Saadullah G Aziz

List of Publications by Year in Descending Order

83 papers	1,491 citations	23 h-index	36 g-index
91 ext. papers	1,677 ext. citations	4.7 avg, IF	4.55 L-index

#	Paper	IF	Citations
83	Zn-Schiff Base Complex as an "On-Off-On" Molecular Switch and a Fluorescence Probe for Cu and Ag Ions.. *Journal of Fluorescence*, **2022**, 32, 691	2.4	0
82	Formation of the oxonium phenol ion in the stepwise hydration of the phenyl cation in the gas phase. *Journal of Molecular Liquids*, **2021**, 322, 114541	6	0
81	Solvation and speciation of cobalt(II). A theoretical X-ray absorption and RIXS study. *Chemical Physics*, **2020**, 532, 110681	2.3	4
80	Synthesis, characterization, computational study, DNA binding and molecular docking studies of chromium (III) drug-based complexes. *Journal of Molecular Structure*, **2020**, 1215, 128283	3.4	2
79	Solvent-assisted excited state proton transfer and photoacidity of 2-hydroxypyridine. A nonadiabatic dynamics study. *Molecular Simulation*, **2019**, 45, 165-177	2	2
78	Proton-coupled electron transfer in dye-sensitized solar cells: a theoretical perspective. *Structural Chemistry*, **2018**, 29, 983-997	1.8	8
77	Characterization of the structural, mechanical, and electronic properties of fullerene mixtures: a molecular simulations description. *Journal of Materials Chemistry C*, **2018**, 6, 3642-3650	7.1	8
76	Impact of Hydroxylation and Hydration on the Reactivity of □Fe2O3 (0001) and (102) Surfaces under Environmental and Electrochemical Conditions. *Advanced Energy Materials*, **2018**, 8, 1800545	21.8	7
75	Theoretical insights into dehydrogenative chemisorption of alkylaromatics on Pt(1 0 0) and Ni(1 0 0). *Journal of Catalysis*, **2018**, 363, 197-203	7.3	3
74	Ultrafast Spin-State Dynamics in Transition-Metal Complexes Triggered by Soft-X-Ray Light. *Physical Review Letters*, **2017**, 118, 023001	7.4	6
73	Nuclear Dynamical Correlation Effects in X-ray Spectroscopy from a Theoretical Time-Domain Perspective. *Journal of Physical Chemistry Letters*, **2017**, 8, 992-996	6.4	6
72	Observation of covalent and electrostatic bonds in nitrogen-containing polycyclic ions formed by gas phase reactions of the benzene radical cation with pyrimidine. *Physical Chemistry Chemical Physics*, **2017**, 19, 6422-6432	3.6	4
71	Understanding the effects of electronic polarization and delocalization on charge-transport levels in oligoacene systems. *Journal of Chemical Physics*, **2017**, 146, 224705	3.9	12
70	Density matrix-based time-dependent configuration interaction approach to ultrafast spin-flip dynamics. *Molecular Physics*, **2017**, 115, 1898-1907	1.7	4
69	Toward better understanding of the support effect: Test cases for CO dissociation on Fen/TiO2(1 1 0), n = 4, 5. *Chemical Physics Letters*, **2017**, 684, 30-35	2.5	1
68	Time dependent □density functional theory characterization of organic dyes for dye-sensitized solar cells. *Molecular Simulation*, **2017**, 43, 1523-1531	2	13
67	Light-induced relaxation dynamics of the ferricyanide ion revisited by ultrafast XUV photoelectron spectroscopy. *Physical Chemistry Chemical Physics*, **2017**, 19, 14248-14255	3.6	24

