Mwadham M Kabanda

List of Publications by Year in Descending Order

52 papers	1,989 citations	26 h-index	44 g-index
53 ext. papers	2,249 ext. citations	3.1 avg, IF	5.28 L-index

#	Paper	IF	Citations
52	Hydrogen bonding between 1-ethyl-3-methyl-imidazolium dicyanamide ionic liquid and selected co-solvents with varying polarity: A DFT study. *Journal of Molecular Liquids*, **2022**, 119418	6	1
51	A DFT and MP2 mechanistic and kinetic study on hypohalogenation reaction of cysteine and N-acetylcysteine in aqueous solution. *Journal of Molecular Liquids*, **2021**, 349, 118191	6	0
50	Proportional coexistence of okanin chalcone glycoside and okanin flavanone glycoside in leaves and theoretical investigation on the antioxidant properties of their aglycones. *Free Radical Research*, **2021**, 55, 53-70	4	4
49	LC-MS based validation and DFT investigation on the antioxidant properties of clovamide: •OH and •OOH scavenging and Cu(II) chelation mechanisms. *Journal of Molecular Structure*, **2021**, 1236, 130349	3.4	1
48	A Theoretical Study of the Preferred Reaction Mechanism Between Chloroacetic Acid and Thiourea. *Progress in Theoretical Chemistry and Physics*, **2020**, 119-142	0.6	
47	A DFT mechanistic and kinetic study on the reaction of phloroglucinol with •OH in different media: Hydrogen atom transfer versus oxidation. *Journal of Theoretical and Computational Chemistry*, **2019** , 18, 1950017	1.8	3
46	A DFT mechanistic, thermodynamic and kinetic study on the reaction of 1, 3, 5-trihydroxybenzene and 2, 4, 6-trihydroxyacetophenone with •OOH in different media. *Journal of Theoretical and Computational Chemistry*, **2019**, 18, 1950023	1.8	3
45	A Theoretical study on the degradation of 2-mercaptobenzothiazole and 2-mercaptobenzimidazole by OH in vacuo and aqueous media. *Computational and Theoretical Chemistry*, **2018**, 1125, 112-127	2	4
44	A DFT study on the addition and abstraction reactions of thiourea with hydroxyl radical. *Journal of Sulfur Chemistry*, **2018**, 39, 23-46	2.3	12
43	Structural Elucidation of cis/trans Dicaffeoylquinic Acid Photoisomerization Using Ion Mobility Spectrometry-Mass Spectrometry. *Journal of Physical Chemistry Letters*, **2017**, 8, 1381-1388	6.4	33
42	An appraisal of the hydrogen atom transfer mechanism for the reaction between thiourea derivatives and . *Computational and Theoretical Chemistry*, **2017**, 1101, 83-95	2	12
41	A theoretical study on the antioxidant properties of methoxy-substituted chalcone derivatives: A case study of kanakugiol and pedicellin through their Fe (II and III) coordination ability. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650048	1.8	15
40	Synthesis, crystal structure, thermal and theoretical studies of bis(N-ethyl-N-phenyldithiocarbamato) Ni(II) and (N-ethyl-N-phenyldithiocarbamato) (isothiocyanato) (triphenylphosphine) Ni(II). *Journal of Chemical Sciences*, **2016**, 128, 1081-1093	1.8	9
39	Investigation of the adsorption characteristics of some selected sulphonamide derivatives as corrosion inhibitors at mild steel/hydrochloric acid interface: Experimental, quantum chemical and QSAR studies. *Journal of Molecular Liquids*, **2016**, 215, 763-779	6	52
38	Antioxidant and antimalarial properties of butein and homobutein based on their ability to chelate iron (II and III) cations: a DFT study in vacuo and in solution. *European Food Research and Technology*, **2016**, 242, 71-90	3.4	19
37	Quinoxaline derivatives as corrosion inhibitors for mild steel in hydrochloric acid medium: Electrochemical and quantum chemical studies. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 76, 109-126	3	90
36	The Effect of Geometrical Isomerism of 3,5-Dicaffeoylquinic Acid on Its Binding Affinity to HIV-Integrase Enzyme: A Molecular Docking Study. *Evidence-based Complementary and Alternative Medicine*, **2016**, 2016, 4138263	2.3	13

