Mohamed K Awad

List of Publications by Year
in descending order

68 papers	2,219 citations	257357 24 h-index	233338 45 g-index
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.	3.1	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.	3.0	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.	3.0	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.	6.6	103
6	Semiempirical investigation of the inhibition efficiency of thiourea derivatives as corrosion inhibitors. Journal of Electroanalytical Chemistry, 2004, 567, 219-225.	1.9	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.	2.9	93
8	Dielectrical, conduction mechanism and thermal properties of rhodanine azodyes. Materials Science in Semiconductor Processing, 2014, 19, 150-162.	1.9	62
9	Dual emission of chalcone-analogue dyes emitting in the red region. Chemical Physics, 2004, 303, 317-326.	0.9	60
10	Photodimerization of cyclohexene and methane by decatungstate anions: molecular orbital theory. Journal of the American Chemical Society, 1990, 112, 1603-1606.	6.6	49
11	Theoretical investigation of the inhibition of corrosion by some triazole Schiff bases. Materials and Corrosion - Werkstoffe Und Korrosion, 2009, 60, 813-819.	0.8	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.	2.3	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.	1.8	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.	1.8	35
16	DFT theoretical studies of antipyrine Schiff bases as corrosion inhibitors. Materials and Corrosion - Werkstoffe Und Korrosion, 2010, 61, 709-714.	0.8	35
17	Synthesis, characterization, and biological activity studies of copper(II)â€“metal(II) binuclear complexes of dipyridylglyoxal bis(2-hydroxybenzoyl hydrazone). Journal of Coordination Chemistry, 2010, 63, 330-345.	0.8	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.	1.8	35

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19	New Ni(II), Pd(II) and Pt(II) complexes coordinated to azo pyrazolone ligand with a potent antiâ€tumor activity: Synthesis, characterization, DFT and DNA cleavage studies. Applied Organometallic Chemistry, 2018, 32, e4104.	1.7	35
20	Design, synthesis, molecular modeling, and biological evaluation of novel Î±-aminophosphonates based quinazolinone moiety as potential anticancer agents: DFT, NBO and vibrational studies. Journal of Molecular Structure, 2018, 1173, 128-141.	1.8	28
21	Effect of protonation on the molecular structure and reactivity of a typical merocyanine dye: experimental and theoretical investigation. The Journal of Physical Chemistry, 1993, 97, 3160-3165.	2.9	27
22	Molecular docking, molecular modeling, vibrational and biological studies of some new heterocyclic Î±-aminophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 78-88.	2.0	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. Carbohydrate Research, 2020, 487, 107894.	1.1	26
24	Photoactivation of water by p-benzoquinone and the role of manganese(III) complexes in oxygen evolution: molecular orbital theory. Journal of the American Chemical Society, 1989, 111, 802-806.	6.6	24
25	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. Journal of Molecular Structure, 1996, 378, 103-110.	1.8	24
26	Characterization of synthetic and commercial trisiloxane surfactant materials. Applied Organometallic Chemistry, 2004, 18, 28-38.	1.7	24
27	Effect of alkyl substituents on the thermal degradation of poly(alkyl methacrylate): a molecular orbital study using the ASED-MO method. Polymer Degradation and Stability, 1995, 49, 339-346.	2.7	23
28	Pd (II) complexes of bidentate chalcone ligands: Synthesis, spectral, thermal, antitumor, antioxidant, antimicrobial, DFT and SAR studies. Journal of Molecular Structure, 2018, 1160, 348-359.	1.8	21
29	Binding of Ru, O, and RuOn (n=1â€“4) to the Ru(001) surface: Structures, stabilities, and diffusion barriers. Surface Science, 1987, 183, 289-301.	0.8	20
30	Nuclear quadrupole resonance and molecular orbital studies of charge distribution in H-bonded complexes of 2-chloro-4-nitrobenzoic acid. Magnetic Resonance in Chemistry, 1995, 33, 476-480.	1.1	19
31	Quantum chemical studies and molecular modeling of the effect of polyethylene glycol as corrosion inhibitors of an aluminum surface. Canadian Journal of Chemistry, 2013, 91, 283-291.	0.6	18
32	Design of blue fluorescence emitter star-shaped macromolecules based on pyrene and anthracene. Polymer, 2016, 98, 210-228.	1.8	16
33	Molecular dynamic simulation studies and surface characterization of carbon steel corrosion with changing green inhibitors concentrations and temperatures. AEJ - Alexandria Engineering Journal, 2022, 61, 2492-2519.	3.4	16
34	MP2 and DFT theoretical studies of the geometry, vibrational and electronic absorption spectra of 2-aminopyrimidine. Research on Chemical Intermediates, 2013, 39, 2741-2761.	1.3	14
35	Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. Photochemical and Photobiological Sciences, 2013, 12, 1220-1231.	1.6	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. Journal of Molecular Liquids, 2021, 337, 116541.	2.3	14