66	Electronic structure and acidBase properties of Kojic acid and its dimers. A DFT and quantum topology study. *Molecular Physics*, **2017**, 115, 2565-2576	1.7	5
65	Effect of substitution on the optoelectronic properties of dyes for DSSC. A DFT approach. *Journal of Theoretical and Computational Chemistry*, **2017**, 16, 1750018	1.8	6
64	Ultrafast Spin Crossover in [Fe (bpy)] : Revealing Two Competing Mechanisms by Extreme Ultraviolet Photoemission Spectroscopy. *ChemPhysChem*, **2017**, 18, 465-469	3.2	24
63	Gas phase hydration of halogenated benzene cations. Is it hydrogen or halogen bonding?. *Physical Chemistry Chemical Physics*, **2017**, 19, 18603-18611	3.6	4
62	Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New C-N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. *Journal of the American Chemical Society*, **2017**, 139, 11923-11932	16.4	7
61	A time-correlation function approach to nuclear dynamical effects in X-ray spectroscopy. *Journal of Chemical Physics*, **2017**, 146, 224203	3.9	4
60	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. *Journal of Chemical Theory and Computation*, **2017**, 13, 5846-5860	6.4	33
59	Ultrafast kinetics of linkage isomerism in Na[Fe(CN)NO] aqueous solution revealed by time-resolved photoelectron spectroscopy. *Structural Dynamics*, **2017**, 4, 044031	3.2	8
58	The electronic structure of alloxan monohydrate. Spectroscopic and density functional synergic approach. *Journal of Molecular Structure*, **2017**, 1130, 487-496	3.4	1
57	Packing and Disorder in Substituted Fullerenes. *Journal of Physical Chemistry C*, **2016**, 120, 17242-17250	3.8	23
56	Joint Analysis of Radiative and Non-Radiative Electronic Relaxation Upon X-ray Irradiation of Transition Metal Aqueous Solutions. *Scientific Reports*, **2016**, 6, 24659	4.9	35
55	Towards an ab initio theory for metal L-edge soft X-ray spectroscopy of molecular aggregates. *Structural Dynamics*, **2016**, 3, 062601	3.2	25
54	Efficient extraction of sulfate from water using a Zr-metal-organic framework. *Dalton Transactions*, **2016**, 45, 93-7	4.3	43
53	Photochemical dissociation of HOBr. A nonadiabatic dynamics study. *Journal of Photochemistry and Photobiology A: Chemistry*, **2016**, 324, 8-13	4.7	3
52	Xe-bearing hydrocarbon ions: Observation of Xe.acetylene+ and Xe.benzene+ radical cations and calculations of their ground state structures. *Chemical Physics Letters*, **2016**, 649, 8-14	2.5	0
51	Unconventional CH(ǂ)N hydrogen bonding interactions in the stepwise solvation of the naphthalene radical cation by hydrogen cyanide and acetonitrile molecules. *Physical Chemistry Chemical Physics*, **2016**, 18, 2580-90	3.6	4
50	The Thermodynamic and Kinetic Properties of 2-Hydroxypyridine/2-Pyridone Tautomerization: A Theoretical and Computational Revisit. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	18
49	UV excitations of halons. *Journal of Chemical Physics*, **2016**, 145, 184306	3.9	6