35	Preferential alkali metal adduct formation by cis geometrical isomers of dicaffeoylquinic acids allows for efficient discrimination from their trans isomers during ultra-high-performance liquid chromatography/quadrupole time-of-flight mass spectrometry. *Rapid Communications in Mass Spectrometry*, **2016**, 30, 1011-8	2.2	28
34	Experimental and theoretical studies on some selected ionic liquids with different cations/anions as corrosion inhibitors for mild steel in acidic medium. *Journal of the Taiwan Institute of Chemical Engineers*, **2016**, 64, 252-268	5.3	93
33	Influence of the geometric isomers on the radical scavenging properties of 3,5-dicaffeoylquinic acid: A DFT study in vacuo and in solution. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650052	1.8	2
32	A theoretical study of the antioxidant properties of phenolic acid amides investigated through the radical-scavenging and metal chelation mechanisms. *European Food Research and Technology*, **2015**, 241, 553-572	3.4	9
31	Some Quinoxalin-6-yl Derivatives as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid: Experimental and Theoretical Studies. *Journal of Physical Chemistry C*, **2015**, 119, 16004-16019	3.8	301
30	Experimental and theoretical studies on the corrosion inhibition of mild steel by some sulphonamides in aqueous HCl. *RSC Advances*, **2015**, 5, 28743-28761	3.7	77
29	Synthesized photo-cross-linking chalcones as novel corrosion inhibitors for mild steel in acidic medium: experimental, quantum chemical and Monte Carlo simulation studies. *RSC Advances*, **2015**, 5, 76675-76688	3.7	47
28	Conformational, electronic and antioxidant properties of lucidone, linderone and methyllinderone: DFT, QTAIM and NBO studies. *Molecular Physics*, **2015**, 113, 683-697	1.7	31
27	Antioxidant Radical Scavenging Properties of Phenolic Pent-4-En-1-Yne Derivatives Isolated From Hypoxis Rooperi. A DFT Study in vacuo and in Solution. *International Journal of Food Properties*, **2015**, 18, 149-164	3	19
26	Adsorption and Corrosion Inhibition Studies of Some Selected Dyes as Corrosion Inhibitors for Mild Steel in Acidic Medium: Gravimetric, Electrochemical, Quantum Chemical Studies and Synergistic Effect with Iodide Ions. *Molecules*, **2015**, 20, 16004-29	4.8	71
25	Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl. *Materials*, **2015**, 8, 3607-3632	3.5	72
24	Some Phthalocyanine and Naphthalocyanine Derivatives as Corrosion Inhibitors for Aluminium in Acidic Medium: Experimental, Quantum Chemical Calculations, QSAR Studies and Synergistic Effect of Iodide Ions. *Molecules*, **2015**, 20, 15701-34	4.8	35
23	Porphyrins as Corrosion Inhibitors for N80 Steel in 3.5% NaCl Solution: Electrochemical, Quantum Chemical, QSAR and Monte Carlo Simulations Studies. *Molecules*, **2015**, 20, 15122-46	4.8	52
22	Antioxidant Properties of Kanakugiol Revealed Through the Hydrogen Atom Transfer, Electron Transfer and M2+ (M2+ = Cu(II) or Co(II) Ion) Coordination Ability Mechanisms. A DFT Study In Vacuo and in Solution. *Food Biophysics*, **2015**, 10, 342-359	3.2	21
21	A computational study of pyrazinamide: Tautomerism, acid–base properties, micro-solvation effects and acid hydrolysis mechanism. *Computational and Theoretical Chemistry*, **2014**, 1046, 30-41	2	23
20	MP2, DFT and DFT-D study of the dimers of diazanaphthalenes: a comparative study of their structures, stabilisation and binding energies. *Molecular Simulation*, **2014**, 40, 1131-1146	2	8
19	Metronidazole as environmentally safe corrosion inhibitor for mild steel in 0.5 M HCl: Experimental and theoretical investigation. *Journal of Environmental Chemical Engineering*, **2013**, 1, 431-439	6.8	131
18	Isolation, identification and radical scavenging activity of phlorotannin derivatives from brown algae, Ecklonia maxima: An experimental and theoretical study. *Free Radicals and Antioxidants*, **2013**,	1.7	4

