Ahmed M El-Nahas

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6485799/publications.pdf

Version: 2024-02-01

98 papers	2,029 citations	279701 23 h-index	289141 40 g-index
100 all docs	100 docs citations	100 times ranked	2061 citing authors

#	Article	IF	Citations
1	Cubically cage-shaped mesoporous ordered silica for simultaneous visual detection and removal of uranium ions from contaminated seawater. Mikrochimica Acta, 2022, 189, 3.	2.5	7
2	Biophysicochemical studies of a ruthenium (II) nitrosyl thioetherâ€thiolate complex binding to BSA: Mechanistic information, molecular docking, and relationship to antibacterial and cytotoxic activities. Applied Organometallic Chemistry, 2022, 36, .	1.7	9
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.	1.9	9
4	Theoretical investigations on the unimolecular decomposition mechanisms of isopropyl acetate. Journal of Molecular Structure, 2022, 1262, 133006.	1.8	6
5	Structures, Energetics, and Spectra of (NH) and (OH) Tautomers of 2-(2-Hydroxyphenyl)-1-azaazulene: A Density Functional Theory/Time-Dependent Density Functional Theory Study. ACS Omega, 2022, 7, 14222-14238.	1.6	4
6	Wide Nematogenic Azomethine/Ester Liquid Crystals Based on New Biphenyl Derivatives: Mesomorphic and Computational Studies. Molecules, 2022, 27, 4150.	1.7	18
7	Attenuation of Redox Switching and Rectification in Azulenequinones/Hydroquinones after B and N Doping: A Firstâ€Principles Investigation. Advanced Theory and Simulations, 2021, 4, 2000203.	1.3	2
8	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.	1.1	15
9	Atmospheric chemistry of oxazole: the mechanism and kinetic studies of the oxidation reaction initiated by OH radicals. New Journal of Chemistry, 2021, 45, 2237-2248.	1.4	15
10	A W1 computational study on the kinetics of initial pyrolysis of a biodiesel model: methyl propanoate. New Journal of Chemistry, 2021, 45, 19531-19541.	1.4	7
11	Ab initio-based kinetics of hydrogen atom abstraction from methyl propionate by H and CH3 radicals: a biodiesel model. Structural Chemistry, 2021, 32, 1857-1872.	1.0	12
12	Synthesis, spectral characterization, density functional theory studies, and biological screening of some transition metal complexes of a novel hydrazideâ€“hydrazone ligand of isonicotinic acid. Applied Organometallic Chemistry, 2021, 35, e6205.	1.7	20
13	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. Fuel, 2021, 290, 119970.	3.4	22
14	Exploring reactions of amines-model compounds with NH2: In relevance to nitrogen conversion chemistry in biomass. Fuel, 2021, 291, 120076.	3.4	12
15	Updated yields of nitrogenated species in flames of ammonia/benzene via introducing an aniline sub-mechanism. Combustion and Flame, 2021, 228, 433-442.	2.8	7
16	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	8
17	Biodiesel combustion: Kinetics and thermochemistry of H-atom abstraction from methyl propionate by Ã– (3P) and O2H radicals: ab initio study. Journal of Molecular Structure, 2021, 1243, 130896.	1.8	0
18	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.	1.4	10

