Nelson Yaw Dzade

Assistant Professor of Energy and Mineral Engineering

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PERSONAL PROFILE

Dr Dzade is a highly experienced and skilled computational materials and minerals scientist. He leads the Materials and Minerals Theory Group, which specializes in the development and application of 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 for the understanding of (i) complex heterogeneous catalytic reaction mechanisms at surfaces, (ii) chemical reaction dynamics and transport processes at interfaces between highly dissimilar materials, e.g. organic-inorganic and epitaxial inorganic interfaces. An important context for his research has been renewable energy, where novel materials, sulphides, oxides, perovskites, organics, and interfaces feature prominently. A skilled writer and an effective communicator with an interactive teaching style that promotes effective participation and enthusiasm while facilitating learning. Highly organized and able to effectively prioritize and coordinate multiple tasks to accomplish projects with creativity and enthusiasm. Exceptionally flexible, able to adapt to new situations and environments, work independently as well as thrive in a team environment.

EDUCATION

2010–2014 | **PhD Computational Materials Science**
University College London (UCL), London, United Kingdom

SUPERVISORS: Professor Nora de Leeuw (n.h.deleeuw@leeds.ac.uk)
Professor Richard Catlow (catlowr@cardiff.ac.uk)
THESIS TITLE: "*Computational Study of the Interactions of Small Pollutant Molecules with the Surfaces of Iron-Bearing Minerals*"
DATE AWARDED: October 28th 2014

2009–2010 | **Postgraduate Diploma (PGDip) Materials Science**
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India

SUPERVISORS: Professor Umesh Waghmare (waghmare@jncasr.ac.in)
Professor C.N.R. Rao (cnrrao@jncasr.ac.in)
THESIS TITLE: "*Phonon Softening Near Crack Opening: A First-Principles DFT Study*"
DATE AWARDED: May 21st 2010

2008–2009 | **MSc Materials Science (Distinction)**
African University of Science and Technology, Abuja, Nigeria

SUPERVISOR: Professor Umesh Waghmare (waghmare@jncasr.ac.in)
THESIS TITLE: "*Energetics and Stabilities of Molecule-Electrode Interfaces: A First-Principles Study*"
DATE AWARDED: December 19th 2010

2003–2007	**BSc Mathematical Science (Statistics option), First Class Honours** University for Development Studies, Tamale, Ghana SUPERVISOR: Professor Kaku Sagary Nokoe (nokoemaths@gmail.com) THESIS TITLE: *"Line Transect Sampling: An evaluation of Models and Field Experiments"* DATE AWARDED: December 19th 2010

PROFESSIONAL RESEARCH POSITIONS & APPOINTMENTS

2021 - Date	**Assistant Professor of Energy and Mineral Engineering** John and Willie Leone Family Department of Energy and Mineral Engineering The Pennsylvania State University, USA
2018 – 2021	**EPSRC (Engineering & Physical Sciences Research Council) Innovation Fellow** School of Chemistry, Cardiff University, UK. PI for the Project: Computer-Aided Design of Zinc Phosphide Heterojunctions for Efficient Solar Energy Conversion
2018-date	**Visiting Assistant Professor of Materials Science and Engineering** African University of Science and Technology (AUST), Abuja-FCT, Nigeria
2018 – date	**PhD Assessor (External Based Abroad)** • University of South Australia, Australia • University Of Johannesburg, South Africa • Africa University of Science and Technology, Nigeria • University of New South Wales, Australia • University of Limpopo, South Africa • University of KwaZulu-Natal, Westville, South Africa • University of Namibia, Namibia • Savitribai Phule Pune University, India
2015 – date	**Co-investigator/Trainer on Chem4Energy Africa Research Consortium** "New Materials for a Sustainable Energy Future" funded by the UK Department of International Development, to strengthen research and training capacity in Kwame Nkrumah University of Science and Technology (KNUST) Ghana, and University of Namibia and University Botswana.
2014 –2018	**Postdoctoral Research Fellow** Utrecht University, Department of Earth Sciences Funded by Netherlands Organization for Scientific Research (NWO). Mentors: Professor Nora H. de Leeuw Professor Jan Philipp Hofmann Research project: "Computer-Aided Design of Iron-Sulphide Nano-Catalysts for Solar-Driven Conversion of CO_2 to Fuels".
2012 – 2013	**Research Associate, British Petroleum (BP), UK** University College London Mentors: Professor Nora H. de Leeuw Dr Martin Gold Research project: "Computer Simulations of the Effect of Fuel Additives on Metal Oxides Surfaces", an important problem in chemical fouling of fuel pipeline in car engines.
2007 – 2008	**Teaching Assistant (Ghana National Service)** Department of Mathematics, University for Development studies, Ghana.

