Adelia J A Aquino

List of Publications by Year
in descending order

94 papers	3,432 citations	172207 29 h-index	149479 56 g-index
96 all docs	96 docs citations	96 times ranked	3585 citing authors

#	Article	IF	Citations
1	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21453-21458.	3.3	362
2	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	23.0	287
3	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. Physical Chemistry Chemical Physics, 2010, 12, 4959.	1.3	208
4	Excited-State Intramolecular Proton Transfer:Â A Survey of TDDFT and RI-CC2 Excited-State Potential Energy Surfaces. Journal of Physical Chemistry A, 2005, 109, 3201-3208.	1.1	175
5	Ultrafast internal conversion pathway and mechanism in 2-(2â€²-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. Physical Chemistry Chemical Physics, 2009, 11, 1406.	1.3	174
6	Solvent Effects on Hydrogen BondsA Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871.	1.1	167
7	Isomeric Separation of Permethylated Glycans by Porous Graphitic Carbon (PGC)-LC-MS/MS at High Temperatures. Analytical Chemistry, 2017, 89, 6590-6597.	3.2	96
8	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145.	1.3	84
9	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255.	1.1	84
10	Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	77
11	The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227.	1.5	73
12	The decay mechanism of photoexcited guanine â˜’ A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304.	1.2	70
13	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2â€²-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 9016.	1.3	69
14	Electronically Excited States in Poly(p-phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 2181-2189.	1.1	65
15	Ultrafast two-step process in the non-adiabatic relaxation of the CH2 molecule. Molecular Physics, 2006, 104, 1053-1060.	0.8	64
16	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the Ï€Ïƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	1.1	60
17	Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255.	6.6	59
18	Ï€â€“Ï€ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310.	1.3	57

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19	Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. Environmental Science & Technology, 2011, 45, 8411-8419.	4.6	54
20	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. Journal of Chemical Theory and Computation, 2014, 10, 3280-3289.	2.3	54
21	Fluorination of an Alumina Surface: Modeling Aluminumâ€“Fluorine Reaction Mechanisms. ACS Applied Materials & Interfaces, 2017, 9, 24290-24297.	4.0	49
22	Stabilizing Capacity of Water Bridges in Nanopore Segments of Humic Substances: A Theoretical Investigation. Journal of Physical Chemistry C, 2009, 113, 16468-16475.	1.5	47
23	The functionality of cation bridges for binding polar groups in soil aggregates. International Journal of Quantum Chemistry, 2011, 111, 1531-1542.	1.0	46
24	Excited-State Properties and Environmental Effects for Protonated Schiff Bases: A Theoretical Study. ChemPhysChem, 2006, 7, 2089-2096.	1.0	43
25	Excited-State Proton Transfer in 7-Hydroxy-4-methylcoumarin along a Hydrogen-Bonded Water Wire. Journal of Physical Chemistry A, 2007, 111, 127-135.	1.1	43
26	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
27	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. Journal of Chemical Physics, 2019, 150, 124302.	1.2	35
28	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. Physical Chemistry Chemical Physics, 2019, 21, 9077-9088.	1.3	34
29	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669.	6.6	31
30	Singlet L_a and L_b Bands for N-Acenes (N = 2â€“7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306.	2.3	30
31	The electronically excited states of RDX (hexahydroâ€1,3,5â€trinitroâ€1,3,5â€triazine): Vertical excitations. International Journal of Quantum Chemistry, 2009, 109, 2348-2355.	1.0	27
32	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. Journal of Physical Chemistry C, 2020, 124, 14327-14337.	1.5	25
33	Restructuring of a Peat in Interaction with Multivalent Cations: Effect of Cation Type and Aging Time. PLoS ONE, 2013, 8, e65359.	1.1	24
34	Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. Journal of Organic Chemistry, 2018, 83, 244-252.	1.7	24
35	How to efficiently tune the biradicaloid nature of acenes by chemical doping with boron and nitrogen. Physical Chemistry Chemical Physics, 2017, 19, 19225-19233.	1.3	23
36	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	1.3	23