#	Article	IF	Citations
19	A green approach for enhancing the hydrophobicity of UiO-66(Zr) catalysts for biodiesel production at 298 K. RSC Advances, 2020, 10, 41283-41295.	1.7	14
20	A computational study on the kinetics of pyrolysis of isopropyl propionate as a biodiesel model: DFT and ab initio investigation. Fuel, 2020, 281, 118798.	3.4	18
21	Chitosan, magnetite, silicon dioxide, and graphene oxide nanocomposites: Synthesis, characterization, efficiency as cisplatin drug delivery, and DFT calculations. International Journal of Biological Macromolecules, 2020, 154, 621-633.	3.6	71
22	Synthesis, structural, spectroscopic, and thermal studies of some transitionâ€metal complexes of a ligand containing the amino mercapto triazole moiety. Applied Organometallic Chemistry, 2020, 34, e5591.	1.7	28
23	Simulated kinetics of the atmospheric removal of aniline during daytime. Chemosphere, 2020, 255, 127031.	4.2	18
24	Electronic transport investigation of redox-switching of azulenequinones/hydroquinones via first-principles studies. Physical Chemistry Chemical Physics, 2019, 21, 17859-17867.	1.3	2
25	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. Scientific Reports, 2019, 9, 15361.	1.6	17
26	A Series of UiO-66(Zr)-Structured Materials with Defects as Heterogeneous Catalysts for Biodiesel Production. Industrial & Engineering Chemistry Research, 2019, 58, 21961-21971.	1.8	29
27	First-principle studies on the gas phase OH-initiated oxidation of O-toluidine. Computational and Theoretical Chemistry, 2019, 1170, 112634.	1.1	13
28	Adsorption of Cu²⁺ and Mg²⁺ ions on silica gel derived from rice hulls ash: Experimental and theoretical studies. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950026.	1.8	2
29	A thermochemical computational study on hydroxyquinolines and their azulene analogues. Journal of Molecular Structure, 2019, 1183, 70-77.	1.8	4
30	Synthesis of polyaminophosphonic acid-functionalized poly(glycidyl methacrylate) for the efficient sorption of La(III) and Y(III). Chemical Engineering Journal, 2019, 375, 121932.	6.6	46
31	Thermochemistry and Kinetics of the Thermal Degradation of 2-Methoxyethanol as Possible Biofuel Additives. Scientific Reports, 2019, 9, 4535.	1.6	20
32	Structure, stability and conversions of tautomers and rotamers of azulene-based uracil analogue. Journal of Molecular Structure, 2019, 1182, 271-282.	1.8	7
33	Oxidation of Methyl Propanoate by the OH Radical. Russian Journal of Physical Chemistry A, 2018, 92, 2476-2484.	0.1	6
34	A computational study on molecular structure and stability of tautomers of dipyrrole-based phenanthroline analogue. Computational and Theoretical Chemistry, 2018, 1145, 6-14.	1.1	3
35	DFT/TD-DFT calculations of the electronic and optical properties of bis-N,N-dimethylaniline-based dyes for use in dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 367, 332-346.	2.0	17
36	A thermochemistry and kinetic study on the thermal decomposition of ethoxyquinoline and ethoxyisoquinoline. International Journal of Chemical Kinetics, 2018, 50, 604-611.	1.0	1

#	Article	IF	Citations
37	The First Synthesis of 3-O-Methylcyanidin and the Effect of 3-O-Substitution on Stability Under Acidic Conditions. Heterocycles, 2018, 97, 946.	0.4	2
38	Electrical Conductance and Diode-Like Behavior of Substituted Azulene. Journal of Physical Chemistry C, 2017, 121, 2504-2511.	1.5	13
39	Functionalized cellulose-magnetite nanocomposite catalysts for efficient biodiesel production. Chemical Engineering Journal, 2017, 322, 167-180.	6.6	56
40	Selective Recovery of Silver(I) Ions from Eâ€Waste using Cubically Multithiolated Cage Mesoporous Monoliths. European Journal of Inorganic Chemistry, 2017, 2017, 4823-4833.	1.0	37
41	Electrical conductivity of dithiophene-based diblock molecular junctions. Computational and Theoretical Chemistry, 2017, 1099, 64-74.	1.1	2
42	First-Principles Calculations of Electron Transport through Azulene. Journal of Physical Chemistry C, 2016, 120, 9043-9052.	1.5	18
43	Oxidative Stress Induced by Pt(IV) Pro-drugs Based on the Cisplatin Scaffold and Indole Carboxylic Acids in Axial Position. Scientific Reports, 2016, 6, 29367.	1.6	56
44	Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1â€“C5 oxygenates. Molecular Physics, 2015, 113, 1630-1635.	0.8	8
45	Synthesis and Photophysical Property Studies of the 2,6,8-Triaryl-4-(phenylethynyl)quinazolines. Molecules, 2014, 19, 795-818.	1.7	26
46	Synthesis and Photophysical Properties of the 2-(3-(2-Alkyl-6,8-diaryl-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)propyl)-6,8-diarylquinazolin-4(3H)-ones. Molecules, 2014, 19, 9712-9735.	1.7	4
47	Synthesis, Characterization and Theoretical Studies of Novel Phosphonates as uPA Inhibitors. Current Organic Chemistry, 2014, 18, 629-639.	0.9	3
48	Preparation and characterization of a novel system of CdS nanoparticles embedded in borophosphate glass matrix. Journal of Alloys and Compounds, 2013, 555, 161-168.	2.8	19
49	Thermochemistry and kinetics of isobutanol oxidation by the OH radical. Fuel, 2013, 106, 431-436.	3.4	10
50	Theoretical investigation of the conducting properties of substituted phosphole oligomers. Computational and Theoretical Chemistry, 2012, 980, 68-72.	1.1	7
51	A computational study on the structures and energetics of isobutanol pyrolysis. Computational and Theoretical Chemistry, 2012, 997, 94-102.	1.1	9
52	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
53	Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. Journal of Physical Chemistry A, 2011, 115, 2837-2846.	1.1	36
54	Thermodynamic and kinetic stability of magnesium dication solvated by tetramethylethylenediamine. Computational and Theoretical Chemistry, 2011, 978, 104-109.	1.1	4