SCHOLARSHIPS and AWARDS

2020–2021	**DUO-India Professor Fellowship Award, Cardiff University, UK** DUO-India Fellowship Programme
2018–2021	**EPSRC Innovation Research Fellowship Award, Cardiff University, UK** UK Research and Innovation
2007–2008	**Teaching Assistant (Ghana National Service)** Department of Mathematics, University for Development studies, Ghana.
2010–2014	**Overseas Research Scholarship** University College London, UK
2010–2014	**Faculty of Mathematical and Physical Sciences Studentship** University College London, UK
2008–2009	**World Bank Scholarship** African University of Science and Technology, Nigeria
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
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 Developments Studies, Tamale, Ghana.

RESEARCH GRANTS

- **Principal Investigator**: Penn State Institutes of Energy and the Environment – IEE ICDS Seed Grant Program. "Rational Design of Bio-inspired and Earth-abundant Catalysts for Carbon Dioxide Reduction into Fuels and Fine Chemicals". Funded value: $15,000.
- **Co-Principal Investigator**: European Innovation Council (EIC) PathFinder Grant. "SOLARUP -Advanced Strategies For Development Of Sustainable Semiconductors For Scalable Solar Cell Applications". Funded value: €2,450,878.
- **Principal Investigator**: Penn State Institute for Computational and Data Sciences – ICDS Seed Grant Program. "*Toward the Rational Design of Chalcogenide Perovskites Heterojunction Photovoltaics*". Funded value: $50,000.
- **Principal Investigator**: DUO-India Professor Fellowship Award "*Rationally Design of Novel ABO_3 Compounds and their Nano-Hetero-Architectures for Catalytic PEC Water Splitting Applications*" Funded value: £6,000; Funded Period: Jan. 2020–Dec. 2020).
- **Principal Investigator**: Engineering and Physical Sciences Research Council (EPSRC) Innovation Research Fellowship Grant "*Computer-Aided Design of Zinc Phosphide Heterojunctions for Efficient Solar Energy Conversion"*. Funded value: £525,254; Funded Period: June 2018–June 2021).
- **Co-Principal Investigator**: Natural Environment Research Council (NERC) Research Grant "*International Innovation Project on the Computer-aided High Throughput Development and Upscaling of Tailored Zeolites as Wastewater Filters in Ghana*". Funded value: £107,175; Funded Period Nov 2017- Apr 2020).
- **Co-Principal Investigator**: Netherlands Organization for Scientific Research (NWO) ECHO grant "*Earth-abundant materials for the sustainable catalysis of CO_2 to fuels and chemicals: Linking computation to experiment*". Funded value: €250,000; Funded Period Dec 2018 - Dec 2021).

UNDERGRADUATE/POSTGRADUATE STUDENTS SUPERVISION

CURRENT STUDENTS

- **Main supervisor:** Nikhil Komalla, PhD Candidate (2022-2026), The Pennsylvania State University, "*Rational Design of Transition Metal Chalcogenides Electrocatalysts for Green Hydrogen Production"*
- **Main supervisor:** Henry I. Eya, PhD Candidate (2022-2026), The Pennsylvania State University, "*Interface Engineering Lead-free Chalcogenide Perovskite Thin-Film Solar Cells*."

