Nelson Yaw Dzade

List of Publications by Year in Descending Order

84 papers	1,074 citations	19 h-index	28 g-index
93 ext. papers	1,554 ext. citations	5.1 avg, IF	5.31 L-index

#	Paper	IF	Citations
84	Solution-processed Cd-substituted CZTS nanocrystals for sensitized liquid junction solar cells. *Journal of Alloys and Compounds*, **2022**, 890, 161575	5.7	1
83	Photocatalytic Degradation of Rhodamine B Dye and Hydrogen Evolution by Hydrothermally Synthesized NaBH-Spiked ZnS Nanostructures.. *Frontiers in Chemistry*, **2022**, 10, 835832	5	0
82	Terbium-doped and dual passivated CsPb(I Br) inorganic perovskite solar cells with improved air-thermal stability and high efficiency.. *Advanced Materials*, **2022**, e2203204	24	2
81	Rotated domains in selective area epitaxy grown ZnP: formation mechanism and functionality. *Nanoscale*, **2021**, 13, 18441-18450	7.7	1
80	Insights from density functional theory calculations into the effects of the adsorption and dissociation of water on the surface properties of zinc diphosphide (ZnP) nanocrystals. *Physical Chemistry Chemical Physics*, **2021**, 23, 26482-26493	3.6	0
79	Ternary CuSnS: Synthesis, Structure, Photoelectrochemical Activity, and Heterojunction Band Offset and Alignment. *Chemistry of Materials*, **2021**, 33, 1983-1993	9.6	6
78	Experimental and Theoretical Investigation of the Structural and Opto-electronic Properties of Fe-Doped Lead-Free Cs AgBiCl Double Perovskite. *Chemistry - A European Journal*, **2021**, 27, 7408-7417	4.8	11
77	Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method. *Journal of Physical Chemistry A*, **2021**, 125, 2770-2781	2.8	0
76	Structural and optical properties of ionic liquid-based hybrid perovskitoid: A combined experimental and theoretical investigation. *Functional Materials Letters*, **2021**, 14, 2150008	1.2	1
75	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	6.7	8
74	Photocatalytic behavior of Ba(Sb/Ta)2O6 perovskite for reduction of organic pollutants: Experimental and DFT correlation. *Journal of the Taiwan Institute of Chemical Engineers*, **2021**, 122, 201-209	5.3	2
73	Theoretical Insights into the Hydrogen Evolution Reaction on the Ni3N Electrocatalyst. *Catalysts*, **2021**, 11, 716	4	2
72	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	4.2	4
71	Indium-doped ZnOas 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	2.6	
70	DFT and experimental investigations on the photocatalytic activities of NiO nanobelts for removal of organic pollutants. *Journal of Alloys and Compounds*, **2021**, 855, 157337	5.7	12
69	Investigations of the structural, optoelectronic and band alignment properties of Cu2ZnSnS4 prepared by hot-injection method towards low-cost photovoltaic applications. *Journal of Alloys and Compounds*, **2021**, 854, 157093	5.7	8
68	First-principles DFT insights into the adsorption of hydrazine on bimetallic -NiZn catalyst: Implications for direct hydrazine fuel cells. *Applied Surface Science*, **2021**, 536, 147648	6.7	3

67	Hierarchically interconnected ZnO nanowires for low-temperature-operated reducing gas sensors: experimental and DFT studies. *New Journal of Chemistry*, **2021**, 45, 1404-1414	3.6	2
66	Activating the FeS (001) Surface for CO2 Adsorption and Reduction through the Formation of Sulfur Vacancies: A DFT-D3 Study. *Catalysts*, **2021**, 11, 127	4	2
65	Revealing the electronic structure, heterojunction band offset and alignment of CuZnGeSe: a combined experimental and computational study towards photovoltaic applications. *Physical Chemistry Chemical Physics*, **2021**, 23, 9553-9560	3.6	1
64	Combined electrochemical and DFT investigations of iron selenide: a mechanically bendable solid-state symmetric supercapacitor. *Sustainable Energy and Fuels*, **2021**, 5, 5001-5012	5.8	12
63	Structural, Electronic, and Optical Properties of Lead-Free Halide Double Perovskite Rb2AgBiI6: A Combined Experimental and DFT Study. *ES Materials & Manufacturing*, **2021**,	3.7	4
62	Towards defect-free thin films of the earth-abundant absorber zinc phosphide by nanopatterning. *Nanoscale Advances*, **2021**, 3, 326-332	5.1	9
61	Identification of Photoexcited Electron Relaxation in a Cobalt Phosphide Modified Carbon Nitride Photocatalyst. *ChemPhotoChem*, **2021**, 5, 330-334	3.3	6
60	Implementing Dopant-Free Hole-Transporting Layers and Metal-Incorporated CsPbIBr for Stable All-Inorganic Perovskite Solar Cells. *ACS Energy Letters*, **2021**, 6, 778-788	20.1	21
59	First-Principles Density Functional Theory Characterisation of the Adsorption Complexes of H3AsO3 on Cobalt Ferrite (Fe2CoO4) Surfaces. *Minerals (Basel, Switzerland)*, **2021**, 11, 195	2.4	0
58	First-principles insights into the electronic structure, optical and band alignment properties of earth-abundant CuSrSnS solar absorber. *Scientific Reports*, **2021**, 11, 4755	4.9	3
57	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	9.5	25
56	Highly efficient field emission properties of vertically aligned 2D CuSe nanosheets: An experimental and theoretical investigation. *Journal of Alloys and Compounds*, **2021**, 875, 159987	5.7	4
55	Enhanced Performance of Perovskite Solar Cells via Reactive Post-treatment Process Utilizing Guanidine Acetate as Interface Modifier. *Solar Rrl*, **2021**, 5, 2100547	7.1	3
54	Highly active methanol oxidation electrocatalyst based on 2D NiO porous nanosheets:a combined computational and experimental study. *Electrochimica Acta*, **2021**, 394, 139143	6.7	3
53	An interlinked computational experimental investigation into SnS nanoflakes for field emission applications. *New Journal of Chemistry*, **2021**, 45, 11768-11779	3.6	0
52	Electronic Structure and Surface Properties of Copper Thiocyanate: A Promising Hole Transport Material for Organic Photovoltaic Cells. *Materials*, **2020**, 13,	3.5	3
51	Modified Activation Process for Supercapacitor Electrode Materials from African Maize Cob. *Materials*, **2020**, 13,	3.5	9
50	Experimental and Theoretical Study into Interface Structure and Band Alignment of the CuZn Cd SnS Heterointerface for Photovoltaic Applications. *ACS Applied Energy Materials*, **2020**, 3, 5153-5162	6.1	13