#	Article	IF	Citations
55	Theoretical studies on the isomers and tautomers of 22-membered macrocyclic ligand. Computational and Theoretical Chemistry, 2011, 967, 75-80.	1.1	1
56	The effect of constitutional and conformational isomerization on the electrical properties of diblock molecular diode. Organic Electronics, 2011, 12, 1080-1092.	1.4	11
57	Structural studies and anticancer activity of a novel (N6O4) macrocyclic ligand and its Cu(II) complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 360-370.	2.0	71
58	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
59	Structures and Energetics of Unimolecular Thermal Degradation of Isopropyl Butanoate as a Model Biofuel: Density Functional Theory and Ab Initio Studies. Journal of Physical Chemistry A, 2010, 114, 7996-8002.	1.1	14
60	Effect of structural properties of acid dyes on their adsorption behaviour from aqueous solutions by amine modified silica. Journal of Hazardous Materials, 2009, 161, 1544-1550.	6.5	158
61	Erratum to â€œStructures, stabilities and tautomerizations of uracil and diphosphouracil tautomersâ€• [Chem. Phys. 332 (2007) 152â€“161]. Chemical Physics, 2008, 348, 254.	0.9	0
62	Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. Computational and Theoretical Chemistry, 2008, 851, 54-62.	1.5	9
63	Thermochemistry and kinetics of acetonylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. Physical Chemistry Chemical Physics, 2008, 10, 7139.	1.3	19
64	DFT/Ab initio Study on the Pathways for the Reaction of CH3SH with NO3Radical. Chemistry Letters, 2007, 36, 400-401.	0.7	1
65	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels:Â Ethyl Propanoate and Methyl Butanoateâ€. Journal of Physical Chemistry A, 2007, 111, 3727-3739.	1.1	145
66	Experimental and Modeling Study of C5H10O2Ethyl and Methyl Estersâ€. Journal of Physical Chemistry A, 2007, 111, 4001-4014.	1.1	157
67	Quantum chemical calculations on the structure and stability of Mg2+XH3OH complexes in the gas phase (X=C, Si, and Ge). International Journal of Mass Spectrometry, 2007, 263, 267-275.	0.7	10
68	Structures, stabilities and tautomerizations of uracil and diphosphouracil tautomers. Chemical Physics, 2007, 332, 152-161.	0.9	26
69	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	1.1	52
70	Relative reactivity and regioselectivity of halogen-substituted ethenes and propene toward addition of an OH radical or O (3P) atom: An ab initio study. Computational and Theoretical Chemistry, 2006, 770, 59-65.	1.5	13
71	Adsorption of Oleic Acid on Silica Gel Derived from Rice Ash Hulls: Experimental and Theoretical Studies. Adsorption Science and Technology, 2006, 24, 797-814.	1.5	10
72	Hydrogen abstraction from dimethyl ether (DME) and dimethyl sulfide (DMS) by OH radical: a computational study. Computational and Theoretical Chemistry, 2005, 722, 9-19.	1.5	43

