

Mohamed K Awad

List of Publications by Year in descending order

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68
papers

2,219
citations

257450

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h-index

233421

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68
all docs

68
docs citations

68
times ranked

1932
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational simulation of the molecular structure of some triazoles as inhibitors for the corrosion of metal surface. Computational and Theoretical Chemistry, 2010, 959, 66-74.	1.5	243
2	Quantum chemical studies on the inhibition of corrosion of copper surface by substituted uracils. Applied Surface Science, 2008, 255, 2433-2441.	6.1	206
3	Three novel di-quaternary ammonium salts as corrosion inhibitors for API X65 steel pipeline in acidic solution. Part I: Experimental results. Corrosion Science, 2014, 81, 54-64.	6.6	184
4	The role of structural chemistry in the inhibitive performance of some aminopyrimidines on the corrosion of steel. Corrosion Science, 2010, 52, 2387-2396.	6.6	165
5	Factors determining carbon monoxide adsorption sites on palladium and platinum (100) and (111) surfaces: theoretical study. Journal of the American Chemical Society, 1985, 107, 7854-7857.	13.7	103
6	Semiempirical investigation of the inhibition efficiency of thiourea derivatives as corrosion inhibitors. Journal of Electroanalytical Chemistry, 2004, 567, 219-225.	3.8	98
7	Experimental and quantum chemical studies of the effect of poly ethylene glycol as corrosion inhibitors of aluminum surface. Journal of Industrial and Engineering Chemistry, 2014, 20, 796-808.	5.8	93
8	Dielectrical, conduction mechanism and thermal properties of rhodanine azodyes. Materials Science in Semiconductor Processing, 2014, 19, 150-162.	4.0	62
9	Dual emission of chalcone-analogue dyes emitting in the red region. Chemical Physics, 2004, 303, 317-326.	1.9	60
10	Photodimerization of cyclohexene and methane by decatungstate anions: molecular orbital theory. Journal of the American Chemical Society, 1990, 112, 1603-1606.	13.7	49
11	Theoretical investigation of the inhibition of corrosion by some triazole Schiff bases. Materials and Corrosion - Werkstoffe Und Korrosion, 2009, 60, 813-819.	1.5	44
12	High performance corrosion inhibition of novel tricationic surfactants on carbon steel in formation water: Electrochemical and computational evaluations. Journal of Molecular Liquids, 2018, 262, 363-375.	4.9	43
13	Theoretical studies of the effect of structural parameters on the inhibition efficiencies of mercapto-1,2,4-triazoline derivatives. Computational and Theoretical Chemistry, 2000, 531, 105-117.	1.5	41
14	Absorption, fluorescence, and semiempirical ASED-MO studies on a typical Brooker's merocyanine dye. Journal of Molecular Structure, 2005, 754, 16-24.	3.6	35
15	Solvatochromism, molecular and electronic structures of trans and cis isomers of a typical styryl pyridinium cyanine dye. Journal of Molecular Structure, 2009, 920, 332-341.	3.6	35
16	DFT theoretical studies of antipyrine Schiff bases as corrosion inhibitors. Materials and Corrosion - Werkstoffe Und Korrosion, 2010, 61, 709-714.	1.5	35
17	Synthesis, characterization, and biological activity studies of copper(II)-metal(II) binuclear complexes of dipyrityldiglyoxal bis(2-hydroxybenzoyl hydrazone). Journal of Coordination Chemistry, 2010, 63, 330-345.	2.2	35
18	Computational simulation of the effect of quantum chemical parameters on the molecular docking of HMG-CoA reductase drugs. Journal of Molecular Structure, 2014, 1075, 311-326.	3.6	35

