



DR NELSON YAW DZADE

Address: John and Willie Leone Family Department of Energy and Mineral Engineering, The Pennsylvania State University, Hosler Building, University Park, PA 16802, USA.

Email: Nxd5313@psu.edu; DzadeNY@cardiff.ac.uk; Dzanelly@gmail.com

Mobile: +18148265004; **Office Tel:** +18148674227

Research Group Webpage URL: <https://sites.google.com/view/nelsondzade>

PERSONAL PROFILE

Highly motivated computational materials and minerals scientist with over a decade experience in the development and application of the state-of-the-art computational materials modelling and simulation techniques in synergy with novel experimental approaches to (a) predict structure-property relationships and accelerate the discovery and rational design of advanced functional materials for catalytic and optoelectronic applications including solar cells; (b) describe surface and interface phenomena and provide mechanistic insights into catalytic reactions that are critical to the development of active and selective heterogeneous catalysts; (c) obtain information about the atomic structure and electronic states that may be hard to access experimentally; and (d) provide detailed atomic-level insights into environmentally relevant reactions and geochemical processes occurring at mineral surfaces/interfaces. 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 Chemistry and Materials Science**, University College London (UCL), London, United Kingdom. Dissertation entitled: *“Computational study of the interactions of small pollutant molecules with the surfaces of iron-bearing minerals”* Under the guidance of Professor Nora de Leeuw and Professor Richard Catlow.
- 2009–2010 **Postgraduate Diploma (PGDip) Materials Science**, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Thesis entitled: *“Phonon softening near crack opening: a first-principles DFT study”*. Under the guidance of Professor Umesh Waghmare and Professor C. N. R. Rao.
- 2008–2009 **MSc Materials Science, Distinction**, African University of Science and Technology, Abuja, Nigeria. Thesis entitled: *“Energetics and stabilities of molecule-electrode interfaces: A First-principles Study”*
- 2003–2007 **BSc Mathematical Science (Statistics option), First Class Honours**, University for Development Studies, Tamale, Ghana. Project work: *“Line Transect Sampling: An evaluation of models and field experiments”* under the guidance of Prof. Kaku Sagary Nokoe.

PROFESSIONAL RESEARCH EXPERIENCE and POSITIONS

- 2021–Date **Assistant Professor (Tenure Track)**, John and Willie Leone Family Department of Energy and Mineral Engineering, The Pennsylvania State University, USA
- 2018–2021 **EPSRC-UKRI Innovation Fellow and Independent Research Group Leader**, School of Chemistry, Cardiff University, UK.
- 2018–date **Visiting Assistant Professor**, African University of Science and Technology (AUST), Abuja-FCT, Nigeria
- 2020–date **Assessor (External Based Abroad)**, University of Limpopo, South Africa.
- 2020–date **Assessor (External Based Abroad)**, University of KwaZulu-Natal, Westville South Africa
- 2020–date **Assessor (External Based Abroad)**, University of Namibia, Namibia.
- 2020–date **Assessor (External Based Abroad)**, Savitribai Phule Pune University, India
- 2018–date **Assessor (External Based Abroad)**, University of Johannesburg, South Africa.
- 2015–date **Co-investigator/Trainer on the 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 Universities of Namibia and Botswana.
- 2012–2019 **Visiting Research Fellow**, Kwame Nkrumah University of Science and Technology via the UCL-KNUST Leverhulme-Royal Society Africa Award initiative program on *“Computational design of materials for energy efficiency”*.
- Feb–Jun 2018 **Research Associate in Computational Materials Chemistry**, School of Chemistry, Cardiff University. Research Project title *“Electronic structure characterization of the geometric and electronic structures of multi-phase sulfide materials for solar energy applications”*.

- 2014–2017 **Postdoctoral Research Fellow**, Utrecht University, Funded by Netherlands Organization for Scientific Research (NWO). Research project title: “Computer-aided design of iron-sulfide nanocatalysts for the solar-driven conversion of CO₂ to fuels”.
- 2012–2013 **Research Fellow**, British Petroleum (BP), Pangbourne technology centre, 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**, Department of Mathematics, University for Development studies, Ghana.

SCHOLARSHIPS and AWARDS

- 2020–date DUO-India Professor Fellowship Award, Cardiff University, UK
- 2018–date EPSRC-UKRI Innovation Research Fellowship Award, Cardiff University, UK
- 2010–2014 Overseas Research Scholarship, University College London, UK.
- 2010–2014 UCL Faculty of Mathematical and Physical Sciences Studentship, UK.
- 2012–2013 British Petroleum (BP) Research 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 for brilliant students, 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 of the 2006/2007 academic year, University for Developments Studies, Tamale, Ghana.

