Safwat Abdel-Azeim

List of Publications by Year
in descending order

49	1,078	430874	454955
papers	citations	18 h-index	30 g-index

49	49	49	1697
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Phosphate ions interfacial drift layer to improve the performance of CoFeâ˜Prussian blue hematite photoanode toward water splitting. Applied Catalysis B: Environmental, 2022, 304, 121014.	20.2	24
2	Highly exfoliated Ti₃C₂T_x MXene nanosheets atomically doped with Cu for efficient electrochemical CO₂ reduction: an experimental and theoretical study. Journal of Materials Chemistry A, 2022, 10, 1965-1975.	10.3	60
3	Solvent-free synthesis and characterization of Ca2+-doped UiO-66(Zr) as heterogeneous catalyst for esterification of oleic acid with methanol: a joint experimental and computational study. Materials Today Sustainability, 2022, 18, 100110.	4.1	9
4	N-Vinyl Caprolactam/Maleic-Based Copolymers as Kinetic Hydrate Inhibitors: The Effect of Internal Hydrogen Bonding. Energy & Fuels, 2022, 36, 3088-3096.	5.1	10
5	Three new turn-on fluorescent sensors for the selective detection of Zn2+: Synthesis, properties and DFT studies. Arabian Journal of Chemistry, 2022, 15, 104002.	4.9	8
6	Phosphonated Lower-Molecular-Weight Polyethyleneimines as Oilfield Scale Inhibitors: An Experimental and Theoretical Study. Industrial & Engineering Chemistry Research, 2022, 61, 9586-9599.	3.7	2
7	Structures, energetics, and kinetics of H-atom abstraction from methyl propionate by molecular oxygen: Ab initio and DFT investigations. Computational and Theoretical Chemistry, 2021, 1196, 113119.	2.5	15
8	(E)-2-styryl-1H-benzo[d]imidazole as novel green corrosion inhibitor for carbon steel: Experimental and computational approach. Journal of Molecular Liquids, 2021, 324, 115010.	4.9	31
9	A W1 computational study on the kinetics of initial pyrolysis of a biodiesel model: methyl propanoate. New Journal of Chemistry, 2021, 45, 19531-19541.	2.8	7
10	Specificity and Synergy at the Oilâ€“Brine Interface: New Insights from Experiments and Molecular Dynamics Simulations. Energy & Fuels, 2021, 35, 14647-14657.	5.1	15
11	Antiscaling Evaluation and Quantum Chemical Studies of Nitrogen-Free Organophosphorus Compounds for Oilfield Scale Management. Industrial & Engineering Chemistry Research, 2021, 60, 12175-12188.	3.7	12
12	Experimental and Theoretical Investigation of the Synergy Effect of Zr and Ce on the Catalytic Efficiency of NiMoS Grafted on SBA-15 for Oil Hydrodesulfurization. Energy & Fuels, 2021, 35, 2579-2589.	5.1	12
13	Mechanistic insights of the degradation of an O-anisidine carcinogenic pollutant initiated by OH radical attack: theoretical investigations. New Journal of Chemistry, 2021, 45, 5907-5924.	2.8	10
14	Electrochemical and Computational Insights on the Application of Expired Metformin Drug as a Novel Inhibitor for the Sweet Corrosion of C1018 Steel. ACS Omega, 2021, 6, 65-76.	3.5	29
15	Investigation of the Antiscaling Performance of Phosphonated Chitosan for Upstream Petroleum Industry Application. ACS Sustainable Chemistry and Engineering, 2021, 9, 16494-16505.	6.7	12
16	Revisiting OPLS-AA Force Field for the Simulation of Anionic Surfactants in Concentrated Electrolyte Solutions. Journal of Chemical Theory and Computation, 2020, 16, 1136-1145.	5.3	20
17	Photophysical and photocatalytic properties of structurally modified UiO-66. Inorganica Chimica Acta, 2020, 501, 119287.	2.4	15
18	Molecular simulation of kerogen-water interaction: Theoretical insights into maturity. Journal of Molecular Liquids, 2020, 299, 112224.	4.9	11