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19	New Ni(II), Pd(II) and Pt(II) complexes coordinated to azo pyrazolone ligand with a potent anti-tumor activity: Synthesis, characterization, DFT and DNA cleavage studies. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4104.	3.5	35
20	Design, synthesis, molecular modeling, and biological evaluation of novel β -aminophosphonates based quinazolinone moiety as potential anticancer agents: DFT, NBO and vibrational studies. <i>Journal of Molecular Structure</i> , 2018, 1173, 128-141.	3.6	28
21	Effect of protonation on the molecular structure and reactivity of a typical merocyanine dye: experimental and theoretical investigation. <i>The Journal of Physical Chemistry</i> , 1993, 97, 3160-3165.	2.9	27
22	Molecular docking, molecular modeling, vibrational and biological studies of some new heterocyclic β -aminophosphonates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 78-88.	3.9	27
23	New N-ribosides and N-mannosides of rhodanine derivatives with anticancer activity on leukemia cell line: Design, synthesis, DFT and molecular modelling studies. <i>Carbohydrate Research</i> , 2020, 487, 107894.	2.3	26
24	Photoactivation of water by p-benzoquinone and the role of manganese(III) complexes in oxygen evolution: molecular orbital theory. <i>Journal of the American Chemical Society</i> , 1989, 111, 802-806.	13.7	24
25	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. <i>Journal of Molecular Structure</i> , 1996, 378, 103-110.	3.6	24
26	Characterization of synthetic and commercial trisiloxane surfactant materials. <i>Applied Organometallic Chemistry</i> , 2004, 18, 28-38.	3.5	24
27	Effect of alkyl substituents on the thermal degradation of poly(alkyl methacrylate): a molecular orbital study using the ASED-MO method. <i>Polymer Degradation and Stability</i> , 1995, 49, 339-346.	5.8	23
28	Pd (II) complexes of bidentate chalcone ligands: Synthesis, spectral, thermal, antitumor, antioxidant, antimicrobial, DFT and SAR studies. <i>Journal of Molecular Structure</i> , 2018, 1160, 348-359.	3.6	21
29	Binding of Ru, O, and RuO _n (n=1-4) to the Ru(001) surface: Structures, stabilities, and diffusion barriers. <i>Surface Science</i> , 1987, 183, 289-301.	1.9	20
30	Nuclear quadrupole resonance and molecular orbital studies of charge distribution in H-bonded complexes of 2-chloro-4-nitrobenzoic acid. <i>Magnetic Resonance in Chemistry</i> , 1995, 33, 476-480.	1.9	19
31	Quantum chemical studies and molecular modeling of the effect of polyethylene glycol as corrosion inhibitors of an aluminum surface. <i>Canadian Journal of Chemistry</i> , 2013, 91, 283-291.	1.1	18
32	Design of blue fluorescence emitter star-shaped macromolecules based on pyrene and anthracene. <i>Polymer</i> , 2016, 98, 210-228.	3.8	16
33	Molecular dynamic simulation studies and surface characterization of carbon steel corrosion with changing green inhibitors concentrations and temperatures. <i>AEJ - Alexandria Engineering Journal</i> , 2022, 61, 2492-2519.	6.4	16
34	MP2 and DFT theoretical studies of the geometry, vibrational and electronic absorption spectra of 2-aminopyrimidine. <i>Research on Chemical Intermediates</i> , 2013, 39, 2741-2761.	2.7	14
35	Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1220-1231.	2.9	14
36	Chemical, electrochemical, theoretical (DFT & MEP), thermodynamics and surface morphology studies of carbon steel during gas and oil production using three novel di-cationic amphiphiles as corrosion inhibitors in acidic medium. <i>Journal of Molecular Liquids</i> , 2021, 337, 116541.	4.9	14