RESEARCH GRANTS

FUNDED/AWARDED

- **Principal Investigator:** DUO-India Professor Fellowship Award “*Rationally design of novel ABO₃ 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-Investigator:** Natural Environment Research Council (NERC) research grant for the project “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-Investigator:** Netherlands Organisation for Scientific Research (NWO) ECHO grant “Earth-abundant materials for the sustainable catalysis of CO₂ to fuels and chemicals: Linking computation to experiment”. Funded value: €250,000; Funded Period Dec 2018 - Dec 2021).

UNDER EVALAUTION

- **Co-Applicant:** European Innovation Council Pathfinder - Consortium Grant. “*SOLARUP: Advanced Strategies for Development of Sustainable Semiconductors for Scalable Solar Cell Applications*”. Submitted (2021). Total amount requested: €3,110,615.65 (amount to be received by me: €568,148.15)

GRADUATE/POSTGRADUATE STUDENTS SUPERVISION

ONGOING

- **Main supervisor:** Ricardo Amaral, PhD Candidate, Pennsylvania State University, “*Rational design of earth-abundant heterojunction photocatalysts for carbon dioxide conversion*”
- **Main supervisor:** Russell William Cross, PhD Candidate, Cardiff University, “*Computer-aided design of improved transition metal phosphides catalysts for efficient hydrogen evolution reaction (HER)*”
- **Co-supervisor:** Dario Campisi, PhD research, Leiden University, working on “*Computational investigation of polycyclic aromatic hydrocarbons (PAHs) interactions of olivine surface (typical minerals found in meteorites)*”
- **Co-supervisor:** Cecil H. Botchway, PhD research, NJUST, working on “*Mechanistic study of ethanol conversion to hydrocarbons over zeolites perlielite and ferrierite*”

COMPLETED (PAST STUDENTS)

- **Main supervisor:** Dr Sachin Rondiya, Postdoctoral Research Associate, Cardiff University, worked on the project “*Rational design of zinc phosphide heterojunctions for efficient solar energy conversion*” 2019-2021

- **Main supervisor:** Dr Patrick Heasman, Postdoctoral Research Associate, Cardiff University, worked on project “*Ab initio investigation of O₂ adsorption on SmCoO₃-based cathode materials for solid oxide fuel cells*” 2019-2020
- **Main supervisor:** Sophie Colton, MChem research project, Cardiff University. “*Computational design of chalcogenide perovskites for solar energy conversion applications*”
- **Main supervisor:** Eloise Lewis, MChem research project, Cardiff University, “*First-principles mechanistic insight into the adsorption of arsenic on cobalt ferrite (Fe₂CoO₄) surfaces: Implications for water purification.*”
- **Main supervisor:** Connor Duggan, BSc research project, Cardiff University, “*XPS valence band spectra of BaZrS₃: insights from density functional theory calculations*”
- **Main supervisor:** Lewis Old, BSc research project, Cardiff University, “*Optoelectronic properties of CaZrSe chalcogenide perovskite calculated from first principles theory*”
- **Main Supervisor:** Kigozi Moses, PhD thesis 2021, African University of Science and Technology, worked on “*Activated carbon and graphene oxide for supercapacitor and batteries application*”
- **Main Supervisor:** Jemima Moorcroft, BSc research project 2019, Cardiff University, worked on “*CO₂ adsorption and activation on bimetallic Fe-Ni catalysts: A dispersion-corrected DFT analysis*”
- **Co-supervisor:** Elliot S. Menkah, PhD thesis 2019, KNUST-Ghana, worked on “*Computational design of bimetallic Ni-Ru catalysts for the conversion of syngas to synthetic fuels*”
- **Main Supervisor:** Timoteüs F. J. Bögels, MSc research 2019, Utrecht University, worked on “*Analyzing hydrogen evolution reaction catalytic sites of nickel sulfides, a first-principle DFT study*”
- **Co-supervisor:** Albert Aniagyei, PhD thesis 2018, KNUST-Ghana, worked on “*Theoretical studies of oxygen (O₂) reduction on calcium-, strontium- and barium-doped lanthanum manganite (LaMnO₃) as cathode materials in solid oxide fuel cells.*”
- **Main supervisor:** Jasper Huijsmans BSc project 2018, Utrecht University, worked on “*Computational study of the influence of inorganic solution components on lithium carbonate crystal growth*”
- **Co-supervisor:** Caroline R. Kwawu, PhD thesis 2017, KNUST-Ghana, worked on “*Computational study of the conversion of CO₂ to fuel or chemicals on pure and Ni-coated iron surfaces*”
- **Main supervisor:** Manon Dierkx, BSc project 2017, Utrecht University, worked on “*Computer simulation of the effects of pH on phosphate adsorption to iron-oxides*”
- **Co-supervisor:** Isaac W. Boateng, MPhil thesis 2016, KNUST-Ghana, worked on “*Computational study of hydrogen adsorption on the (010) surface of Lanthanum ferrite (LaFeO₃)*”
- **Co-supervisor:** Joel Baffour Awuah, MPhil thesis 2015, KNUST-Ghana, “*Computational study arsenic immobilization by the Al(III)-modified zeolite clinoptilolite*”

