

Nelson Yaw Dzade

List of Publications by Citations

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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	A Density Functional Theory Study of the Adsorption of Benzene on Hematite ($\alpha\text{-Fe}_2\text{O}_3$) Surfaces. <i>Minerals (Basel, Switzerland)</i> , 2014 , 4, 89-115	2.4	77
83	Adsorption of hydrazine on the perfect and defective copper (111) surface: A dispersion-corrected DFT study. <i>Surface Science</i> , 2014 , 622, 1-8	1.8	68
82	The Origin of High Activity of Amorphous MoS in the Hydrogen Evolution Reaction. <i>ChemSusChem</i> , 2019 , 12, 4383-4389	8.3	54
81	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. <i>Advanced Materials</i> , 2016 , 28, 9602-9607	24	53
80	Activation and dissociation of CO ₂ on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. <i>Journal of Chemical Physics</i> , 2015 , 143, 094703	3.9	40
79	Silicene and transition metal based materials: prediction of a two-dimensional piezomagnet. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 375502	1.8	40
78	Adsorption of methylamine on mackinawite (FeS) surfaces: a density functional theory study. <i>Journal of Chemical Physics</i> , 2013 , 139, 124708	3.9	38
77	Enhancing the electrocatalytic activity of 2H-WS for hydrogen evolution via defect engineering. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 6071-6079	3.6	35
76	Structures and Properties of As(OH) Adsorption Complexes on Hydrated Mackinawite (FeS) Surfaces: A DFT-D2 Study. <i>Environmental Science & Technology</i> , 2017 , 51, 3461-3470	10.3	34
75	The surface chemistry of NO(x) on mackinawite (FeS) surfaces: a DFT-D2 study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 15444-56	3.6	33
74	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 32007-32020	3.6	27
73	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21441-21450	3.8	26
72	Unraveling the Role of Lithium in Enhancing the Hydrogen Evolution Activity of MoS: Intercalation versus Adsorption. <i>ACS Energy Letters</i> , 2019 , 4, 1733-1740	20.1	25
71	High Stability and Long Cycle Life of Rechargeable Sodium-Ion Battery Using Manganese Oxide Cathode: A Combined Density Functional Theory (DFT) and Experimental Study. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 11433-11441	9.5	25
70	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). <i>Journal of Chemical Physics</i> , 2016 , 144, 174704	3.9	23
69	A DFT+U investigation of hydrogen adsorption on the LaFeO(010) surface. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 7399-7409	3.6	22
68	Structural and Optical Properties of ZnO Thin Films Prepared by Molecular Precursor and Sol-Gel Methods. <i>Crystals</i> , 2020 , 10, 132	2.3	21