49	First-Principles Mechanistic Insights into the Hydrogen Evolution Reaction on Ni2P Electrocatalyst in Alkaline Medium. *Catalysts*, **2020**, 10, 307	4	6
48	Structural and Optical Properties of ZnO Thin Films Prepared by Molecular Precursor and Sol□Gel Methods. *Crystals*, **2020**, 10, 132	2.3	21
47	Enhanced Field Emission Properties of Au/SnSe Nano-heterostructure: A Combined Experimental and Theoretical Investigation. *Scientific Reports*, **2020**, 10, 2358	4.9	8
46	First-Principles Investigation of the Structural, Elastic, Electronic, and Optical Properties of □and □SrZrS: Implications for Photovoltaic Applications. *Materials*, **2020**, 13,	3.5	8
45	Optical, structural and morphological study of CdS nanoparticles: role of sulfur source. *Nanomaterials and Energy*, **2020**, 9, 72-81	1.1	8
44	Thermoluminescence, photoluminescence and optically stimulated luminescence characteristics of CaSO4:Eu phosphor: Experimental and density functional theory (DFT) investigations. *Journal of Luminescence*, **2020**, 221, 117051	3.8	7
43	First-Principles Insights into the Interface Chemistry between 4-Aminothiophenol and Zinc Phosphide (ZnP) Nanoparticles. *ACS Omega*, **2020**, 5, 1025-1032	3.9	7
42	ZnO/CuSCN Nano-Heterostructure as a Highly Efficient Field Emitter: a Combined Experimental and Theoretical Investigation. *ACS Omega*, **2020**, 5, 6715-6724	3.9	8
41	Cu Electrodeposition on Nanostructured MoS2 and WS2 and Implications for HER Active Site Determination. *Journal of the Electrochemical Society*, **2020**, 167, 116517	3.9	2
40	Structural, Optoelectronic, and Photoelectrochemical Investigation of CdSe NCs Prepared by Hot Injection Method. *ES Materials & Manufacturing*, **2020**,	3.7	4
39	Photoelectrochemical Investigation on the Cadmium Sulfide (CdS) Thin Films Prepared using Spin Coating Technique. *ES Materials & Manufacturing*, **2020**,	3.7	10
38	Unravelling the early oxidation mechanism of zinc phosphide (ZnP) surfaces by adsorbed oxygen and water: a first-principles DFT-D3 investigation. *Physical Chemistry Chemical Physics*, **2020**, 22, 1444-1456	3.6	12
37	Electronic Structure and Interface Energetics of CuBiO Photoelectrodes. *Journal of Physical Chemistry C*, **2020**, 124, 22416-22425	3.8	13
36	Uncovering the origin of enhanced field emission properties of rGO-MnO heterostructures: a synergistic experimental and computational investigation.. *RSC Advances*, **2020**, 10, 25988-25998	3.7	6
35	Enhanced photocatalytic activity of N, P, co-doped carbon quantum dots: An insight from experimental and computational approach. *Vacuum*, **2020**, 180, 109589	3.7	7
34	Influence of Topology and Br□sted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI. *Catalysts*, **2020**, 10, 1342	4	6
33	CO2 and H2O Coadsorption and Reaction on the Low-Index Surfaces of Tantalum Nitride: A First-Principles DFT-D3 Investigation. *Catalysts*, **2020**, 10, 1217	4	5
32	Characteristics of K2Ca2(SO4)3:Eu TLD nanophosphor for its applications in electron and gamma rays dosimetry. *Optical Materials*, **2020**, 109, 110272	3.3	4