TEACHING EXPERIENCE

January 2020	CH0002: Thermodynamics, Kinetics and Equilibria, School of Chemistry, Cardiff University
Nov. 12-30, 2018	Visiting Lectures, “PHY 901: Materials Modeling and Simulation” Postgraduates, African University of Science and Technology (AUST), Abuja, Nigeria.
April-May 2018	Guest lectures, “Surface geochemistry and computational mineralogy”, on the MSc Advanced mineralogy AW-4004 course; Geochemistry, Utrecht University, The Netherlands.
September 2017	Visiting lectures through Africa Research Consortium in Renewable Energy, “ <i>Chemistry of Materials</i> ”, Postgraduates, Chemistry, University of Namibia, Windhoek, Namibia.
March-April 2017	Guest lectures, “Surface chemical reactions and transition state theory”, on the MSc Geo4-1426 Kinetic Processes course; Geochemistry, Utrecht University, The Netherlands.
Aug-Sept 2016	Visiting lectures: <i>Materials discovery and design from first-principles calculations</i> ; Postgraduates Chemistry, KNUST, Ghana.
July-August 2013	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.
Aug 2007- Jul 2008	Teaching Assistant: MAT 104 Introduction to Statistics, MTH 281 Computational Mathematics I, and STS 351 Statistical Computing; Undergraduates, Department of Mathematics, UDS, Ghana.

LIST OF PEER-REVIEWED PUBLICATIONS (*Corresponding author)

82. Russell W. Cross, Sachin R Rondiya, **Nelson Y. Dzade*** “*Theoretical insights into the hydrogen evolution reaction on the Ni₃N electrocatalyst*” *Catalysts* (2021), 11(6), 716

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
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), <https://doi.org/10.1016/j.jallcom.2021.161575>
79. Bidhan Pandit, Sachin R. Rondiya, Shyamal Shegokar, Lakshmana K. Bommineedi, Russell William Cross, **Nelson Yaw Dzade** and Babasaheb R. Sankapal. "Reciprocated Electrochemical and DFT Investigations of Iron Selenide: Mechanically Bendable Solid-State Symmetric Supercapacitor" *Sustainable Energy Fuels*, (2021), Accepted Manuscript. DOI: <https://doi.org/10.1039/D1SE00074H>
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 Cu₄O₃ (paramelaconite): the role of native impurities" *Pure Appl. Chem.* (2021), DOI: <https://doi.org/10.1515/pac-2021-0114>.
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
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
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 CsPbI₂Br for Stable All-Inorganic Perovskite Solar Cells." *ACS Energy Letters*, (2021), 6, 778–788.
74. **Nelson Y. Dzade***. First-principles insights into the electronic structure, band alignment, and optical properties of CSTS: an earth-abundant material for photovoltaics. *Scientific Reports*, (2021), 1, 4755.
73. Sachin R. Rondiya, Dilara Gokcen Buldu, Guy Brammertz, Yogesh Jadhav, Russell William Cross, Hirendra N. Ghosh, Thomas Davies, Sandesh R Jadkar, **Nelson Yaw Dzade*** and Bart Vermang. "Revealing the Electronic Structure, Heterojunction Band Offset and Alignment of Cu₂ZnGeSe₄: A Combined Experimental and Computational Study towards Photovoltaic Applications". *Phys. Chem. Chem. Phys.*, (2021), 23, 9553-9560.
72. Chandradip D. Jadhav, Sachin R. Rondiya, Reshma C. Hambire, Devshri R. Baviskar, Russell W. Cross, **Nelson Y. Dzade**, Padmakar G. Chavan. "Highly Efficient Field Emission Properties of Vertically Aligned 2D CuSe Nanosheets: an Experimental and Theoretical Investigation" *Journal of Alloys and Compounds*, (2021), 875 159987.
71. M. S. Patil, N. Kitchamsetti, S. R. Mulani, S. R. Rondiya, R. W. Cross, N. Y. Dzade, P. S. Patil, Y.-R. Ma, R. S. Devan. "Photocatalytic behavior of Ba(Sb/Ta)₂O₆ perovskite for reduction of organic pollutants: Experimental and DFT correlation" *Journal of the Taiwan Institute of Chemical Engineer* (2021), 122, 201-209.
70. Dario Campisi, Thanja Lamberts, **Nelson Y. Dzade**, Rocco Martinazzo, Inge Loes ten Kate, and Alexander G. G. M. Tielens. "Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method." *J. Phys. Chem. A* (2021), 125, 13, 2770–2781
69. B. H. Mamatha, Sachin R. Rondiya, M. G. Ashritha, **Nelson Y. Dzade**, S. D. Dhole, Jim Williams, K. Hareesh. " Polymer-wrapped reduced graphene oxide/nickel-cobalt ferrite nanocomposites as tertiary hybrid supercapacitors: insights from experiment and simulation" *Journal of Science: Advanced Materials and Devices*, (2021), 6, 291-301.
68. Sagar B. Jathar, Sachin R. Rondiya, Yogesh A. Jadhav, Dhanaraj S. Nilegave, Russell W. Cross, Sunil V. Barma, Mamta P. Nasane, Shankar A. Gaware, Bharat R. Bade, Sandesh R. Jadkar, Adinath M. Funde, **Nelson Y. Dzade***. "Ternary