17	Weight Loss, Electrochemical, Quantum Chemical Calculation, and Molecular Dynamics Simulation Studies on 2-(Benzylthio)-1,4,5-triphenyl-1H-imidazole as an Inhibitor for Carbon Steel Corrosion in Hydrochloric Acid. *Industrial & Engineering Chemistry Research*, **2013**, 52, 14315-14327	3.9	59
16	Structures, stabilization energies, and binding energies of quinoxaline(H2O)(n), quinoxaline dimer, and quinoxalineCu complexes: a theoretical study. *Journal of Physical Chemistry A*, **2013**, 117, 1583-95	2.8	18
15	DFT STUDY OF THE PROTONATION AND DEPROTONATION ENTHALPIES OF BENZOXAZOLE, 1,2-BENZISOXAZOLE AND 2,1-BENZISOXAZOLE AND IMPLICATIONS FOR THE STRUCTURES AND ENERGIES OF THEIR ADDUCTS WITH EXPLICIT WATER MOLECULES. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1350070	1.8	11
14	Antioxidant activity of rooperol investigated through Cu (I and II) chelation ability and the hydrogen transfer mechanism: a DFT study. *Chemical Research in Toxicology*, **2012**, 25, 2153-66	4	34
13	Electrochemical and Quantum Chemical Investigation of Some Azine and Thiazine Dyes as Potential Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution. *Industrial & Engineering Chemistry Research*, **2012**, 51, 12940-12958	3.9	113
12	Experimental and Quantum Chemical Studies of Some Bis(trifluoromethyl-sulfonyl) Imide Imidazolium-Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution. *Industrial & Engineering Chemistry Research*, **2012**, 51, 13282-13299	3.9	136
11	A comparative study of the dimers of selected hydroxybenzenes. *International Journal of Quantum Chemistry*, **2012**, 112, 519-531	2.1	17
10	Computational study of the patterns of weaker intramolecular hydrogen bonds stabilizing acylphloroglucinols. *International Journal of Quantum Chemistry*, **2012**, 112, 2650-2658	2.1	31
9	The conformational preferences of acylphloroglucinols promising class of biologically active compounds. *International Journal of Quantum Chemistry*, **2012**, 112, 3691-3702	2.1	35
8	A computational study of the carboxylic acid of phloroglucinol in vacuo and in water solution. *International Journal of Quantum Chemistry*, **2010**, 110, 595-623	2.1	31
7	Adducts of acylphloroglucinols with explicit water molecules: Similarities and differences across a sufficiently representative number of structures. *International Journal of Quantum Chemistry*, **2010**, 110, n/a-n/a	2.1	3
6	Interplay of intramolecular hydrogen bonds, OH orientations, and symmetry factors in the stabilization of polyhydroxybenzenes. *International Journal of Quantum Chemistry*, **2010**, 111, n/a-n/a	2.1	1
5	A study of the intramolecular hydrogen bond in acylphloroglucinols. *Computational and Theoretical Chemistry*, **2009**, 901, 210-219		59
4	A computational study of the effects of different solvents on the characteristics of the intramolecular hydrogen bond in acylphloroglucinols. *Journal of Physical Chemistry A*, **2009**, 113, 15064-77	2.8	50
3	A computational study of the interactions of the caespitate molecule with water. *International Journal of Quantum Chemistry*, **2008**, 108, 1772-1791	2.1	26
2	A computational study of the interactions of the phloroglucinol molecule with water. *Computational and Theoretical Chemistry*, **2008**, 852, 36-45		26
1	Model structures for the study of acylated phloroglucinols and computational study of the caespitate molecule. *Computational and Theoretical Chemistry*, **2007**, 805, 39-52		44