- **Main supervisor:** Ricardo Amaral, PhD Candidate (2021-2025), The Pennsylvania State University, "*First-Principles Design and Engineering of Heterostructured Materials for Efficient and Stable Lithium–Sulfur Batteries*"
- **Main supervisor:** Russell William Cross, PhD Candidate ((2018-2022)), Cardiff University, "*Computer–aided Design of Transition Metal Phosphides Catalysts for Efficient Hydrogen Evolution Reaction (HER)*"
- **Co-supervisor:** Cecil H. Botchway, PhD Candidate (2018-2022), KNUST, Ghana, working on "*Mechanistic Study of Ethanol Conversion to Hydrocarbons over Zeolites Perlialite and Ferrierite*"

PAST STUDENTS

- **Main supervisor**: Dr Sachin Rondiya, Postdoctoral Research Associate (2019-2021), Cardiff University, Project: "*Earth-Abundant Next Generation Materials for Solar Energy: Synthesis and Device Fabrication*".
- **Main supervisor:** Dr Patrick Heasman, Postdoctoral Research Associate (2019-2020), Cardiff University, Project: "*Ab Initio Investigation of O_2 Adsorption on $SmCoO_3$-based Cathode Materials for Solid Oxide Fuel Cells*".
- **Main supervisor**: Sophie Colton, MChem Thesis (2019-2020), Cardiff University. "*Computational Design of Chalcogenide Perovskites for Solar Energy Conversion Applications)*".
- **Main supervisor**: Eloise Lewis, MChem Thesis (2019-2020), Cardiff University, "*First-Principles Mechanistic Insight into the Adsorption of Arsenic on Cobalt Ferrite (Fe_2CoO_4) Surfaces: Implications for Water Purification*"
- **Main supervisor**: Lewis Old, BSc Thesis (202-2021), Cardiff University, "*Optoelectronic Properties of CaZrSe Chalcogenide Perovskite Calculated from First-Principles Theory*".
- **Main supervisor**: Connor Duggan, BSc Thesis (2019-2020), Cardiff University, "*XPS Valence Band Spectra of $BaZrS_3$: Insights from Density Functional Theory Calculations*".
- **Main supervisor:** Kigozi Moses, PhD Thesis (2017-2021), African University of Science and Technology, worked on "*Activated Carbon and Graphene Oxide for Supercapacitor and Battery Application*".
- **Main supervisor:** Jemima Moorcroft, BSc Thesis (2018-2019), Cardiff University, worked on "*CO_2 Adsorption and Activation on Bimetallic Fe-Ni Catalysts: A Dispersion-Corrected DFT Analysis*"
- **Co-supervisor:** Elliot S. Menkah, PhD Thesis (2013-2019), KNUST-Ghana, "*Computational Design of Bimetallic Ni-Ru Catalysts for the Conversion of Syngas to Synthetic Fuels*".
- **Main Supervisor:** Timoteüs F.J. Bögels, MSc Thesis (2019), Utrecht University, "*Analyzing Hydrogen Evolution Reaction Catalytic Sites of Nickel Sulfides: A First-Principle DFT Study*".
- **Co-supervisor:** Albert Aniagyei, PhD Thesis (2013-2018), KNUST-Ghana, "*Theoretical Studies of Oxygen Reduction on Calcium-, Strontium- and Barium-Doped Lanthanum Manganite ($LaMnO_3$) as Cathode Materials in Solid Oxide Fuel Cells*".
- **Main supervisor:** Jasper Huijsmans BSc Thesis (2018), Utrecht University, "*Computational Study of the Influence of Inorganic Solution Components on Lithium Carbonate Crystal Growth*".
- **Co-supervisor:** Caroline R. Kwawu, PhD Thesis (2013-2017), KNUST-Ghana, "*Computational Study of the Conversion of CO_2 to Fuel or Chemicals on Pure and Ni-Coated Iron Surfaces*".
- **Main supervisor:** Manon Dierkx, BSc Thesis (2017), Utrecht University, "*Computer Simulation of the Effects of pH on Phosphate Adsorption to Iron-oxides*".
- **Co-supervisor:** Isaac W. Boateng, MPhil Thesis (2013-2016), KNUST-Ghana, "*Computational study of hydrogen adsorption on the (010) surface of Lanthanum ferrite ($LaFeO_3$)*".
- **Co-supervisor:** Joel Baffour Awuah, MPhil thesis (2013-2015), KNUST-Ghana, "*Computational study arsenic immobilization by the Al(III)-modified zeolite clinoptilolite*".