- Cu₂SnS₃: synthesis, structure, photoelectrochemical activity, and heterojunction band offset and Alignment*". **Chemistry of Materials**, (2021), 33, 6, 1983–1993.
67. Sachin Thawarkar, Sachin R. Rondiya, Prem Jyoti Singh Rana, Ramanujan Narayan, **Nelson Y. Dzade**, Surya Prakash Singh. "Structural and optical properties of ionic liquid-based hybrid perovskite: a combined experimental and theoretical investigation." **Functional Materials Letters**, (2021), Accepted. DOI: [10.1142/S1793604721500089](https://doi.org/10.1142/S1793604721500089)
 66. Bidhan Pandit, Sachin R. Rondiya, **Nelson Y. Dzade**, Shoyebmohamad F. Shaikh, Nitish Kumar, Emad S. Goda, Abdullah A. Al-Kahtani, Rajaram S. Mane, Sanjay Mathur, Rahul R. Salunkhed. "High stability and long cycle life of rechargeable sodium-ion battery using manganese oxide cathode: A combined density functional theory (DFT) and experimental study." **ACS Applied Materials & Interfaces**, (2021), 13, 11433–11441.
 65. Sachin Thawarkar, Sachin R. Rondiya, Nageshwar D. Khupse, **Nelson Y. Dzade**, Sandesh Jadkar. "Experimental and Theoretical Investigation of the Structural and Opto-electronic Properties of Fe-Doped Lead-Free Cs₂AgBiCl₆ Double Perovskite." **Chemistry - A European Journal**, (2021), 27, 1–11.
 64. Eloise Lewis and **Nelson Y. Dzade***. "First-Principles Density Functional Theory Characterisation of the Adsorption Complexes of H₃AsO₃ on Cobalt Ferrite (Fe₂CoO₄) Surfaces". **Minerals**, (2021), 11(2), 195.
 63. Ajinkya Bhorde, Ravindra Waykar, Sachin R. Rondiya, Shruthi Nair, Ganesh Lonkar, Adinath Funde, **Nelson Y. Dzade***, Sandesh Jadkar. "Structural, Electronic, and Optical Properties of Lead-Free Halide Double Perovskite Rb₂AgBiI₆: A Combined Experimental and DFT Study." **ES Materials & Manufacturing**, (2021), 12, 43-52.
 62. Girish P. Patil, Sachin R. Rondiya, Vivekanand S. Bagal, Sugam Shivhare, Russell W. Cross, **Nelson Y. Dzade**, Sandesh R. Jadkar, Padmakar. G. Chavan. "Field Emission Characteristics of Double Walled TiO₂ Nanotubes." **ES Materials & Manufacturing**, (2021), 13, 76-81.
 61. **Nelson Y. Dzade***, and Nora H. de Leeuw. "Activating the FeS (001) Surface for CO₂ Adsorption and Reduction through the Formation of Sulfur Vacancies: A DFT-D3 Study." **Catalysts**, (2021), 11(1), 127.
 60. Guang Xian Pei, **Nelson Y. Dzade**, Yue Zhang, Jan P. Hofmann, Nora H. de Leeuw, Bert M. Weckhuysen. "Identification of Photoexcited Electron Relaxation in a Cobalt Phosphide Modified Carbon Nitride Photocatalyst." **ChemPhotoChem**, (2021), 5, 1–6.
 59. M.G. Ashritha, S.R. Rondiya, R. W. Cross, **N. Y. Dzade**, S. Dhole, D.V. Sunitha, K. Hareesh. "Experimental and computational studies of sonochemical assisted anchoring of carbon quantum dots on reduced graphene oxide sheets towards the photocatalytic activity." **Applied Surface Science**, (2021), 545, 148962.
 58. N. Kitchamsetti; M. S Ramteke; S. R. Rondiya, S. R. Mulani; M. S. Patil, R. W. Cross, **N. Y. Dzade**; R. Devan. "Experimental and DFT correlations on the photocatalytic activities of NiO nanobelts for removal of organic pollutants." **Journal of Alloys and Compounds**, (2021), 855, 157337.
 57. Bharat R. Bade, Sachin Rondiya, Yogesh A. Jadhav, Mahesh M. Kamble, Sunil V. Barma, Sandesh R. Jadkar, Adinath M. Funde, **Nelson Y. Dzade***. "Investigations of the structural, optoelectronic, and band alignment properties of Cu₂ZnSnS₄ nanocrystals: prepared by hot-injection method towards low-cost photovoltaic applications." **Journal of Alloys and Compounds**, (2021), 854, 157093.
 56. Russell W. Cross, Sachin R. Rondiya and **Nelson Y. Dzade***. "First-principles DFT Insights into the Adsorption of Hydrazine on Bimetallic β 1-AB Catalyst: Implications for Direct Hydrazine Fuel Cells." **Applied Surface Science**, (2021), 536, 147648.
 55. Ganesh K. Rahane, Sagar B. Jathar, Sachin R. Rondiya, Yogesh A. Jadhav, Sunil V. Barma, Avinash Rokade, Russell W. Cross, Mamta P. Nasane, Vijaya Jadkar, **Nelson Y. Dzade**, Sandesh R. Jadkar. "Photoelectrochemical Investigation on the Cadmium Sulfide (CdS) Thin Films Prepared using Spin Coating Technique." **ES Materials & Manufacturing**, (2021), 11, 57-64.
 54. Parameshwar R. Chikate, Alfa Sharma, Sachin R. Rondiya, Russel W. Cross, **Nelson Y. Dzade**, Parasharam M. Shirage, and Rupesh S. Devan. "Hierarchically interconnected ZnO nanowires for low temperature operated reducing gas sensors: Experimental and DFT studies." **New J. Chem.**, (2021), 45, 1404-1414.

