

Safwat Abdel-Azeim

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1730224/publications.pdf>

Version: 2024-02-01

49
papers

1,078
citations

430874

18
h-index

454955

30
g-index

49
all docs

49
docs citations

49
times ranked

1697
citing authors

#	ARTICLE	IF	CITATIONS
1	Targeting STAT1 by myricetin and delphinidin provides efficient protection of the heart from ischemia/reperfusion-induced injury. <i>FEBS Letters</i> , 2009, 583, 531-541.	2.8	80
2	Limits for Recombination in a Low Energy Loss Organic Heterojunction. <i>ACS Nano</i> , 2016, 10, 10736-10744.	14.6	79
3	Compact, flexible conducting polymer/graphene nanocomposites for supercapacitors of high volumetric energy density. <i>Composites Science and Technology</i> , 2018, 160, 50-59.	7.8	62
4	Highly exfoliated Ti_3C_2 MXene nanosheets atomically doped with Cu for efficient electrochemical CO_2 reduction: an experimental and theoretical study. <i>Journal of Materials Chemistry A</i> , 2022, 10, 1965-1975.	10.3	60
5	Insight into the apoptosis-inducing action of \pm -bisabolol towards malignant tumor cells: Involvement of lipid rafts and Bid. <i>Archives of Biochemistry and Biophysics</i> , 2008, 476, 113-123.	3.0	57
6	Highly Efficient Permeation and Separation of Gases with Metal-Organic Frameworks Confined in Polymeric Nanochannels. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 49992-50001.	8.0	49
7	Dynamics, Aggregation, and Interfacial Properties of the Partially Hydrolyzed Polyacrylamide Polymer for Enhanced Oil Recovery Applications: Insights from Molecular Dynamics Simulations. <i>Energy & Fuels</i> , 2018, 32, 3335-3343.	5.1	48
8	Higher order structural effects stabilizing the reverse Watson-Crick Guanine-Cytosine base pair in functional RNAs. <i>Nucleic Acids Research</i> , 2014, 42, 714-726.	14.5	43
9	Molybdenum Nitride Nanocrystals Anchored on Phosphorus-Incorporated Carbon Fabric as a Negative Electrode for High-Performance Asymmetric Pseudocapacitor. <i>IScience</i> , 2019, 16, 50-62.	4.1	43
10	Well-Defined Surface Species $[(Si^+O^-)W(O)Me_3]$ Prepared by Direct Methylation of $[(Si^+O^-)W(O)Cl_3]$, a Catalyst for Cycloalkane Metathesis and Transformation of Ethylene to Propylene. <i>ACS Catalysis</i> , 2015, 5, 2164-2171.	11.2	35
11	Biochemical stability and molecular dynamic characterization of <i>Aspergillus fumigatus</i> cystathionine β -lyase in response to various reaction effectors. <i>Enzyme and Microbial Technology</i> , 2015, 81, 31-46.	3.2	33
12	(E)-2-styryl-1H-benzo[d]imidazole as novel green corrosion inhibitor for carbon steel: Experimental and computational approach. <i>Journal of Molecular Liquids</i> , 2021, 324, 115010.	4.9	31
13	Molecular and electronic structure elucidation of Fe^{2+}/Fe^{3+} complexed chelators used in iron sulphide scale removal in oil and gas wells. <i>Canadian Journal of Chemical Engineering</i> , 2019, 97, 2021-2027.	1.7	30
14	MDcons: Intermolecular contact maps as a tool to analyze the interface of protein complexes from molecular dynamics trajectories. <i>BMC Bioinformatics</i> , 2014, 15, S1.	2.6	29
15	Electrochemical and Computational Insights on the Application of Expired Metformin Drug as a Novel Inhibitor for the Sweet Corrosion of C1018 Steel. <i>ACS Omega</i> , 2021, 6, 65-76.	3.5	29
16	Phosphate ions interfacial drift layer to improve the performance of CoFe-Prussian blue hematite photoanode toward water splitting. <i>Applied Catalysis B: Environmental</i> , 2022, 304, 121014.	20.2	24
17	Revisiting OPLS-AA Force Field for the Simulation of Anionic Surfactants in Concentrated Electrolyte Solutions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1136-1145.	5.3	20
18	Tethering Metal Ions to Photocatalyst Particulate Surfaces by Bifunctional Molecular Linkers for Efficient Hydrogen Evolution. <i>ChemSusChem</i> , 2014, 7, 2575-2583.	6.8	19