THESIS EXAMINATION (EXTERNAL ASSESSOR BASED ABROAD)

- Mohammed Al-Fars, Materials Science and Engineering, The University of New South Wales, "*Computational materials discovery: Ab initio modelling of new, high performance semiconductors for top cells in multi-junction tandems on silicon solar cells*". MSc in Materials Science and Engineering, Graduated 2022.
- Seiso Emmanuel Tsoeu, Chemistry, University Of Johannesburg, "*First-Principles Design of Hybrid Carbon Nitride (C2n) with Gallium Sulphide and Gallium Selenide Two-Dimensional (2D) Materials as High-Performance Photovoltaic Cells*". MSc in Chemistry, Graduated: 2021.
- Bismark Amankwaa-Kyeremeh, Minerals and Resources, University of South Australia "*Sensing and Optimisation of Flotation Circuits and Integration with Grinding*", PhD in Minerals and Resources Engineering, Graduated: 2022.

- Jadhavar Ashok Arun, Physics, Savitribai Phule Pune University, "*Synthesis of intrinsic and doped nanocrystalline hydrogenated silicon (nc-Si:H) by using plasma enhanced chemical vapor deposition (PE-CVD)and evaluation of their opto-electronic properties for photovoltaic applications*". PhD in Physics, Graduated: 2020.
- Subhash Maruti Pandharkar, Physics, Savitribai Phule Pune University, "*Synthesis and study of quaternary chalcogenide absorbers for solar cell applications*". PhD in physics, Ggraduated: 2021.
- Aher Rahul Ashokrao, Physics, Savitribai Phule Pune University, "*Synthesis of graphene analogous layered ternary topological insulators and their sensing, field emission and other application*." PhD in physics, Graduated: 2021.
- Shruthi Sethumadhavan Nair, Physics, Savitribai Phule Pune University, "*Lead-free halide perovskite materials for photovoltaic applications: experimental and theoretical approach*." PhD in physics, Graduated: 2021.
- Ephraim Muriithi Kiarii, Chemistry, University Of Johannesburg, "*High Thermoelectric Performance and Electronic Structure of Traditional Thermoelectric/2D Hetero-Thermoelectric Materials for Efficient Energy Conversion: A first-Principles Study*". PhD in Chemistry, Graduated: 2020.
- Nemutudi Bradley, Physics, University Of Limpopo, "*Computational Modelling Studies of PtAs, PtAsS and Pd_2As Mineral Surfaces*". MSc in Physics, Graduated 2020.
- Elizeth Afonso Humba, Chemistry, The University of Namibia, "*Computational Study of the Structure and Electronic Properties of Ag- and Au-Doped $(TiO_2)_n$ Clusters (n = 2-6)*". MSc in Chemistry, Graduated: 2020.
- Sharlene-Asia Naicker, Physics, University of KwaZulu-Natal, Westville, South Africa, "*A Computational Study of Corrosive Sulphur on Metal Surfaces*". PhD in Physics, Graduated: 2020.
- Ephraim F. Marondedze, Chemistry, University Of Johannesburg, "*In-Silico Design Of A Novel Probe For The Potential Early Detection Of Alzheimer's Disease*". PhD in Chemistry, Graduated: 2019.
- Wahab Olaide Olalekan, Chemistry, University Of Johannesburg, "*Theoretical Prediction Of Solubility, Reactivity And Degradation Pathways Of Selected Azo Disperse Dyes*". PhD in Chemistry, Graduated: 2019.
- Francis Opoku, Chemistry, University Of Johannesburg, "*First–Principles Studies On The Development Of Semiconductor–Based Photocatalyst Materials For Applications In Photocatalytic Water Splitting And Degradation Of Pollutants*". PhD in Chemistry, Graduated: 2018.