53. Sunil V. Barma, Sachin R. Rondiya, Yogesh A. Jadhav, Sagar B. Jathar, Ganesh K. Rahane, Avinash Rokade, Russell W. Cross, Mamta P. Nasane, Vijaya Jadhkar, **Nelson Y. Dzade**, Sandesh R. Jadhkar. "Structural, Optoelectronic, and Photoelectrochemical Investigation of CdSe NCs Prepared by Hot Injection Method." *ES Materials & Manufacturing*, (2021), 11, 50-56.
52. Bonaventure A. Odeke, Gyang D. Chung, Jesutofunmi A. Fajemisin, Kabir S. Suraj, Kiplangat D. Tonui, Ayinla R. Tobi, Thomas C. Bewaale, Jamiu A. Ajibola, **Nelson Y. Dzade***. "Electronic Structure and Surface Properties of Copper Thiocyanate: A Promising Hole Transport Material for Organic Photovoltaic Cells." *Materials*, (2020), 13(24), 5765.
51. S. E. Steinvall, E. Stutz, R. Paul, M. Zamani, **N. Y. Dzade**, V. Piazza, M. Friedl, V. de Mestral, J.B. Leran, R. R. Zamani, A. F. i Morral. "Towards Defect-Free Thin Films of the Earth-Abundant Absorber Zinc Phosphide by Nano-patterning." *Nanoscale Advances*, (2020), 3, 326-332.
50. Cecil H. Botchway, Richard Tia, Evans Adei, Alex O'Malley, **Nelson Y. Dzade***, Carlos Hernandez-Tamargo, Nora H. de Leeuw. "Influence of Topology and Brønsted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI." *Catalysts* (2020), 10(11), 1342.
49. Kigozi Moses, Ravi Kali, Abdulhakeem Bello, Balaji Padya, Azikiwe Peter Onwualu, Pawan Kumar Jain, **Nelson Y. Dzade***. "Modified Activation Process for Supercapacitor Electrode Materials from African Maize Cob." *Materials* (2020), 13(23), 5412.
48. **Nelson Y. Dzade*** "First-Principles Mechanistic Insights into the Coadsorption and Reaction of CO₂ and H₂O on Tantalum Nitride Surfaces." *Catalysts* (2020), 10(10), 1217.
47. Freddy E. Oropeza, **Nelson Y. Dzade**, Amalia Pons-Martí, Zhenni Yang, Kelvin H. L. Zhang, Nora H. de Leeuw, Emiel J. M. Hensen, and Jan P. Hofmann. "Electronic Structure and Interface Energetics of CuBi₂O₄ Photoelectrodes." *J. Phys. Chem. C* (2020), 124, 41, 22416–22425
46. Mandlika, N. T.; Sahare, P. D.; Rondiya, S. R.; **Dzade, N. Y.**; Deore, A. V.; Dahiwal, S. S.; Dhole, S. D. "Characteristics of K₂Ca₂(SO₄)₃:Eu TLD Nanophosphor for its Applications in Electron and Gamma Rays Dosimetry." *of Optical Materials*, (2020), 109, 110272.
45. Nyepetsi, M.; Mbaiwa, F.; Oyetunji, O. A., **Dzade, N.Y.***; N.H. de Leeuw. "The Carbonate-Catalysed Transesterification of Sunflower Oil for Biodiesel Production: In Situ Monitoring and Density Functional Theory Calculations." *Accepted: South African Journal of Chemistry*, (2020).
44. Botchway, C. H.; Tia, R.; Adei, E.; **Dzade, N. Y.***; Nora H. de Leeuw. "Methanol Adsorption and Conversion to Ethanol and Dimethyl Ether Catalyzed by Ferrierite Zeolites: A First-Principles DFT Study." *Accepted: South African Journal of Chemistry*, (2020).
43. Yashwanth, H. J.; Rondiya, S. R.; **Dzade, N. Y.** Dhole, S.D.; Hareesh, K. "Enhanced photocatalytic activity of N, P, co-doped carbon quantum dots: An insight from experimental and computational approach." *Journal of Vacuum*, (2020), 180, 109589.
42. Wu, L.; **Dzade, N. Y.**; Chen, N.; van Dijk, B.; Balasubramanyam, S.; Sharma, A.; Gao, L.; Hettterscheid, D. G. H.; Hensen, E. J. M.; Bol, A. A.; de Leeuw, N. H.; Hofmann, J. P. "Cu Electrodeposition on Nanostructured MoS₂ and WS₂ and Implications for HER Active Site Determination." *J. Electrochem. Soc.* (2020), 167 116517.
41. Rondiya, S. R.; Karbhal, I.; Jadhav, C. D.; Nasane, M. P.; Davies, T.; Shelke, M. V.; Jadhkar, S. R.; Chavan, P. G.; **Dzade, N. Y.*** "Uncovering the origin of enhanced field emission properties of rGO-MnO₂ heterostructures: a synergistic experimental and computational investigation." *RSC Advances*, (2020), 10, 25988-25998.
40. Rondiya, S. R.; Jadhav, Y.; **Dzade, N. Y.**; Ahammed, R.; Goswami, T.; Sarkar, A. D.; Jadhkar, S. R.; Haram, S.; Ghosh, H. N. "An Experimental and Theoretical Study into Interface Structure and Band Alignment of the Cu₂Zn_{1-x}Cd_xSnS₄ Heterointerface for Photovoltaic Applications." *ACS Applied Energy Materials*, (2020), 3, 5153–5162.
39. Baviskar, P. K.; Rondiya, S. R.; Patil, G. P.; Sankapal, B. R.; Pathan, H. M.; Chavan, P. G.; **Dzade, N. Y.*** "ZnO/CuSCN Nano-heterostructure as a Highly Efficient Field Emitter: A Combined Experimental and Theoretical Investigation." *ACS Omega*, (2020), 5, 6715-6724.