#	Article	IF	Citations
73	Theoretical study of H3AXH3 and H3AYH2 (A=B, Al, Ga; X=N, P, As and Y=O, S, and Se), electrostatic and hyperconjugative interactions roles. Chemical Physics, 2005, 313, 159-168.	0.9	13
74	Tautomeric 2-arylquinolin-4(1H)-one derivatives- spectroscopic, X-ray and quantum chemical structural studies. Journal of Molecular Structure, 2004, 688, 129-136.	1.8	37
75	Theoretical study on the structures and dissociation channels of metal dications solvated by acetonitrile ligands. International Journal of Mass Spectrometry, 2004, 233, 87-98.	0.7	12
76	Formation and unimolecular dissociation of Al3+(DMSO)n complexes. International Journal of Mass Spectrometry, 2004, 237, 47-54.	0.7	4
77	Conformational studies of potentially tautomeric 2-phenyl- and 3-phenyl-1,4-benzoxazepin-5(4H)-one derivatives. Computational and Theoretical Chemistry, 2004, 668, 157-162.	1.5	4
78	Quantum chemical predictions of structures and vibrational spectra of formaldehyde and related molecules. Computational and Theoretical Chemistry, 2004, 671, 125-132.	1.5	13
79	Spectroscopic and quantum chemical studies on the structure of 2-arylquinoline-4(1H)-thione derivatives. Journal of Molecular Structure, 2004, 690, 151-157.	1.8	11
80	Density-Functional Study on the Structures, Stabilities, and Dissociation Pathways of Sc3+(DMSO)nComplexes (n= 1â^'6). Journal of Physical Chemistry A, 2004, 108, 5322-5332.	1.1	4
81	Reverse SiC Bond Polarization as a Means for Stabilization of Silabenzenes:Â A Computational Investigation. Organometallics, 2003, 22, 5556-5566.	1.1	15
82	Solution phase, solid state and computational structural studies of the 2-aryl-3-bromoquinolin-4(1H)-one derivatives1. Perkin Transactions II RSC, 2002, , 2159-2164.	1.1	14
83	Quantum chemical calculations on metal dications solvated by formaldehyde, acetone and DMSO ligands. Chemical Physics Letters, 2002, 365, 251-259.	1.2	14
84	Thermochemically stable M2+OH2 complexes in the gas phase: M=Mn, Fe, Co, Ni, and Cu. Chemical Physics Letters, 2001, 345, 325-330.	1.2	28
85	Monohydrated alkaline earth metal dications do exist. Chemical Physics Letters, 2001, 348, 483-490.	1.2	15
86	On the existence of Cu2+(NH3)1,2 and Cu2+(OH2)1,2 in the gas phase. Chemical Physics Letters, 2000, 329, 176-178.	1.2	25
87	Do Cu2+NH3 and Cu2+OH2 exist?: theory confirms `yes!'. Chemical Physics Letters, 2000, 318, 333-339.	1.2	44
88	Be2+ V- Dipole and Adsorptivity of Atomic H on LiH(001) Surface: ab initio Study. Journal of Molecular Modeling, 2000, 6, 26-34.	0.8	1
89	Complexation of Li+and Cu+with HX (X = F, Cl, OH, SH, NH2, and PH2) Molecules by B3LYP and CCSD(T) Methods. Journal of Physical Chemistry A, 2000, 104, 138-144.	1.1	21
90	A theoretical study on 2-hydroxypyrazine and 2,3-dihydroxypyrazine: tautomerism, intramolecular hydrogen bond, solvent effects. Computational and Theoretical Chemistry, 1999, 459, 229-237.	1.5	21

#	Article	IF	Citations
91	Binding energies and electronic structures of Cu + (OH 2) n and Cu + (NH 3) n (n =1â€“4): anomaly of the two ligand Cu + complexes. Computational and Theoretical Chemistry, 1999, 469, 201-213.	1.5	33
92	A theoretical study on the catalysis of Cu-exchanged zeolite for the decomposition of nitric oxide. Physical Chemistry Chemical Physics, 1999, 1, 3823-3830.	1.3	47
93	Quantum chemical studies on structures and spectra of 2,5-distyrylpyrazine (DSP) laser dye. Journal of Computational Chemistry, 1998, 19, 585-592.	1.5	2
94	Semiempirical and Ab Initio Calculations of Tautomerism in 2,3-Dihydroxypyrazine. Journal of Chemical Research Synopses, 1998, , 222-223.	0.3	5
95	Theoretical Study on Photophysical and Photochemical Properties of a Merocyanine Dye. Journal of Physical Chemistry A, 1998, 102, 9739-9744.	1.1	18
96	Bond functions and many-body effects of the helium trimer. Theoretical Chemistry Accounts, 1997, 96, 217-222.	0.5	5
97	AM1 and PM3 Calculations on the Effect of Substituents on the Stabilities of Carbocations in the Gas Phase and in Solution. Journal of Organic Chemistry, 1995, 60, 8023-8027.	1.7	14
98	Structures and stabilization energies of methyl anions with main group substituents from the first five periods. Journal of Computational Chemistry, 1994, 15, 596-626.	1.5	44