48	Substituent effects on the absorption and vibrational spectra of some 2-hydroxy Schiff bases: DFT/TDDFT, natural bond orbital and experimental study. *Journal of Structural Chemistry*, **2015**, 56, 414-427	0.9	1
47	Magnetite Fe3O4 (111) Surfaces: Impact of Defects on Structure, Stability, and Electronic Properties. *Chemistry of Materials*, **2015**, 27, 5856-5867	9.6	78
46	Unraveling the Electronic Structure of Photocatalytic Manganese Complexes by L-Edge X-ray Spectroscopy. *Journal of Physical Chemistry C*, **2015**, 119, 19192-19200	3.8	35
45	Towards understanding the decomposition/isomerism channels of stratospheric bromine species: ab initio and quantum topology study. *International Journal of Molecular Sciences*, **2015**, 16, 6783-800	6.3	6
44	Static and Dynamic Energetic Disorders in the C60, PC61BM, C70, and PC71BM Fullerenes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3657-62	6.4	89
43	Communication: Ion mobility of the radical cation dimers: (Naphthalene)2(+) and naphthalene(+)-benzene: Evidence for stacked sandwich and T-shape structures. *Journal of Chemical Physics*, **2015**, 142, 191102	3.9	10
42	Effect of Solvent Additives on the Solution Aggregation of Phenyl-C61-Butyl Acid Methyl Ester (PCBM). *Chemistry of Materials*, **2015**, 27, 8261-8272	9.6	23
41	Photochemistry of methyl hypobromite (CH3OBr): excited states and photoabsorption spectrum. *RSC Advances*, **2015**, 5, 97003-97015	3.7	2
40	Electronic structure of alloxan and its dimers: QM/QD simulations and quantum chemical topology analysis. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 2121-32	3.6	2
39	Interaction of polar and nonpolar organic pollutants with soil organic matter: sorption experiments and molecular dynamics simulation. *Science of the Total Environment*, **2015**, 508, 276-87	10.2	51
38	Protonation and deprotonation enthalpies of alloxan and implications for the structure and energy of its complexes with water: a computational study. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 897-910	3.6	6
37	Multi-reference approach to the calculation of photoelectron spectra including spin-orbit coupling. *Journal of Chemical Physics*, **2015**, 143, 074104	3.9	37
36	Quantum Topology of the Charge Density of Chemical Bonds. QTAIM Analysis of the C-Br and O-Br Bonds. *Procedia Computer Science*, **2015**, 51, 1872-1877	1.6	8
35	Gas-Phase Thermal Tautomerization of Imidazole-Acetic Acid: Theoretical and Computational Investigations. *International Journal of Molecular Sciences*, **2015**, 16, 26347-62	6.3	4
34	Experimental and theoretical assignment of the vibrational spectra of triazoles and benzotriazoles. Identification of IR marker bands and electric response properties. *Journal of Molecular Modeling*, **2014**, 20, 2078	2	20
33	Structure and Disorder in Squaraine:C60 Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donor/Acceptor Interface. *Advanced Functional Materials*, **2014**, 24, 3790-3798	15.6	38
32	Theoretical and computational studies of conformation, natural bond orbital and nonlinear optical properties of cis-N-phenylbenzohydroxamic acid. *Computational and Theoretical Chemistry*, **2014**, 1028, 65-71	2	8
31	Impact of Electron Delocalization on the Nature of the Charge-Transfer States in Model Pentacene/C60 Interfaces: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 27648-27656	3.8	67

30	Interplay of alternative conjugated pathways and steric interactions on the electronic and optical properties of donor□cceptor conjugated polymers. *Journal of Materials Chemistry C*, **2014**, 2, 8873-8879	7.1	22
29	Evidence for the Formation of Pyrimidine Cations from the Sequential Reactions of Hydrogen Cyanide with the Acetylene Radical Cation. *Journal of Physical Chemistry Letters*, **2014**, 5, 3392-8	6.4	23
28	Influence of Molecular Shape on Solid-State Packing in Disordered PC61BM and PC71BM Fullerenes. *Journal of Physical Chemistry Letters*, **2014**, 5, 3427-33	6.4	37
27	Hydrogen bonding of the naphthalene radical cation to water and methanol and attachment of the naphthalene ion to extended hydrogen bonding chains. *Chemical Physics Letters*, **2014**, 613, 45-53	2.5	14
26	Synthesis and optophysical properties of dimeric aza-BODIPY dyes with a push-pull benzodipyrrolidone core. *Chemical Communications*, **2014**, 50, 11540-2	5.8	37
25	A density functional theory investigation of the electronic structure and spin moments of magnetite. *Science and Technology of Advanced Materials*, **2014**, 15, 044202	7.1	57
24	Molecular design of donor-acceptor dyes for efficient dye-sensitized solar cells I: a DFT study. *Journal of Molecular Modeling*, **2014**, 20, 2241	2	28
23	Theoretical Study of the Local and Charge-Transfer Excitations in Model Complexes of Pentacene-C60 Using Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 2379-88	6.4	65
22	Origin of the Extra Stability of Alloxan. A Computation Study. *Procedia Computer Science*, **2014**, 29, 1366-1375	1.6	
21	Exploring the Conical Intersection Seam in Cytosine: A DFT and CASSCF Study. *Procedia Computer Science*, **2014**, 29, 1384-1391	1.6	
20	Theoretical description of the geometric and electronic structures of organic-organic interfaces in organic solar cells: a brief review. *Science China Chemistry*, **2014**, 57, 1330-1339	7.9	5
19	Does prop-2-ynylideneamine, HC?CCH=NH, exist in space? A theoretical and computational investigation. *International Journal of Molecular Sciences*, **2014**, 15, 11064-81	6.3	1
18	Proton-bound dimers of nitrogen heterocyclic molecules: substituent effects on the structures and binding energies of homodimers of diazine, triazine, and fluoropyridine. *Journal of Chemical Physics*, **2014**, 140, 114313	3.9	10
17	Unconventional hydrogen bonding to organic ions in the gas phase: stepwise association of hydrogen cyanide with the pyridine and pyrimidine radical cations and protonated pyridine. *Journal of Chemical Physics*, **2014**, 141, 054305	3.9	17
16	How soil organic matter composition controls hexachlorobenzene-soil-interactions: adsorption isotherms and quantum chemical modeling. *Science of the Total Environment*, **2014**, 476-477, 98-106	10.2	19
15	Hydration of the pyrimidine radical cation and stepwise solvation of protonated pyrimidine with water, methanol, and acetonitrile. *Journal of Chemical Physics*, **2013**, 139, 084304	3.9	17
14	Electronic structure and decomposition reaction mechanism of cyclopropenone, phenylcylopropenone and their sulfur analogues: a theoretical study. *Journal of Molecular Modeling* , **2013**, 19, 1339-53	2	4
13	Theoretical Investigation of the Dispersion Interaction in Argon Dimer and Trimer. *Procedia Computer Science*, **2013**, 18, 826-834	1.6	3