38. Cross, R. W.; **Dzade, N. Y.*** "First-principles mechanistic insights into the hydrogen evolution reaction on Ni₂P electrocatalyst in alkaline medium." *Catalysts*, (2020), 10, 307.
37. Amakali, T.; Daniel, L. S.; Uahengo, V.; **Dzade, N. Y.***; Nora H. de Leeuw. "Structural and Optical Properties of ZnO Thin Films Prepared by Molecular Precursor and Sol-gel Methods." *Crystals* (2020), 10(2), 132.
36. Rondiya, S. R.; Jadhav, C. D.; Chavan, P. G.; **Dzade, N.Y.*** "Enhanced Field Emission Properties of Au/SnSe Nano-heterostructure: A Combined Experimental and Theoretical Investigation." *Scientific Reports* (2020) 10, 2358.
35. Eya, H. I.; Ntsoenzok, E.; **Dzade, N. Y.*** "First-principles Investigation of the Structural, Elastic, Electronic, and Optical Properties of α - and β -SrZrS₃: Implications for Photovoltaic Applications." *Materials* (2020), 13(4), 978.
34. Mandlik, N. T.; Rondiya, S.; Kulkarni, M. S.; Sahare, P. D.; Bhatt, B. C.; **Dzade, N. Y.** "Thermoluminescence and Optically Stimulated Luminescence Characteristics of CaSO₄:Eu Nanophosphor: An Experimental and Density Functional Theory (DFT) Investigation." *Journal of Luminescence*, (2020), 221, 117051.
33. Kamble, M. M.; Bade, B. R.; Rondiya, S. R.; Nasane, M. P.; **Dzade, N. Y.**; Funde, A. M.; S. R. Jadkar. "Optical, Structural and Morphological Study of CdS Nanoparticles: Role of Sulphur Source." *Nanomaterials and Energy*, (2020), 1, 1-9.
32. **Dzade, N. Y.** "First-Principles Insights into the Interface Chemistry between 4-Aminothiophenol and Zinc Phosphide (Zn₃P₂) Nanoparticles." *ACS Omega*, (2020), 5, 1025–1032.
Featured as Supplementary Cover: ACS Omega, Issue 2 (2020)
31. **Dzade, N. Y.** "Unravelling the early oxidation mechanism of zinc phosphide (Zn₃P₂) surfaces by adsorbed oxygen and water: a first-principles DFT-D3 investigation." *Phys. Chem. Chem. Phys.*, (2020), 22, 1444-1456.
30. Rondiya, S.; Jadhav, Y.; Nasane, M.; Jadkar, J.; **Dzade, N.Y.** "Combined Computational and Experimental Investigation of the Interface Structure and Band Alignment in CZTS/CdS Heterojunction for Solar Cell Applications." *Materials*, (2019), 12, 4040.
29. King, H. E.; Salisbury, A.; Huijsmans, J.; **Dzade, N. Y.**; Plümper, O. "Influence of inorganic solution components on lithium carbonate crystal growth." *Crystal Growth & Design* (2019), 19, 12, 6994-7006.
28. Bade, B. R.; Rondiya S.; Bhopale, S. R.; **Dzade, N. Y.**; Kamble, M. M.; Rokade, A.; Nasane, M. P.; More, M. A.; Jadkar, S. R.; Funde, A. M. "Investigation of Growth Mechanism for Highly Oriented TiO₂ Nanorods: The Role of Reaction Time and Annealing Temperature." *Springer Nature Applied Sciences*, (2019), 1, 1073.
27. Wu, L.; **Dzade, N. Y.**; Yu, M.; Mezari, B.; van Hoof, A. J. F.; Friedrich, H.; de Leeuw, N. H.; Hensen, E. J. M.; Hofmann, J. P. "Unraveling the Role of Lithium in Enhancing the Hydrogen Evolution Activity of MoS₂: Intercalation versus Adsorption." *ACS Energy Letters* (2019), 471733–1740.
26. Wu, L; Longo, A; **Dzade, N.Y.**; Sharma, A.; Hendrix, M. M. R. M.; Bol, A.A; De Leeuw, N.H.; Hensen, E. J. M.; Hofmann, J.P. "The Origin of High Activity of Amorphous MoS₂ in the Hydrogen Evolution Reaction." *ChemSusChem* (2019), (2019), 12,1–8.
Featured as Outside Front Cover: ChemSusChem, Issue 19, 2019.
25. Jossou, E. E.; Malakkal, L.; **Dzade, N. Y.**; Claisse, A.; Szpunar, B.; Szpunar, J. A. "DFT+U Study of the Adsorption and Dissociation of Water on Clean, Defective and Oxygen-Covered U₃Si₂ {001}, {110}, and {111} Surfaces." *J. Phys. Chem. C* (2019), 123, 19453–19467.
24. Živković, A.; Farkaš, B.; Uahengo, V.; de Leeuw, N.H.; **Dzade, N.Y.*** "First-principles DFT insights into the structural, elastic, and optoelectronic properties of α and β -ZnP₂: implications for photovoltaic applications." *J Phys Condens Matter*. (2019), 31, 265501.
23. Menkah, E. S.; **Dzade, N. Y.***; Tia, R.; Adei, E.; de Leeuw, N. H. "Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study." *Applied Surface Science* (2019), 480, 1014-1024.