TEACHING EXPERIENCE

- EGEE 437: Design of Solar Energy Conversion Systems, The Pennsylvania State University
- EME 301: Thermodynamics in Energy and Mineral Engineering, The Pennsylvania State University
- CH0002: Thermodynamics, Kinetics and Equilibria, Cardiff University, UK.
- PHY 901: Materials Modeling and Simulation, African University of Science and Technology (AUST), Nigeria.
- MSc Advanced mineralogy AW-4004, Utrecht University, The Netherlands.
- MSc Geo4-1426 Kinetic Processes course, Utrecht University, The Netherlands.
- Visiting lectures, "Surface chemistry and heterogeneous catalysis" Postgraduates, Chemistry, KNUST, Ghana.
- December 2013, Workshop organizer and instructor, "Electronic Structure Calculations", Centre for High Performance Computing (CHPC) annual National Conference, Cape Town, South Africa.
- Teaching Assistant: MAT 104 Introduction to Statistics, MTH 281 Computational Mathematics I, and STS 351 Statistical Computing; Department of Mathematics, University for Development Studies, Ghana.

LIST OF PEER-REVIEWED PUBLICATIONS (*Corresponding Author)

101. Narasimharao Kitchamsetti, Manopriya Samtham, Diwaka Singh, Ekta Choudhary, Sachin R. Rondiya, Yuan-Ron Ma, Russell W. Cross, 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**). DOI.
100. Rohini Udavant, Sachin Thawarkar, Sachin Rondiya, Ankita Shelke, Rahul Aher, Thalasseril G. Ajithkumar, Russell W. Cross, Nelson Y. Dzade, Sandesh Jadkar. "Lead-Free Solid State Mechanochemical Synthesis of $Cs_2NaBi_{1-x}Fe_xCl_6$ Double Perovskite: Reduces Band Gap and Enhances Optical Properties". ***Inorganic Chemistery*** (**2023**). DOI.
99. 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.