67	Periodic DFT+U investigation of the bulk and surface properties of marcasite (FeS). <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27478-27488	3.6	21
66	Implementing Dopant-Free Hole-Transporting Layers and Metal-Incorporated CsPbI ₃ Br for Stable All-Inorganic Perovskite Solar Cells. <i>ACS Energy Letters</i> , 2021 , 6, 778-788	20.1	21
65	Reactivity of CO on the surfaces of magnetite (FeO), greigite (FeS) and mackinawite (FeS). <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2018 , 376,	3	18
64	Oxidation behaviour of USi: an experimental and first principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 4708-4720	3.6	14
63	Density functional theory characterization of the structures of HAsO and HAsO adsorption complexes on ferrihydrite. <i>Environmental Sciences: Processes and Impacts</i> , 2018 , 20, 977-987	4.3	14
62	Experimental and Theoretical Study into Interface Structure and Band Alignment of the CuZn Cd SnS Heterointerface for Photovoltaic Applications. <i>ACS Applied Energy Materials</i> , 2020 , 3, 5153-5162	6.1	13
61	Electronic Structure and Interface Energetics of CuBiO Photoelectrodes. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 22416-22425	3.8	13
60	Unravelling the early oxidation mechanism of zinc phosphide (ZnP) surfaces by adsorbed oxygen and water: a first-principles DFT-D3 investigation. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 1444-1456	3.6	12
59	DFT and experimental investigations on the photocatalytic activities of NiO nanobelts for removal of organic pollutants. <i>Journal of Alloys and Compounds</i> , 2021 , 855, 157337	5.7	12
58	Combined electrochemical and DFT investigations of iron selenide: a mechanically bendable solid-state symmetric supercapacitor. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 5001-5012	5.8	12
57	Experimental and Theoretical Investigation of the Structural and Opto-electronic Properties of Fe-Doped Lead-Free Cs AgBiCl ₂ Double Perovskite. <i>Chemistry - A European Journal</i> , 2021 , 27, 7408-7417	4.8	11
56	Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS(001), (011), and (111) Surfaces: A Dispersion-Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 359-370	3.8	11
55	Photoelectrochemical Investigation on the Cadmium Sulfide (CdS) Thin Films Prepared using Spin Coating Technique. <i>ES Materials & Manufacturing</i> , 2020 ,	3.7	10
54	Modified Activation Process for Supercapacitor Electrode Materials from African Maize Cob. <i>Materials</i> , 2020 , 13,	3.5	9
53	CO activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 19478-19486	3.6	9
52	Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study. <i>Applied Surface Science</i> , 2019 , 480, 1014-1024	6.7	9
51	Interface Structure and Band Alignment of CZTS/CdS Heterojunction: An Experimental and First-Principles DFT Investigation. <i>Materials</i> , 2019 , 12,	3.5	9
50	Towards defect-free thin films of the earth-abundant absorber zinc phosphide by nanopatterning. <i>Nanoscale Advances</i> , 2021 , 3, 326-332	5.1	9

49	Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study. <i>Applied Surface Science</i> , 2017 , 400, 293-303	6.7	8
48	Investigation of growth mechanism for highly oriented TiO ₂ nanorods: the role of reaction time and annealing temperature. <i>SN Applied Sciences</i> , 2019 , 1, 1	1.8	8
47	Enhanced Field Emission Properties of Au/SnSe Nano-heterostructure: A Combined Experimental and Theoretical Investigation. <i>Scientific Reports</i> , 2020 , 10, 2358	4.9	8
46	First-Principles Investigation of the Structural, Elastic, Electronic, and Optical Properties of Hf ₂ SnS ₂ : Implications for Photovoltaic Applications. <i>Materials</i> , 2020 , 13,	3.5	8
45	Optical, structural and morphological study of CdS nanoparticles: role of sulfur source. <i>Nanomaterials and Energy</i> , 2020 , 9, 72-81	1.1	8
44	ZnO/CuSCN Nano-Heterostructure as a Highly Efficient Field Emitter: a Combined Experimental and Theoretical Investigation. <i>ACS Omega</i> , 2020 , 5, 6715-6724	3.9	8
43	Experimental and computational studies of sonochemical assisted anchoring of carbon quantum dots on reduced graphene oxide sheets towards the photocatalytic activity. <i>Applied Surface Science</i> , 2021 , 545, 148962	6.7	8
42	Investigations of the structural, optoelectronic and band alignment properties of Cu ₂ ZnSnS ₄ prepared by hot-injection method towards low-cost photovoltaic applications. <i>Journal of Alloys and Compounds</i> , 2021 , 854, 157093	5.7	8
41	Thermoluminescence, photoluminescence and optically stimulated luminescence characteristics of CaSO ₄ :Eu phosphor: Experimental and density functional theory (DFT) investigations. <i>Journal of Luminescence</i> , 2020 , 221, 117051	3.8	7
40	First-Principles Insights into the Interface Chemistry between 4-Aminothiophenol and Zinc Phosphide (ZnP) Nanoparticles. <i>ACS Omega</i> , 2020 , 5, 1025-1032	3.9	7
39	A density functional theory study of arsenic immobilization by the Al(III)-modified zeolite clinoptilolite. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 11297-305	3.6	7
38	Influence of Inorganic Solution Components on Lithium Carbonate Crystal Growth. <i>Crystal Growth and Design</i> , 2019 , 19, 6994-7006	3.5	7
37	Enhanced photocatalytic activity of N, P, co-doped carbon quantum dots: An insight from experimental and computational approach. <i>Vacuum</i> , 2020 , 180, 109589	3.7	7
36	Ab initio investigation of O adsorption on Ca-doped LaMnO cathodes in solid oxide fuel cells. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 28685-28698	3.6	7
35	First-Principles Mechanistic Insights into the Hydrogen Evolution Reaction on Ni ₂ P Electrocatalyst in Alkaline Medium. <i>Catalysts</i> , 2020 , 10, 307	4	6
34	DFT + Study of the Adsorption and Dissociation of Water on Clean, Defective, and Oxygen-Covered USi{001}, {110}, and {111} Surfaces. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 19453-19467	3.8	6
33	Uncovering the origin of enhanced field emission properties of rGO-MnO heterostructures: a synergistic experimental and computational investigation.. <i>RSC Advances</i> , 2020 , 10, 25988-25998	3.7	6
32	Influence of Topology and Brønsted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI. <i>Catalysts</i> , 2020 , 10, 1342	4	6