22. Wu, L; van Hoof, A. J. F.; **Dzade, N. Y.**; Gao, L.; Richard, M. I.; Friedrich, H.; De Leeuw, N. H.; Hensen, E. J. M.; Hofmann, J. P. "Enhancing the electrocatalytic activity of 2H-WS₂ for hydrogen evolution via defect engineering." *Phys. Chem. Chem. Phys.*, (2019), 21, 6071-6079.
21. Aniagaeyi, A.; **Dzade, N. Y.***; Tia, R.; Adei, E.; Catlow, C. R. A. and de Leeuw, N.H. "Ab initio investigation of O₂ adsorption on Ca-doped LaMnO₃ cathodes in solid oxide fuel cells." *Phys. Chem. Chem. Phys.*, (2018), 20, 28685-28698.
20. **Dzade, N. Y.*** and de Leeuw, N. H. "Density functional theory characterization of the structures of H₃AsO₃ and H₃AsO₄ adsorption complexes on ferrihydrite." *Environ. Sci.: Processes Impacts*, (2018), 20, 977-987.
19. Jossou, E.; Eduok, U.; **Dzade, N. Y.**; Szpunar, B.; and Szpunar, J. A. "Oxidation behaviour of U₃Si₂: An experimental and first principles investigation." *Phys. Chem. Chem. Phys.*, (2018), 20, 4708-4720.
18. **Dzade, N. Y.*** and de Leeuw, N. H. "Adsorption and desulfurization mechanism of thiophene on layered FeS (001), (011) and (111) surfaces: A DFT-D2 study." *J. Phys. Chem. C*, (2018), 122, 359-370.
17. **Dzade, N. Y.*** and de Leeuw, N. H. "Periodic DFT+U investigation of the bulk and surface properties of marcasite (FeS₂)." *Phys. Chem. Chem. Phys.* (2017), 19, 27478-27488.
16. Santos-Carballal, D.; Roldan, A.; **Dzade, N. Y.** and de Leeuw, N.H. "Reactivity of CO₂ on the surfaces of magnetite (Fe₃O₄), greigite (Fe₃S₄) and mackinawite (FeS)." *Phil. Trans. R. Soc. A* (2017), 376, 20170065.
15. Kwawu, C. R.; Tia, R.; Adei, E.; **Dzade, N. Y.***; Catlow, C. R. A.; and de Leeuw, N. H. "CO₂ activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study." *Phys. Chem. Chem. Phys.* (2017), 19, 19478.
14. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "Structures and properties of As(OH)₃ adsorption complexes on hydrated mackinawite (FeS) surfaces: A DFT-D2 study." *Environ. Sci. Technol.* (2017), 51, 3461-3470.
13. 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 LaFeO₃(010) surface." *Phys. Chem. Chem. Phys.* (2017), 19, 7399-7409.
12. 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.
11. 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.
Featured as Outside Back Cover, Photoelectrochemistry: Advanced Materials, Issue 28, 2016
10. **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.
Featured as Outside Front Cover: PCCP, Issue 47, 2016.
9. **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.
8. 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.
7. **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.
6. **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.
5. **Dzade, N. Y.***; Roldan, A.; and de Leeuw, N. H. "A density functional theory study of the adsorption of benzene on