#	ARTICLE	IF	CITATIONS
19	Zinc–Homocysteine binding in cobalamin–dependent methionine synthase and its role in the substrate activation: DFT, ONIOM, and QM/MM molecular dynamics studies. <i>Journal of Computational Chemistry</i> , 2011, 32, 3154-3167.	3.3	16
20	Molecular Dynamics Characterization of Five Pathogenic Factor X Mutants Associated with Decreased Catalytic Activity. <i>Biochemistry</i> , 2014, 53, 6992-7001.	2.5	15
21	Photophysical and photocatalytic properties of structurally modified UiO-66. <i>Inorganica Chimica Acta</i> , 2020, 501, 119287.	2.4	15
22	Structures, energetics, and kinetics of H-atom abstraction from methyl propionate by molecular oxygen: Ab initio and DFT investigations. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113119.	2.5	15
23	Specificity and Synergy at the Oil–Brine Interface: New Insights from Experiments and Molecular Dynamics Simulations. <i>Energy & Fuels</i> , 2021, 35, 14647-14657.	5.1	15
24	Atomic-Resolution Structures of Discrete Stages on the Reaction Coordinate of the [Fe 4 S 4] Enzyme IspG (GcpE). <i>Journal of Molecular Biology</i> , 2015, 427, 2220-2228.	4.2	14
25	The D173G mutation in ADAMTS-13 causes a severe form of congenital thrombotic thrombocytopenic purpura. <i>Thrombosis and Haemostasis</i> , 2016, 115, 51-62.	3.4	14
26	Mechanistic insights into the reductive dehydroxylation pathway for the biosynthesis of isoprenoids promoted by the IspH enzyme. <i>Chemical Science</i> , 2015, 6, 5643-5651.	7.4	12
27	Antiscalting Evaluation and Quantum Chemical Studies of Nitrogen-Free Organophosphorus Compounds for Oilfield Scale Management. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 12175-12188.	3.7	12
28	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. <i>Energy & Fuels</i> , 2021, 35, 2579-2589.	5.1	12
29	Investigation of the Antiscalting Performance of Phosphonated Chitosan for Upstream Petroleum Industry Application. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 16494-16505.	6.7	12
30	Molecular simulation of kerogen-water interaction: Theoretical insights into maturity. <i>Journal of Molecular Liquids</i> , 2020, 299, 112224.	4.9	11
31	CO migration pathways in cytochrome P450cam studied by molecular dynamics simulations. <i>Protein Science</i> , 2007, 16, 781-794.	7.6	10
32	Effect of ortho-substituted aniline on the corrosion protection of aluminum in 2 mol/L H ₂ SO ₄ solution. <i>Canadian Journal of Chemistry</i> , 2017, 95, 612-619.	1.1	10
33	Boosting the efficiency of water oxidation via surface states on hematite photoanodes by incorporating Bi ³⁺ ions. <i>Sustainable Energy and Fuels</i> , 2020, 4, 4207-4218.	4.9	10
34	Mechanistic insights of the degradation of an O-anisidine carcinogenic pollutant initiated by OH radical attack: theoretical investigations. <i>New Journal of Chemistry</i> , 2021, 45, 5907-5924.	2.8	10
35	N-Vinyl Caprolactam/Maleic-Based Copolymers as Kinetic Hydrate Inhibitors: The Effect of Internal Hydrogen Bonding. <i>Energy & Fuels</i> , 2022, 36, 3088-3096.	5.1	10
36	Reactions of [NH ₃ +H ₂ O] with carbonyl compounds: A McLafferty rearrangement within a complex?. <i>Journal of the American Society for Mass Spectrometry</i> , 2004, 15, 966-971.	2.8	9

#	ARTICLE	IF	CITATIONS
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	Solvent-free synthesis and characterization of Ca ²⁺ -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
39	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
40	Design and synthesis of two new terbium and europium complex-based luminescent probes for the selective detection of zinc ions. Luminescence, 2020, 35, 1238-1247.	2.9	8
41	Unprocessed Viral DNA Could Be the Primary Target of the HIV-1 Integrase Inhibitor Raltegravir. PLoS ONE, 2012, 7, e40223.	2.5	8
42	Three new turn-on fluorescent sensors for the selective detection of Zn ²⁺ : Synthesis, properties and DFT studies. Arabian Journal of Chemistry, 2022, 15, 104002.	4.9	8
43	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
44	Phase Behavior and Interfacial Properties of Salt-Tolerant Polymers: Insights from Molecular Dynamics Simulations. ACS Applied Polymer Materials, 0, , .	4.4	7
45	In Silico and In Vitro Comparison of HIV-1 Subtypes B and CRF02_AG Integrase Susceptibility to Integrase Strand Transfer Inhibitors. Advances in Virology, 2012, 2012, 1-13.	1.1	6
46	Crystalizing the interface – The first X-Ray structure of an oil/surfactant/brine transition layer. Journal of Petroleum Science and Engineering, 2020, 188, 106953.	4.2	5
47	A targeted DNA substrate mechanism for the inhibition of HIV-1 integrase by inhibitors with antiretroviral activity. FEBS Open Bio, 2016, 6, 234-250.	2.3	4
48	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
49	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