31	Ternary CuSnS: Synthesis, Structure, Photoelectrochemical Activity, and Heterojunction Band Offset and Alignment. <i>Chemistry of Materials</i> , 2021 , 33, 1983-1993	9.6	6
30	Identification of Photoexcited Electron Relaxation in a Cobalt Phosphide Modified Carbon Nitride Photocatalyst. <i>ChemPhotoChem</i> , 2021 , 5, 330-334	3.3	6
29	CO ₂ and H ₂ O Coadsorption and Reaction on the Low-Index Surfaces of Tantalum Nitride: A First-Principles DFT-D3 Investigation. <i>Catalysts</i> , 2020 , 10, 1217	4	5
28	Structural, Optoelectronic, and Photoelectrochemical Investigation of CdSe NCs Prepared by Hot Injection Method. <i>ES Materials & Manufacturing</i> , 2020 ,	3.7	4
27	Characteristics of K ₂ Ca ₂ (SO ₄) ₃ :Eu TLD nanophosphor for its applications in electron and gamma rays dosimetry. <i>Optical Materials</i> , 2020 , 109, 110272	3.3	4
26	Polymer-wrapped reduced graphene oxide/nickel cobalt ferrite nanocomposites as tertiary hybrid supercapacitors: insights from experiment and simulation. <i>Journal of Science: Advanced Materials and Devices</i> , 2021 , 6, 291-301	4.2	4
25	Structural, Electronic, and Optical Properties of Lead-Free Halide Double Perovskite Rb ₂ AgBiI ₆ : A Combined Experimental and DFT Study. <i>ES Materials & Manufacturing</i> , 2021 ,	3.7	4
24	Highly efficient field emission properties of vertically aligned 2D CuSe nanosheets: An experimental and theoretical investigation. <i>Journal of Alloys and Compounds</i> , 2021 , 875, 159987	5.7	4
23	Electronic Structure and Surface Properties of Copper Thiocyanate: A Promising Hole Transport Material for Organic Photovoltaic Cells. <i>Materials</i> , 2020 , 13,	3.5	3
22	First-principles DFT insights into the adsorption of hydrazine on bimetallic Ni-NiZn catalyst: Implications for direct hydrazine fuel cells. <i>Applied Surface Science</i> , 2021 , 536, 147648	6.7	3
21	First-principles insights into the electronic structure, optical and band alignment properties of earth-abundant Cu ₂ SnS solar absorber. <i>Scientific Reports</i> , 2021 , 11, 4755	4.9	3
20	Enhanced Performance of Perovskite Solar Cells via Reactive Post-treatment Process Utilizing Guanidine Acetate as Interface Modifier. <i>Solar Rrl</i> , 2021 , 5, 2100547	7.1	3
19	Highly active methanol oxidation electrocatalyst based on 2D NiO porous nanosheets: a combined computational and experimental study. <i>Electrochimica Acta</i> , 2021 , 394, 139143	6.7	3
18	Cu Electrodeposition on Nanostructured MoS ₂ and WS ₂ and Implications for HER Active Site Determination. <i>Journal of the Electrochemical Society</i> , 2020 , 167, 116517	3.9	2
17	Photocatalytic behavior of Ba(Sb/Ta)O ₆ perovskite for reduction of organic pollutants: Experimental and DFT correlation. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021 , 122, 201-209	5.3	2
16	Theoretical Insights into the Hydrogen Evolution Reaction on the Ni ₃ N Electrocatalyst. <i>Catalysts</i> , 2021 , 11, 716	4	2
15	Hierarchically interconnected ZnO nanowires for low-temperature-operated reducing gas sensors: experimental and DFT studies. <i>New Journal of Chemistry</i> , 2021 , 45, 1404-1414	3.6	2
14	Activating the FeS (001) Surface for CO ₂ Adsorption and Reduction through the Formation of Sulfur Vacancies: A DFT-D3 Study. <i>Catalysts</i> , 2021 , 11, 127	4	2