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19	Highly Efficient Permeation and Separation of Gases with Metalâ€“Organic Frameworks Confined in Polymeric Nanochannels. ACS Applied Materials & Interfaces, 2020, 12, 49992-50001.	8.0	49
20	Studies of interaction between bitumen and thermochemical fluid (TCF): Insights from experiment and molecular dynamics simulations. Applied Surface Science, 2020, 527, 146942.	6.1	8
21	Boosting the efficiency of water oxidation via surface states on hematite photoanodes by incorporating Bi³⁺ ions. Sustainable Energy and Fuels, 2020, 4, 4207-4218.	4.9	10
22	Design and synthesis of two new terbium and europium complexâ€based luminescent probes for the selective detection of zinc ions. Luminescence, 2020, 35, 1238-1247.	2.9	8
23	Crystalizing the interface â€“ The first X-Ray structure of an oil/surfactant/brine transition layer. Journal of Petroleum Science and Engineering, 2020, 188, 106953.	4.2	5
24	Molybdenum Nitride Nanocrystals Anchored on Phosphorus-Incorporated Carbon Fabric as a Negative Electrode for High-Performance Asymmetric Pseudocapacitor. IScience, 2019, 16, 50-62.	4.1	43
25	Molecular and electronic structure elucidation of Fe²⁺/Fe³⁺ complexed chelators used in iron sulphide scale removal in oil and gas wells. Canadian Journal of Chemical Engineering, 2019, 97, 2021-2027.	1.7	30
26	Dynamics, Aggregation, and Interfacial Properties of the Partially Hydrolyzed Polyacrylamide Polymer for Enhanced Oil Recovery Applications: Insights from Molecular Dynamics Simulations. Energy & Fuels, 2018, 32, 3335-3343.	5.1	48
27	Compact, flexible conducting polymer/graphene nanocomposites for supercapacitors of high volumetric energy density. Composites Science and Technology, 2018, 160, 50-59.	7.8	62
28	Effect of ortho-substituted aniline on the corrosion protection of aluminum in 2 mol/L H2SO4 solution. Canadian Journal of Chemistry, 2017, 95, 612-619.	1.1	10
29	The D173G mutation in ADAMTS-13 causes a severe form of congenital thrombotic thrombocytopenic purpura. Thrombosis and Haemostasis, 2016, 115, 51-62.	3.4	14
30	A targeted <scp>DNA</scp> substrate mechanism for the inhibition of <scp>HIV</scp>â€1 integrase by inhibitors with antiretroviral activity. FEBS Open Bio, 2016, 6, 234-250.	2.3	4
31	Investigation of Surface Alkylation Strategy in SOMC: In Situ Generation of a Silica-Supported Tungsten Methyl Catalyst for Cyclooctane Metathesis. Organometallics, 2016, 35, 2524-2531.	2.3	4
32	Limits for Recombination in a Low Energy Loss Organic Heterojunction. ACS Nano, 2016, 10, 10736-10744.	14.6	79
33	Mechanistic insights into the reductive dehydroxylation pathway for the biosynthesis of isoprenoids promoted by the IspH enzyme. Chemical Science, 2015, 6, 5643-5651.	7.4	12
34	Atomic-Resolution Structures of Discrete Stages on the Reaction Coordinate of the [Fe 4 S 4] Enzyme IspG (GcpE). Journal of Molecular Biology, 2015, 427, 2220-2228.	4.2	14
35	Well-Defined Surface Species [(â‰¡Siâ€”Oâ€”)W(â•O)Me₃] Prepared by Direct Methylation of [(â‰¡Siâ€”Oâ€”)W(â•O)Cl₃], a Catalyst for Cycloalkane Metathesis and Transformation of Ethylene to Propylene. ACS Catalysis, 2015, 5, 2164-2171.	11.2	35
36	Biochemical stability and molecular dynamic characterization of Aspergillus fumigatus cystathionine Î³-lyase in response to various reaction effectors. Enzyme and Microbial Technology, 2015, 81, 31-46.	3.2	33

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37	Structural Basis for the Recognition in an Idiotype-Anti-Idiotype Antibody Complex Related to Celiac Disease. PLoS ONE, 2014, 9, e102839.	2.5	9
38	Higher order structural effects stabilizing the reverse Watsonâ€“Crick Guanine-Cytosine base pair in functional RNAs. Nucleic Acids Research, 2014, 42, 714-726.	14.5	43
39	Molecular Dynamics Characterization of Five Pathogenic Factor X Mutants Associated with Decreased Catalytic Activity. Biochemistry, 2014, 53, 6992-7001.	2.5	15
40	MDcons: Intermolecular contact maps as a tool to analyze the interface of protein complexes from molecular dynamics trajectories. BMC Bioinformatics, 2014, 15, S1.	2.6	29
41	Tethering Metal Ions to Photocatalyst Particulate Surfaces by Bifunctional Molecular Linkers for Efficient Hydrogen Evolution. ChemSusChem, 2014, 7, 2575-2583.	6.8	19
42	In SilicoandIn VitroComparison of HIV-1 Subtypes B and CRF02_AG Integrases Susceptibility to Integrase Strand Transfer Inhibitors. Advances in Virology, 2012, 2012, 1-13.	1.1	6
43	Unprocessed Viral DNA Could Be the Primary Target of the HIV-1 Integrase Inhibitor Raltegravir. PLoS ONE, 2012, 7, e40223.	2.5	8
44	Zincâ€“Homocysteine binding in cobalaminâ€dependent methionine synthase and its role in the substrate activation: DFT, ONIOM, and QM/MM molecular dynamics studies. Journal of Computational Chemistry, 2011, 32, 3154-3167.	3.3	16
45	Targeting STAT1 by myricetin and delphinidin provides efficient protection of the heart from ischemia/reperfusionâ€induced injury. FEBS Letters, 2009, 583, 531-541.	2.8	80
46	Insight into the apoptosis-inducing action of Î±-bisabolol towards malignant tumor cells: Involvement of lipid rafts and Bid. Archives of Biochemistry and Biophysics, 2008, 476, 113-123.	3.0	57
47	CO migration pathways in cytochrome P450camstudied by molecular dynamics simulations. Protein Science, 2007, 16, 781-794.	7.6	10
48	Reactions of [NH3+Â·, H2O] with carbonyl compounds: A McLafferty rearrangement within a complex?. Journal of the American Society for Mass Spectrometry, 2004, 15, 966-971.	2.8	9
49	Phase Behavior and Interfacial Properties of Salt-Tolerant Polymers: Insights from Molecular Dynamics Simulations. ACS Applied Polymer Materials, 0, , .	4.4	7