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37	Absorption and Fluorescence Spectra of Poly(p-phenylenevinylene) (PPV) Oligomers: An ab Initio Simulation. Journal of Physical Chemistry A, 2015, 119, 1787-1795.	1.1	22
38	Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4-b]thiophene benzodithiophene) by Means of ab Initio and Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 21818-21826.	1.5	22
39	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. Journal of Materials Chemistry C, 2020, 8, 7793-7804.	2.7	22
40	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. Topics in Current Chemistry, 2014, 356, 1-37.	4.0	20
41	Analysis of charge transfer transitions in stacked Ï€-electron donorâ€“acceptor complexes. Physical Chemistry Chemical Physics, 2018, 20, 26957-26967.	1.3	19
42	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. Journal of Physical Chemistry Letters, 2019, 10, 5592-5597.	2.1	18
43	Waterâ€“Ionomer Interfacial Interactions Investigated by Infrared Spectroscopy and Computational Methods. Langmuir, 2013, 29, 13890-13897.	1.6	17
44	The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. Physical Chemistry Chemical Physics, 2015, 17, 12778-12785.	1.3	17
45	Effect of Polar Environments on the Aluminum Oxide Shell Surrounding Aluminum Particles: Simulations of Surface Hydroxyl Bonding and Charge. ACS Applied Materials & Interfaces, 2016, 8, 13926-13933.	4.0	17
46	The electronic transitions of analogs of red wine pyranoanthocyanin pigments. Photochemical and Photobiological Sciences, 2019, 18, 45-53.	1.6	16
47	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for cis-/trans-Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. Journal of Organic Chemistry, 2020, 85, 3664-3675.	1.7	16
48	Post-transition state dynamics and product energy partitioning following thermal excitation of the Fâ‹¯HCH2CN transition state: Disagreement with experiment. Journal of Chemical Physics, 2017, 147, 144301.	1.2	14
49	Lewis acid base chemistry of Bestmann's ylide, Ph₃PCCO, and its bulkier analogue, (cyclohexyl)₃PCCO. Chemical Communications, 2019, 55, 3513-3516.	2.2	14
50	Nonadiabatic Dynamics of Charge-Transfer States Using the Anthraceneâ€“Tetracyanoethylene Complex as a Prototype. Journal of Physical Chemistry A, 2020, 124, 3347-3357.	1.1	13
51	Energy transfer mechanism in luminescence Eu(III) and Tb(III) complexes of coumarin-3-carboxylic acid: A theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 240, 118591.	2.0	12
52	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499.	1.0	11
53	Adsorption process of polar and nonpolar compounds in a nanopore model of humic substances. European Journal of Soil Science, 2020, 71, 845-855.	1.8	11
54	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. Journal of Chemical Physics, 2021, 154, 044306.	1.2	11

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55	The Diverse Manifold of Electronic States Generated by a Single Carbon Defect in a Graphene Sheet: Multireference Calculations Using a Pyrene Defect Model. ChemPhysChem, 2014, 15, 3334-3341.	1.0	10
56	The characterization of electronic defect states of single and double carbon vacancies in graphene sheets using molecular density functional theory. Molecular Physics, 2019, 117, 1519-1531.	0.8	10
57	Chromophores inspired by the colors of fruit, flowers and wine. Pure and Applied Chemistry, 2020, 92, 255-263.	0.9	10
58	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorizationviavalence bond theory and high-level computational approaches. Physical Chemistry Chemical Physics, 2020, 22, 22003-22015.	1.3	10
59	Triple-Columned and Multiple-Layered 3D Polymers: Design, Synthesis, Aggregation-Induced Emission (AIE), and Computational Study. Research, 2021, 2021, 3565791.	2.8	10
60	Molecular Dynamics Simulation of the Excited-State Proton Transfer Mechanism in 3-Hydroxyflavone Using Explicit Hydration Models. Journal of Physical Chemistry A, 2021, 125, 5765-5778.	1.1	10
61	Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. Journal of Physical Chemistry A, 2021, 125, 1152-1165.	1.1	10
62	Anab initio study of the molecules P2O and P2O+. Theoretica Chimica Acta, 1991, 79, 105-114.	0.9	9
63	Electronic Structure and Vibrational Mode Study of Nafion Membrane Interfacial Water Interactions. Journal of Physical Chemistry A, 2015, 119, 1754-1764.	1.1	9
64	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. Journal of Chemical Physics, 2017, 147, 194702.	1.2	9
65	Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. Journal of Physical Chemistry A, 2020, 124, 10954-10966.	1.1	9
66	A computational study of the ground and excited state acidities of synthetic analogs of red wine pyranoanthocyanins. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
67	Effect of Hydration on Promoting Oxidative Reactions with Aluminum Oxide and Oxyhydroxide Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 15017-15026.	1.5	8
68	Cycloaddition of Strained Cyclic Alkenes and Ortho-Quinones: A Distortion/Interaction Analysis. Journal of Organic Chemistry, 2020, 85, 13557-13566.	1.7	8
69	Theoretical Oâ€“CH3 bond dissociation enthalpies of selected aromatic and non-aromatic molecules. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	8
70	Pathways to fluorescence via restriction of intramolecular motion in substituted tetraphenylethylenes. Physical Chemistry Chemical Physics, 2022, 24, 1722-1735.	1.3	8
71	Characterization of Charge Transfer in Excited States of Extended Clusters of Ï€-Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. Journal of Physical Chemistry A, 2019, 123, 4532-4542.	1.1	7
72	Quantum chemical evidence for the origin of the red/blue colors of Hydrangea macrophylla sepals. New Journal of Chemistry, 2019, 43, 7532-7540.	1.4	7