hematite ($\alpha\text{-Fe}_2\text{O}_3$) surfaces." *Journal of Minerals*, (2014), 4, 89–115.

4. **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.
3. 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.
2. **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.
1. **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.

SELECTED INTERNATIONAL CONFERENCE/SERMINAR PRESENTATIONS

- **Keynote Speaker:** Computer-Accelerated Rational Design of Earth-abundant Materials for Renewable Energy Conversion. Engineered Science Publisher Symposium on "Energy Conversion and Storage Devices", 20th March, 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 Speaker:** Computation and Experiment: A Powerful Combination to Rationally Design Functional Materials for Renewable Energy Applications. Invited Seminar, Swiss Federal Institute of Technology Lausanne (EPFL), 17th Feb. 2020.
- **Keynote Speaker:** Rational Design of Transition Metal Chalcogenide based Functional Materials for Renewable Energy Conversion. Int. 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, 21-22 February 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 $\text{FeS}(001)$ 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:** 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:** Organic Functionalization Zinc Phosphide (Zn_3P_2) Surfaces: Implications for PV Application. School of Chemistry Seminar, Cardiff University, August 15, 2018.
- **Contributed:** Characterization of the structures and properties of $\text{As}(\text{OH})_3$ adsorption complexes at mackinawite water interfaces: A DFT-D2 study" Goldschmidt2017, August 13–18, 2017, Paris.
- **Contributed:** 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:** 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:** *Mechanisms of thiophene adsorption and desulfurization of on layered FeS low-index Miller surfaces.* Geochemistry Seminar, September 14, 2016, Utrecht University, The Netherlands.
- **Contributed:** *Enhanced photo-response of FeS₂ 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 CO₂ conversion.* International conference on the Science behind CO₂ 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:** *Computational design of active and selective iron sulfide nano-catalyst for CO₂ activation and conversion.* The 12th Int. Conference on Carbon Dioxide Utilization (ICCDU XII), June, 23–27, 2013, Alexandria, Washington D.C., USA.
- **Contributed:** *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, Durban, South Africa.
- **Contributed:** *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:** *The reactivity of CO₂ with the low-index surfaces of FeS*". London Catalysis Winter Seminar, 19th January 2012, Imperial College London, UK.
- **Contributed:** *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 **Contributed:** Industrial Research, (CSIR), International Convention Centre, Pretoria, South Africa.
- **Contributed:** *Bio-inspired (Fe, Ni)S nano-catalyst for CO₂ activation and reduction.* The World Association of Theoretical & Computational Chemists (WATOC 2011) Congress, July 17–22, 2011, Santiago de Compostela, Spain.
- **Contributed:** *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

- Research Committee Member, School of Chemistry, Cardiff University
- Postgraduate Research (PGR) Progress Monitoring Committee Member
- EPSRC Full College Membership (Reviews EPSRC-UKRI research grant applications)
- Materials Research Society (MRS)
- American Chemical Society (ACS)
- SUPERGEN SUPERSOLAR, The network for solar research in the UK
- European Association of Geochemistry (EAG)

EDITORIAL BOARD

- Frontiers in Catalysis, Editorial Board of Modelling, Theory and Computational Catalysis
- Editorial Board, Journal of Solar Energy Research Updates
- Guest Editor, Engineered Science, Materials and Manufacturing

SCIENTIFIC REVIEWING ACTIVITIES

Currently a reviewer for the following scientific journals: Nature Communications, ACS Energy Letters; Journal 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, etc.,