting and Degradation of Pollutants”*.

MSc. Thesis Committee External Examiner (Based Abroad)

- Mohammed Al-Fars, MSc in Materials Science, The University of New South Wales. Completed: 2022. *“Computational materials discovery: Ab initio modelling of new, high-performance semiconductors for top cells in multi-junction tandems on silicon solar cells”*.
- Seiso E. Tsoeu, MSc in Chemistry, University of Johannesburg, South Africa. Completed: 2021. *“First-Principles Design of Hybrid Carbon Nitride (C₂N) with Gallium Sulphide and Gallium Selenide Two-Dimensional (2D) Materials as High-Performance Photovoltaic Cells”*.
- Elizeth Afonso Humba, MSc in Chemistry, The University of Namibia. Completed: 2020. *“Computational Study of the Structure and Electronic Properties of Ag- and Au-Doped (TiO₂)_n Clusters (n = 2-6)”*.
- Nemutudi Bradley, MSc in Physics, University of Limpopo, South Africa. Completed: 2020. *“Computational Modelling Studies of PtAs, PtAsS and Pd₂As Mineral Surfaces”*.

TEACHING: COURSES TAUGHT AND DEVELOPED

PSU Undergraduate Teaching

- **EGEE 437: Design of Solar Energy Conversion Systems:** Examines the principles of solar energy conversion to build a foundation for explaining the basic concepts and implementation of conversion processes. **Teaching Related Awards:* Served as the Faculty Advisor to six Energy Engineering students (taking EGEE 437) that won consecutive 1st Place Award for the “University of Washington District Use Case” in 2024, and “University of Oregon District Use Case” in 2025 of the DOE Solar District Cup Competition, a national collegiate competition that challenges multidisciplinary student teams to design and model distributed solar energy systems for a campus or district. **CAPSTONE Project Sponsor:** I sponsored two capstone projects of the 2025 Learning Factory to “Designing Solar Systems for Penn State University Park”. One of the teams won the overall 3rd place finish award in the Penn State Spring 2025 Capstone Showcase.
- **EME 301: Thermodynamics in Energy and Mineral Engineering:** Focuses on the principles of classical thermodynamics as applied to energy extraction, processing, and utilization within the mineral and energy industries. **Note:* There has been a significant increase in student engagement and improved performance since I started teaching EME 301.

PSU Graduate-level Teaching

- **EME 597: Molecular Modelling of Materials and Minerals:** Introduce graduate students to advanced materials simulation techniques and their use to characterize a wide range of phenomena from electronic and atomic structure to macroscopic behavior

Courses Taught at Other Universities

- **CH0002: Thermodynamics, Kinetics and Equilibria** (Undergraduate level), Cardiff University, UK.
- **PHY 901: Materials Modeling and Simulation** (Graduate level), AUST, Nigeria.
- **MSc Advanced mineralogy AW-4004** (Graduate level) Utrecht University, The Netherlands.
- **MSc Geo4-1426 Kinetic Processes** (Graduate level), Utrecht University, The Netherlands.

FUNDING AGENCY PROPOSAL REVIEW COMMITTEE MEMBERSHIP

- The National Science Foundation (NSF)
- The European Research Council (ERC)
- UK Research and Innovation (UKRI)
- Full College Member– EPSRC (Engineering & Physical Sciences Research Council)
- South Africa's National Research Foundation (NRF)

JOURNAL EDITORIAL BOARD MEMBERSHIP

- Frontiers in Catalysis, Editorial Board of Modelling, Theory and Computational Catalysis
- Associate Editor, Engineered Science, Materials and Manufacturing

PROFESSIONAL MEMBERSHIP

- Materials Research Society (MRS)
- American Chemical Society (ACS)
- Society for Mining, Metallurgy & Exploration (SME)
- SUPERGEN SUPERSOLAR, The network for solar research in the UK

MEDIA (PRESS RELEASES)

- Penn State News: "[Students to present solar design project at expo on April 30](#)" (April 25, 2025)
- MRI News: "[2025 MRI Interdisciplinary Seed Grants and Transdisciplinary Teaming Initiative Awards](#)"
- Penn State News: "[EMS experts promote research ties at National Academies US-African symposium](#)"
- Penn State News: "[EMS faculty member receives DOE Early Career Research Award](#)" (October 17, 2024).
- Penn State News: Featured Interview, Featured Interview (podcast), "[Growing Impact: Converting CO₂ into Fuel](#)," Institute of Energy and the Environment Podcast. (October 1, 2024). [YouTube video](#).
- Penn State News: "[Penn State students win Solar District Cup division competition](#)" (June 27, 2024).
- University College London (UCL) Careers News: "[What's Academia like in the U.S.](#)"
- Penn State News: "[Scientists develop new method to create stable, efficient next-gen solar cells](#)", Oct 19 2023
- Perovskite-Info News: "[Researchers develop phase-heterojunction all-inorganic perovskite solar cells with over 21.5% efficiency](#)", Aug 19, 2023.
- Technology Networks News: "[Scientists Develop New Method to Create Stable, Efficient Next-Gen Solar Cells](#)", October 24, 2023
- Penn State News: "[EarthTalks: Dzade to discuss engineering for enhanced thin-film solar cells](#)" Oct. 26, 2022

SCIENTIFIC REVIEWING ACTIVITIES

Currently reviews for several scientific journals: Advanced Materials, Advanced Electronic Materials, Advanced Energy Materials, Nature Communications, *npj* Computational Materials, ACS Energy Letters; Applied Surface Science; Solar Energy Materials & Solar Cells; ACS Applied Materials & Interfaces; ACS Environmental Science & Technology; ACS Catalysis; ACS Omega; ACS Chemistry of Materials; ACS Physical Chemistry C; Catalysts (MDPI); Minerals (MDPI); RSC Environmental Science: Nano; RSC Physical Chemistry Chemical Physics; CO₂ Utilization; Surface and Coatings Technology; Computational Material Science; Molecular Catalysis; Journal of Chemical Physics; Journal of Physics and Chemistry of Solids and Journal of Applied Physics; RSC Advances;

Chemical Physics Letters; Advanced Functional Materials; ChemSusChem; ES Materials & Manufacturing; RSC Catalysis Science & Technology, Physical Review B; Journal of Molecular Graphics and Modelling, International Journal of Mining Science and Technology.