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37	Theoretical investigations of the stability of degradation products of polystyrene and poly(4-vinylpyridine). <i>Polymer Degradation and Stability</i> , 1994, 46, 165-170.	5.8	13
38	Design, synthesis, DFT, molecular modelling studies and biological evaluation of novel 3-substituted (E)-5-(arylidene)-1-methyl-2-thioxoimidazolidin-4-ones with potent cytotoxic activities against breast MCF-7, liver HepG2, and lung A549. <i>Journal of Molecular Structure</i> , 2021, 1229, 129805.	3.6	13
39	Design, synthesis and biological evaluation of novel thiohydantoin derivatives as antiproliferative agents: A combined experimental and theoretical assessments. <i>Journal of Molecular Structure</i> , 2022, 1249, 131574.	3.6	13
40	Spectral, magnetic studies and molecular orbital calculations for (4,5-dimethyl-3-pyrazolyl)aldazine copper(II) complexes. <i>Transition Metal Chemistry</i> , 1995, 20, 448-453.	1.4	12
41	Effect of Applied Voltage on the Geometrical and Electronic Structures of Dipyrimidinyl-Diphenyl Diblock as a Molecular Diode: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21728-21735.	3.1	12
42	New Zn (II) and Cd (II) complexes of 2,4-dihydroxy-5-mercapto-1,2,4-triazole-3-yl diazenyl]benzaldehyde: Synthesis, structural characterization, molecular modeling and docking studies, DNA binding and biological activity. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5635.	3.5	12
43	Ethynidyne on the rhodium(100) surface: a theoretical investigation. <i>Langmuir</i> , 1990, 6, 806-816.	3.5	11
44	The effect of constitutional and conformational isomerization on the electrical properties of diblock molecular diode. <i>Organic Electronics</i> , 2011, 12, 1080-1092.	2.6	11
45	Molecular structure of amino alcohols on aluminum surface. <i>Journal of Molecular Structure</i> , 2014, 1063, 51-59.	3.6	11
46	Methane activation by hole sites on AlN: A molecular orbital study. <i>Surface Science</i> , 1989, 218, 543-552.	1.9	10
47	FMO treatment of the reactivity and stereochemistry of the cycloaddition processes using ASE-DFT method. <i>Computational and Theoretical Chemistry</i> , 2000, 505, 185-197.	1.5	10
48	Photophysical properties and semiempirical calculations of perylene-3,4,9,10-tetracarboxylic tetramethylester (PTME). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1063-1069.	3.9	10
49	An assessment to evaluate the validity of different methods for the description of some corrosion inhibitors. <i>Journal of Molecular Modeling</i> , 2014, 20, 2422.	1.8	10
50	Design of Piperazine Organoiron Macromolecules with Antibacterial and Anticancer Activity. <i>Macromolecular Chemistry and Physics</i> , 2016, 217, 987-996.	2.2	10
51	Design, Synthesis and Docking study of Novel Imidazolyl Pyrazolopyridine Derivatives as Antitumor Agents Targeting MCF7 Cell Line. <i>Current Organic Synthesis</i> , 2018, 15, 275-285.	1.3	10
52	Theoretical investigations of [4+2] cycloaddition and stereoselectivity of phthalazin derivatives. <i>Computational and Theoretical Chemistry</i> , 2001, 542, 139-147.	1.5	8
53	Mechanism of Water Attacking on Brooker's Merocyanine Dye and Its Effect on the Molecular and Electronic Structures: Theoretical Study. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 838-844.	3.2	8
54	Effect of N-methylation on both ground and excited states properties of 1-(9-anthryl)-2-(2-benzothiazolyl) ethene. <i>Journal of Molecular Structure</i> , 2009, 919, 12-20.	3.6	8

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55	Quantum chemical studies and atomistic simulations of some inhibitors for the corrosion of al surface. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2016, 52, 156-168.	1.1	8
56	Factors Influencing the Potency of Alzheimer Inhibitors: Computational and Docking Studies. <i>American Journal of Alzheimer's Disease and Other Dementias</i> , 2018, 33, 166-175.	1.9	8
57	Molecular aggregation and photochemical Z/E isomerization of 1-methy-2-[2-(9-phenantheryl)ethenyl] benzothiazolium iodide. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 222, 276-282.	3.9	7
58	Design, synthesis, and computational explorations of novel 2 α -thiohydantoin nucleosides with cytotoxic activities. <i>Journal of Heterocyclic Chemistry</i> , 2022, 59, 664-685.	2.6	7
59	Synthesis of New $\hat{\iota}$ -Amino Phosphonates Containing 3-Amino-4(3H) Quinazolinone Moiety as Anticancer and Antimicrobial Agents: DFT, NBO, and Vibrational Studies. <i>Current Organic Synthesis</i> , 2018, 15, 286-296.	1.3	6
60	UV \hat{a} vis, IR and ^1H NMR spectroscopic studies of some mono- and bis-azo-compounds based on 2,7-dihydroxynaphthalene and aniline derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 980-986.	3.9	5
61	QSAR studies for the computational prediction of HMG-CoA reductase inhibitors by genetic function approximation technique. <i>Canadian Journal of Chemistry</i> , 2013, 91, 263-274.	1.1	5
62	Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 301, 20-31.	3.9	5
63	Resorcinol Derivative as an Environmentally Friendly Low Carbon Steel Inhibitor in HCl Medium. <i>ACS Omega</i> , 2022, 7, 17609-17619.	3.5	5
64	Thermal stabilities, electronic properties and structures of metformin-metal complexes. <i>Journal of Thermal Analysis</i> , 1995, 44, 1493-1498.	0.6	4
65	Investigation of regiospecific oxidative heterocyclization of 2-(N \hat{a} \hat{e} -benzylidene) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 347 Td (129-138.	1.5	4
66	Modification of the electric properties of molecular devices via gradual increase of number of nitrogen atoms: A computational study. <i>Organic Electronics</i> , 2012, 13, 807-814.	2.6	3
67	Synthesis, molecular modeling, TD \hat{a} DFT, antimicrobial, and in vitro therapeutic activity of new spherical nano \hat{e} sized sulfonamide imine ligands and their zinc (II) and copper (II) complexes. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5953.	3.5	3
68	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. <i>Computational and Theoretical Chemistry</i> , 1996, 378, 103-110.	1.5	1