98. H.J. Yashwanth, Sachin R. Rondiya, Henry I. Eya, 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.

97. 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 Fe_3O_4 Support as Pre-Catalysts: An Experimental and In Silico Approach*". ***Molecules*** (**2023**), 28, 659. DOI.
96. Bidhan Pandit, Sachin R. Rondiya, Shoyebmohamad F. Shaikh, Mohd Ubaidullah, Ricardo Amaral, 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.
95. Patrick M. Bacirhonde, Nelson Y. Dzade, Henry I. Eya, 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.
94. 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.
93. H. J. Yashwanth, Sachin R. Rondiya, **Nelson Y. Dzade**, Robert L. Z. Hoye, Ram J. Choudhary, Deodatta M. Phase, Sanjay D. Dhole; K. Hareesh "*Improved photocatalytic activity of TiO_2 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
92. 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.
91. Sawanta S. Mali, Jyoti V. Patil, Sachin R. Rondiya, **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.
90. 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 Mo_2C Nanosheet Network Intimately Embedded in 3D NixMoOy Nanorod Arrays for pH-Universal Hydrogen Evolution*". ***Energy & Environmental Materials***, **(2022),** 0,1–15. DOI.
89. Patrick M. Bacirhonde, **Nelson Y. Dzade***, Carmen Chalony, Jeesoo 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.
88. Bidhan Pandit; Sachin R. Rondiya; Russell W. Cross; **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.
87. Barbara Farkaš, Aleksandar Živković, Veikko Uahengo, **Nelson Y. Dzade*** and Nora H. de Leeuw. "*First-Principles DFT Insights into the Stabilization of Zinc Diphosphide (ZnP_2) Nanocrystals via Surface Functionalization by 4-Aminothiophenol for Photovoltaic Applications"*. ***ACS Appl. Energy Mater.*** **(2022)**, 5, 2, 2318–2328, DOI.
86. Deepak Parmar, Cecil H. Botchway, **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.
85. Barbara Farkaš, Aleksandar Živković, Veikko Uahengo, **Nelson Y. Dzade*** and Nora H. de Leeuw. "*Insights from Density Functional Theory Calculations into the Effects of the Adsorption and Dissociation of Water on the Surface Properties of Zinc Diphosphide (ZnP_2) Nanocrystals"*. ***Phys. Chem. Chem. Phys.,*** **(2021)**, 23, 26482-26493, DOI.
84. Maria C. Spadaro, Simon E. Steinvall, **Nelson Y. Dzade**, Sara Marti-Sanchez, Pol Torres-Vila, Elias Z. Stutz, Mahdi Zamani, Rajrupa Paul, Jean-Baptiste Leran, Anna Fontcuberta i Morral, Jordi Arbiol. "*Rotated Domains in Selective Area Epitaxy Grown Zn_3P_2: Formation Mechanism and Functionality"*. ***Nanoscale,*** **(2021)**,13, 18441-18450, DOI.