31	Investigation of growth mechanism for highly oriented TiO2 nanorods: the role of reaction time and annealing temperature. *SN Applied Sciences*, **2019**, 1, 1	1.8	8
30	Unraveling the Role of Lithium in Enhancing the Hydrogen Evolution Activity of MoS: Intercalation versus Adsorption. *ACS Energy Letters*, **2019**, 4, 1733-1740	20.1	25
29	The Origin of High Activity of Amorphous MoS in the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 4383-4389	8.3	54
28	DFT + Study of the Adsorption and Dissociation of Water on Clean, Defective, and Oxygen-Covered USi{001}, {110}, and {111} Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 19453-19467	3.8	6
27	First-principles DFT insights into the structural, elastic, and optoelectronic properties of and ZnP: implications for photovoltaic applications. *Journal of Physics Condensed Matter*, **2019**, 31, 265501	1.8	1
26	Influence of Inorganic Solution Components on Lithium Carbonate Crystal Growth. *Crystal Growth and Design*, **2019**, 19, 6994-7006	3.5	7
25	The Origin of High Activity of Amorphous MoS2 in the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 4336-4336	8.3	1
24	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	6.7	9
23	Enhancing the electrocatalytic activity of 2H-WS for hydrogen evolution via defect engineering. *Physical Chemistry Chemical Physics*, **2019**, 21, 6071-6079	3.6	35
22	Interface Structure and Band Alignment of CZTS/CdS Heterojunction: An Experimental and First-Principles DFT Investigation. *Materials*, **2019**, 12,	3.5	9
21	Oxidation behaviour of USi: an experimental and first principles investigation. *Physical Chemistry Chemical Physics*, **2018**, 20, 4708-4720	3.6	14
20	Reactivity of CO on the surfaces of magnetite (FeO), greigite (FeS) and mackinawite (FeS). *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	18
19	Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS(001), (011), and (111) Surfaces: A Dispersion-Corrected Density Functional Theory Study. *Journal of Physical Chemistry C*, **2018**, 122, 359-370	3.8	11
18	Ab initio investigation of O adsorption on Ca-doped LaMnO cathodes in solid oxide fuel cells. *Physical Chemistry Chemical Physics*, **2018**, 20, 28685-28698	3.6	7
17	Density functional theory characterization of the structures of HAsO and HAsO adsorption complexes on ferrihydrite. *Environmental Sciences: Processes and Impacts*, **2018**, 20, 977-987	4.3	14
16	A DFT+U investigation of hydrogen adsorption on the LaFeO(010) surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 7399-7409	3.6	22
15	Structures and Properties of As(OH) Adsorption Complexes on Hydrated Mackinawite (FeS) Surfaces: A DFT-D2 Study. *Environmental Science & Technology*, **2017**, 51, 3461-3470	10.3	34
14	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	6.7	8

13	Periodic DFT+U investigation of the bulk and surface properties of marcasite (FeS). *Physical Chemistry Chemical Physics*, **2017**, 19, 27478-27488	3.6	21
12	CO activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 19478-19486	3.6	9
11	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). *Journal of Physical Chemistry C*, **2016**, 120, 21441-21450	3.8	26
10	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. *Advanced Materials*, **2016**, 28, 9602-9607	24	53
9	A density functional theory study of arsenic immobilization by the Al(III)-modified zeolite clinoptilolite. *Physical Chemistry Chemical Physics*, **2016**, 18, 11297-305	3.6	7
8	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). *Journal of Chemical Physics*, **2016**, 144, 174704	3.9	23
7	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. *Physical Chemistry Chemical Physics*, **2016**, 18, 32007-32020	3.6	27
6	Activation and dissociation of CO2 on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. *Journal of Chemical Physics*, **2015**, 143, 094703	3.9	40
5	Adsorption of hydrazine on the perfect and defective copper (111) surface: A dispersion-corrected DFT study. *Surface Science*, **2014**, 622, 1-8	1.8	68
4	The surface chemistry of NO(x) on mackinawite (FeS) surfaces: a DFT-D2 study. *Physical Chemistry Chemical Physics*, **2014**, 16, 15444-56	3.6	33
3	A Density Functional Theory Study of the Adsorption of Benzene on Hematite (□Fe2O3) Surfaces. *Minerals (Basel, Switzerland)*, **2014**, 4, 89-115	2.4	77
2	Adsorption of methylamine on mackinawite (FES) surfaces: a density functional theory study. *Journal of Chemical Physics*, **2013**, 139, 124708	3.9	38
1	Silicene and transition metal based materials: prediction of a two-dimensional piezomagnet. *Journal of Physics Condensed Matter*, **2010**, 22, 375502	1.8	40