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37	Theoretical investigations of the stability of degradation products of polystyrene and poly(4-vinylpyridine). Polymer Degradation and Stability, 1994, 46, 165-170.	2.7	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. Journal of Molecular Structure, 2021, 1229, 129805.	1.8	13
39	Design, synthesis and biological evaluation of novel thiohydantoin derivatives as antiproliferative agents: A combined experimental and theoretical assessments. Journal of Molecular Structure, 2022, 1249, 131574.	1.8	13
40	Spectral, magnetic studies and molecular orbital calculations for (4,5-dimethyl-3-pyrazolyl)aldazine copper(II) complexes. Transition Metal Chemistry, 1995, 20, 448-453.	0.7	12
41	Effect of Applied Voltage on the Geometrical and Electronic Structures of Dipyrimidinylâ^'Diphenyl Diblock as a Molecular Diode: A DFT Study. Journal of Physical Chemistry C, 2010, 114, 21728-21735.	1.5	12
42	New Zn (II) and Cd (II) complexes of 2,4â€dihydroxyâ€5â€[(5â€mercaptoâ€1Hâ€1,2,4â€triazoleâ€3â€yl)diazenyl]benzaldehyde: Synthesis, structural characterization, molecular modeling and docking studies, DNA binding and biological activity. Applied Organometallic Chemistry, 2020, 34, e5635.	1.7	12
43	Ethylidyne on the rhodium(100) surface: a theoretical investigation. Langmuir, 1990, 6, 806-816.	1.6	11
44	The effect of constitutional and conformational isomerization on the electrical properties of diblock molecular diode. Organic Electronics, 2011, 12, 1080-1092.	1.4	11
45	Molecular structure of amino alcohols on aluminum surface. Journal of Molecular Structure, 2014, 1063, 51-59.	1.8	11
46	Methane activation by hole sites on AlN: A molecular orbital study. Surface Science, 1989, 218, 543-552.	0.8	10
47	FMO treatment of the reactivity and stereochemistry of the cycloaddition processes using ASED-MO method. Computational and Theoretical Chemistry, 2000, 505, 185-197.	1.5	10
48	Photophysical properties and semiempirical calculations of perylene-3,4,9,10-tetracarboxylic tetramethylester (PTME). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1063-1069.	2.0	10
49	An assessment to evaluate the validity of different methods for the description of some corrosion inhibitors. Journal of Molecular Modeling, 2014, 20, 2422.	0.8	10
50	Design of Piperazine Organoiron Macromolecules with Antibacterial and Anticancer Activity. Macromolecular Chemistry and Physics, 2016, 217, 987-996.	1.1	10
51	Design, Synthesis and Docking study of Novel Imidazolyl Pyrazolopyridine Derivatives as Antitumor Agents Targeting MCF7 Cell Line. Current Organic Synthesis, 2018, 15, 275-285.	0.7	10
52	Theoretical investigations of [4Ï€S+2Ï€S] cyclodimerization and stereoselectivity of phthalazin derivatives. Computational and Theoretical Chemistry, 2001, 542, 139-147.	1.5	8
53	Mechanism of Water Attacking on Brookerâ€™s Merocyanine Dye and Its Effect on the Molecular and Electronic Structures: Theoretical Study. Bulletin of the Chemical Society of Japan, 2006, 79, 838-844.	2.0	8
54	Effect of N-methylation on both ground and excited states properties of 1-(9-anthryl)-2-(2-benzothiazolyl) ethene. Journal of Molecular Structure, 2009, 919, 12-20.	1.8	8

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55	Quantum chemical studies and atomistic simulations of some inhibitors for the corrosion of al surface. Protection of Metals and Physical Chemistry of Surfaces, 2016, 52, 156-168.	0.3	8
56	Factors Influencing the Potency of Alzheimer Inhibitors: Computational and Docking Studies. American Journal of Alzheimer's Disease and Other Dementias, 2018, 33, 166-175.	0.9	8
57	Molecular aggregation and photochemical Z/E isomerization of 1-methy-2-[2-(9-phenantheryl)ethenyl] benzothiazolium iodide. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 222, 276-282.	2.0	7
58	Design, synthesis, and computational explorations of novel 2â€thiohydantoin nucleosides with cytotoxic activities. Journal of Heterocyclic Chemistry, 2022, 59, 664-685.	1.4	7
59	Synthesis of New Î±-Amino Phosphonates Containing 3-Amino-4(3H) Quinazolinone Moiety as Anticancer and Antimicrobial Agents: DFT, NBO, and Vibrational Studies. Current Organic Synthesis, 2018, 15, 286-296.	0.7	6
60	UVâ€“vis, IR and 1H NMR spectroscopic studies of some mono- and bis-azo-compounds based on 2,7-dihydroxynaphthalene and aniline derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 980-986.	2.0	5
61	QSAR studies for the computational prediction of HMG-CoA reductase inhibitors by genetic function approximation technique. Canadian Journal of Chemistry, 2013, 91, 263-274.	0.6	5
62	Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. Journal of Photochemistry and Photobiology A: Chemistry, 2015, 301, 20-31.	2.0	5
63	Resorcinol Derivative as an Environmentally Friendly Low Carbon Steel Inhibitor in HCl Medium. ACS Omega, 2022, 7, 17609-17619.	1.6	5
64	Thermal stabilities, electronic properties and structures of metformin-metal complexes. Journal of Thermal Analysis, 1995, 44, 1493-1498.	0.7	4
65	Investigation of regiospecific oxidative heterocyclization of 2-(Nâ€²-benzylidene) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 347 T 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. Organic Electronics, 2012, 13, 807-814.	1.4	3
67	Synthesis, molecular modeling, TDâ€ĐFT, antimicrobial, and in vitro therapeutic activity of new spherical nanoâ€sized sulfonamide imine ligands and their zinc (II) and copper (II) complexes. Applied Organometallic Chemistry, 2020, 34, e5953.	1.7	3
68	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. Computational and Theoretical Chemistry, 1996, 378, 103-110.	1.5	1