83. Pramila Patil; Dilpreet Mann; Sachin Rondiya; **Nelson Y. Dzade**; Sung-Nam Kwon; Seok-In Na. "*Enhanced Performance of Perovskite Solar Cells via Reactive Post-Treatment Process Utilizing Guanidine Acetate as Interface Modifier*". ***Sol. RRL* (2021)**, 5, 2100547, DOI.
82. Russell W. Cross, Sachin R Rondiya, **Nelson Y. Dzade*** "*Theoretical Insights into the Hydrogen Evolution Reaction on the Ni_3N Electrocatalyst*". ***Catalysts* (2021)**, 11(6), 716, DOI.
81. Zhiyong Jia, Sachin R. Rondiya, Russell W. Cross, Cheng Wang, **Nelson Y. Dzade***, Chuang Zhang. "*Highly Active Methanol Oxidation Electrocatalyst based on 2D-NiO Porous Nanosheets: A Combined Computational and Experimental Study*". ***Electrochemical Acta* (2021)**, 394, 139143, DOI.
80. Sachin R. Rondiya, Yogesh A. Jadhav, Aleksandar Živković, Sagar B. Jathar, Ganesh K. Rahane, Russell W. Cross, Avinash V. Rokade, Rupesh S. Devan, Sadhu Kolekar, Robert L. Z. Hoye, Hirendra N. Ghosh, Nora H. de Leeuw, Sandesh R. Jadkar, **Nelson Y. Dzade*.** "*Solution-Processed Cd-Substituted CZTS Nanocrystals for Sensitized Liquid Junction Solar Cells*". ***Journal of Alloys and Compounds* (2021)**, 890, 161575, DOI.
79. Bidhan Pandit, Sachin Rondiya, Shyamal Shegokar, Lakshmana K. Bommineedi, Russell Cross, **Nelson Y. Dzade** and Babasaheb R. Sankapal. "*Reciprocated Electrochemical and DFT Investigations of Iron Selenide: Mechanically Bendable Solid-State Symmetric Supercapacitor*". ***Sustainable Energy Fuels* (2021)**, 5, 5001-5012, DOI.
78. Aleksandar Živković, Jacobina Sheehama, Michael E. A. Warwick, Daniel R. Jones, Claire Mitchel, Daniel Likius, Veikko Uahengo, **Nelson Y. Dzade**, Sankar Meenakshisundaram, Charles W. Dunnill and Nora H. de Leeuw. "*Structural and Electronic Properties of CuxOy (Paramelaconite): The Role of Native Impurities*". ***Pure and Applied Chemistry* (2021)**, 93, 1229-1244, DOI.
77. Ratna Chauhan, Manish Shinde, Yogesh Sethi, Yogesh Waghadkar, Sachin R Rondiya**,** **Nelson Y. Dzade**, Suresh Gosavi, Mohd Muddassir. "*Indium-doped ZnO as Efficient Photosensitive Material for Sunlight-driven Hydrogen Generation and DSSC Applications: Integrated Experimental and Computational Approach*". ***Journal of Solid State Electrochemistry* (2021)**, 25, 2279–2292, DOI.
76. Mamta P. Nasane, Sachin R. Rondiya, Chandradip D. Jadhav, Ganesh R. Rahane, Russell W. Cross, Sagar Jathar, Yogesh Jadhav, Sunil Barma, Dhanaraj Nilegave, Vijaya Jadkar, Avinash Rokade, Adinath Funde, Padmakar G. Chavan, Robert L. Z. Hoye, **Nelson Y. Dzade*** & Sandesh Jadkar* "*An Interlinked Computational–Experimental Investigation into SnS Nanoflakes for Field Emission Applications*". ***New J. Chem.*, (2021)**, 45, 11768-11779, DOI.
75. Sawanta S. Mali, Jyoti V. Patil, Pravin S. Shinde, Gustavo de Miguel, Sachin R. Rondiya, **Nelson Y. Dzade**, and Chang Kook Hong. "*Implementing Dopant-Free Hole Transporting Layers and Metal Incorporated $CsPbI_2Br$ for Stable All-Inorganic Perovskite Solar Cells*". ***ACS Energy Letters*, (2021)**, 6, 778−788, DOI.
74. ***Nelson Y. Dzade**** "*First-principles Insights into the Electronic Structure, Band Alignment, and Optical Properties of Cu_2SrSnS_4: An Earth-Abundant Material for Photovoltaics*". ***Scientific Reports*, (2021)**, 1, 4755, DOI.
73. Sachin R. Rondiya, Dilara Gokcen Buldu, Guy Brammertz, Yogesh Jadhav, Russell W. Cross, Hirendra N. Ghosh, Thomas Davies, Sandesh R Jadkar, **Nelson Y. Dzade*** and Bart Vermang. "*Revealing the Electronic Structure, Heterojunction Band Offset and Alignment of $Cu_2ZnGeSe_4$: A Combined Experimental and Computational Study towards Photovoltaic Applications*". ***Phys. Chem. Chem. Phys.*, (2021)**, 23, 9553-9560, DOI.
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BOOK CHAPTERS

1. Sachin R. Rondiy, 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.
2. Moses Kigozi, 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

- **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 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, @ 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 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 training:** "*Literature Review Online Training (Learning the Basics of Research)*", Giant 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, Ozar, Nashik, 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 Publisher Symposium: "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 17th. 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, Gaborone, Botswana.
- **Invited speaker:** "*Band-gap 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 NOx at mackinawite (FeS) surfaces*". The Centre for High Performance Computing National Conference, December 2–6, 2012, Durban International Convention Centre, Durban, 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 CO_2 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 CO_2 activation and reduction*". The World Association of Theoretical & Computational Chemists (WATOC) Congress, July 17–22, 2011, Santiago de Compostela, Spain.
- **Contributed talk:** "*Silicene and transition metal-based materials: prediction of a two-dimensional piezomagnet*" Poster, School and Conference on "Emergent Properties and Novel Behaviour at the Nanoscale", Jawaharlal Nehru Centre for Advanced Scientific Research, April 19–24, 2010, Bangalore, India.

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
- European Association of Geochemistry (EAG)
- EPSRC Full College Membership (Reviews EPSRC-UKRI research grant applications)

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