12	Substituent effects on noncovalent bonds: complexes of ionized benzene derivatives with hydrogen cyanide. *Journal of Physical Chemistry A*, **2013**, 117, 10588-97	2.8	7
11	Theoretical characterization of gas-phase thermolysis products of ethane-1,2-diol, 2-chloroethanol and 2-fluoroethanol. *Molecular Physics*, **2013**, 111, 643-659	1.7	4
10	Effects of protonation and deprotonation on the reactivity of quinolone: A theoretical study. *Science Bulletin*, **2012**, 57, 1665-1671		7
9	Eclipsed acetaldehyde as a precursor for producing vinyl alcohol. *International Journal of Molecular Sciences*, **2012**, 13, 15360-72	6.3	3
8	Understanding the decomposition reaction mechanism of chrysanthemic acid: a computational study. *Chemistry Central Journal*, **2011**, 5, 66		4
7	Theoretical investigation of the photochemical reaction mechanism of cyclopropenone decarbonylation. *Molecular Physics*, **2011**, 109, 1785-1795	1.7	5
6	Sequential in situ STM imaging of electrodissolving copper in different aqueous acid solutions. *Electrochimica Acta*, **1998**, 43, 3-12	6.7	18
5	Sequential in situ STM imaging of electrodissolving copper single-crystal domains in aqueous perchloric acid: Kinetics and mechanism of the interface evolution. *Physical Review B*, **1997**, 56, 4166-4175	3.3	8
4	Thermodynamic and kinetic factors in chloride ion pitting and nitrogen donor ligand inhibition of aluminium metal corrosion in aggressive acid media. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 795		25
3	Kinetic-Thermodynamic and Adsorption Isotherms Analyses for the Inhibition of the Acid Corrosion of Steel by Cyclic and Open-Chain Amines. *Journal of the Electrochemical Society*, **1992**, 139, 2149-2154	3.9	198
2	The production and spectroscopic identification of bromothioborine, BrB?S from the thermolysis of 2,4,6-Trisbromo-cyclo-1,3,5-trithia-2,4,6-triborane, (BrBS)3. *Inorganica Chimica Acta*, **1988**, 146, 167-171	2.7	7
1	On the Electronic Structure of Azolides. Part II: Electronic Absorption Spectra of N-Acylimidazoles. A MO Approach to Cross- and Linear Conjugation. *Applied Spectroscopy*, **1986**, 40, 556-562	3.1	5