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73	Stress-altered aluminum powder dust combustion. Journal of Applied Physics, 2020, 127, .	1.1	7
74	Regulating magnesium combustion using surface chemistry and heating rate. Combustion and Flame, 2021, 226, 419-429.	2.8	7
75	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. Journal of Physical Chemistry A, 2018, 122, 9464-9473.	1.1	6
76	Photoacidity of the 7â€Hydroxyflavylium Cation. Photochemistry and Photobiology, 2019, 95, 1339-1344.	1.3	6
77	Theoretical Study of O-CH₃ Bond Dissociation Enthalpy in Anisole Systems. ACS Omega, 2021, 6, 21952-21959.	1.6	6
78	Fluorescence and Phosphorescence of Flavylium Cation Analogues of Anthocyanins. Photochem, 2022, 2, 423-434.	1.3	6
79	Ab Initio Molecular Dynamics Simulations on the Hydrated Structures of Na+â€“Nafion Models. Journal of Physical Chemistry C, 2017, 121, 11215-11225.	1.5	5
80	Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	5
81	Benchmark ab initio calculations on intermolecular structures and the exciton character of poly(p-phenylenevinylene) dimers. Journal of Chemical Physics, 2020, 152, 044306.	1.2	5
82	Highâ€level Ab Initio Absorption Spectra Simulations of Neutral, Anionic and Neutral+ Chromophore of Green Fluorescence Protein Chromophore Models in Gas Phase and Solution. Photochemistry and Photobiology, 2017, 93, 1356-1367.	1.3	4
83	A quantum dynamical study of the rotation of the dihydrogen ligand in the Fe(H)2(H2)(PEtPh2)3 coordination complex. Journal of Chemical Physics, 2018, 148, 154303.	1.2	4
84	Structures and binding energies for complexations of different spin states of Ni⁺ and Ni²⁺ to aromatic molecules. Molecular Physics, 2019, 117, 1392-1403.	0.8	4
85	Synthesis and characterization of polymeric films with stress-altered aluminum particle fillers. Journal of Materials Science, 2020, 55, 14229-14242.	1.7	4
86	Microhydration of Polymer Electrolyte Membranes: A Comparison of Hydrogen-Bonding Networks and Spectral Properties of Nafion and Bis[(perfluoroalkyl)sulfonyl] Imide. Journal of Physical Chemistry B, 2019, 123, 9899-9911.	1.2	3
87	Conical intersections and the weak fluorescence of betalains. Photochemical and Photobiological Sciences, 2019, 18, 1972-1981.	1.6	3
88	Influence of water molecule bridges on sequestration of phenol in soil organic matter of sapric histosol. Environmental Chemistry, 2019, 16, 541.	0.7	3
89	A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. International Journal of Mass Spectrometry, 2021, 461, 116495.	0.7	3
90	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	0.8	3

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91	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. Journal of Chemical Physics, 2021, 154, 104308.	1.2	2
92	Quantum chemical investigation of the ground- and excited-state acidities of a dihydroxyfuranoflavylium cation. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
93	Ab initio calculation of the excited states of nitropyrenes. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
94	Adsorption and exchange reactions of iodine molecules at the alumina surface: modelling alumina-iodine reaction mechanisms. Physical Chemistry Chemical Physics, 2022, , .	1.3	0