13	Terbium-doped and dual passivated $\text{ECsPb}(\text{I Br})$ inorganic perovskite solar cells with improved air-thermal stability and high efficiency.. <i>Advanced Materials</i> , 2022 , e2203204	24	2
12	First-principles DFT insights into the structural, elastic, and optoelectronic properties of Pb and ZnP : implications for photovoltaic applications. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 265501	1.8	1
11	The Origin of High Activity of Amorphous MoS_2 in the Hydrogen Evolution Reaction. <i>ChemSusChem</i> , 2019 , 12, 4336-4336	8.3	1
10	Rotated domains in selective area epitaxy grown ZnP : formation mechanism and functionality. <i>Nanoscale</i> , 2021 , 13, 18441-18450	7.7	1
9	Structural and optical properties of ionic liquid-based hybrid perovskitoid: A combined experimental and theoretical investigation. <i>Functional Materials Letters</i> , 2021 , 14, 2150008	1.2	1
8	Revealing the electronic structure, heterojunction band offset and alignment of CuZnGeSe : a combined experimental and computational study towards photovoltaic applications. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 9553-9560	3.6	1
7	Solution-processed Cd -substituted CZTS nanocrystals for sensitized liquid junction solar cells. <i>Journal of Alloys and Compounds</i> , 2022 , 890, 161575	5.7	1
6	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. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26482-26493	3.6	0
5	Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 2770-2781	2.8	0
4	First-Principles Density Functional Theory Characterisation of the Adsorption Complexes of H_3AsO_3 on Cobalt Ferrite (Fe_2CoO_4) Surfaces. <i>Minerals (Basel, Switzerland)</i> , 2021 , 11, 195	2.4	0
3	An interlinked computational&experimental investigation into SnS nanoflakes for field emission applications. <i>New Journal of Chemistry</i> , 2021 , 45, 11768-11779	3.6	0
2	Photocatalytic Degradation of Rhodamine B Dye and Hydrogen Evolution by Hydrothermally Synthesized NaBH -Spiked ZnS Nanostructures.. <i>Frontiers in Chemistry</i> , 2022 , 10, 835832	5	0
1	Indium-doped ZnO s efficient photosensitive material for sunlight driven hydrogen generation and DSSC applications: integrated experimental and computational approach. <i>Journal of Solid State Electrochemistry</i> , 2021 , 25, 2279-2292	2.6	