

Adelia J A Aquino

List of Publications by Year in descending order

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3,432
citations

172457

29
h-index

149698

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.	7.1	362
2	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
3	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. Physical Chemistry Chemical Physics, 2010, 12, 4959.	2.8	208
4	Excited-State Intramolecular Proton Transfer: A Survey of TDDFT and RI-CC2 Excited-State Potential Energy Surfaces. Journal of Physical Chemistry A, 2005, 109, 3201-3208.	2.5	175
5	Ultrafast internal conversion pathway and mechanism in 2-(2-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. Physical Chemistry Chemical Physics, 2009, 11, 1406.	2.8	174
6	Solvent Effects on Hydrogen Bonds: A Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871.	2.5	167
7	Isomeric Separation of Permethylated Glycans by Porous Graphitic Carbon (PGC)-LC-MS/MS at High Temperatures. Analytical Chemistry, 2017, 89, 6590-6597.	6.5	96
8	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145.	2.8	84
9	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255.	2.5	84
10	Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	77
11	The charge-transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227.	3.3	73
12	The decay mechanism of photoexcited guanine: A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304.	3.0	70
13	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 9016.	2.8	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.	2.5	65
15	Ultrafast two-step process in the non-adiabatic relaxation of the CH ₂ molecule. Molecular Physics, 2006, 104, 1053-1060.	1.7	64
16	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the π^* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	2.5	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.	13.7	59
18	π - π stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310.	2.8	57

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19	Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. <i>Environmental Science & Technology</i> , 2011, 45, 8411-8419.	10.0	54
20	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3280-3289.	5.3	54
21	Fluorination of an Alumina Surface: Modeling Aluminum-Fluorine Reaction Mechanisms. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 24290-24297.	8.0	49
22	Stabilizing Capacity of Water Bridges in Nanopore Segments of Humic Substances: A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16468-16475.	3.1	47
23	The functionality of cation bridges for binding polar groups in soil aggregates. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1531-1542.	2.0	46
24	Excited-State Properties and Environmental Effects for Protonated Schiff Bases: A Theoretical Study. <i>ChemPhysChem</i> , 2006, 7, 2089-2096.	2.1	43
25	Excited-State Proton Transfer in 7-Hydroxy-4-methylcoumarin along a Hydrogen-Bonded Water Wire. <i>Journal of Physical Chemistry A</i> , 2007, 111, 127-135.	2.5	43
26	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42
27	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. <i>Journal of Chemical Physics</i> , 2019, 150, 124302.	3.0	35
28	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9077-9088.	2.8	34
29	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. <i>Journal of the American Chemical Society</i> , 2012, 134, 13662-13669.	13.7	31
30	Singlet L_a and L_b Bands for N-Acenes ($N = 2-7$): A CASSCF/CASPT2 Study. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4297-4306.	5.3	30
31	The electronically excited states of RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine): Vertical excitations. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2348-2355.	2.0	27
32	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14327-14337.	3.1	25
33	Restructuring of a Peat in Interaction with Multivalent Cations: Effect of Cation Type and Aging Time. <i>PLoS ONE</i> , 2013, 8, e65359.	2.5	24
34	Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2018, 83, 244-252.	3.2	24
35	How to efficiently tune the biradicaloid nature of acenes by chemical doping with boron and nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19225-19233.	2.8	23
36	Dynamics of benzene excimer formation from the parallel-displaced dimer. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13916-13924.	2.8	23

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37	Absorption and Fluorescence Spectra of Poly(<i>p</i> -phenylenevinylene) (PPV) Oligomers: An <i>ab Initio</i> Simulation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1787-1795.	2.5	22
38	Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4- <i>b</i>]thiophene benzodithiophene) by Means of <i>ab Initio</i> and Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21818-21826.	3.1	22
39	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7793-7804.	5.5	22
40	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. <i>Topics in Current Chemistry</i> , 2014, 356, 1-37.	4.0	20
41	Analysis of charge transfer transitions in stacked π -electron donor-acceptor complexes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26957-26967.	2.8	19
42	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5592-5597.	4.6	18
43	Water-Ionomer Interfacial Interactions Investigated by Infrared Spectroscopy and Computational Methods. <i>Langmuir</i> , 2013, 29, 13890-13897.	3.5	17
44	The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12778-12785.	2.8	17
45	Effect of Polar Environments on the Aluminum Oxide Shell Surrounding Aluminum Particles: Simulations of Surface Hydroxyl Bonding and Charge. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 13926-13933.	8.0	17
46	The electronic transitions of analogs of red wine pyranoanthocyanin pigments. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 45-53.	2.9	16
47	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for <i>cis</i> -/ <i>trans</i> -Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. <i>Journal of Organic Chemistry</i> , 2020, 85, 3664-3675.	3.2	16
48	Post-transition state dynamics and product energy partitioning following thermal excitation of the $\tilde{A}^1\text{HCH}_2\text{CN}$ transition state: Disagreement with experiment. <i>Journal of Chemical Physics</i> , 2017, 147, 144301.	3.0	14
49	Lewis acid base chemistry of Bestmann's ylide, Ph_3PCCO , and its bulkier analogue, (cyclohexyl) $_3\text{PCCO}$. <i>Chemical Communications</i> , 2019, 55, 3513-3516.	4.1	14
50	Nonadiabatic Dynamics of Charge-Transfer States Using the Anthracene-Tetracyanoethylene Complex as a Prototype. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3347-3357.	2.5	13
51	Energy transfer mechanism in luminescence Eu(III) and Tb(III) complexes of coumarin-3-carboxylic acid: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 240, 118591.	3.9	12
52	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. <i>ChemPhysChem</i> , 2018, 19, 2492-2499.	2.1	11
53	Adsorption process of polar and nonpolar compounds in a nanopore model of humic substances. <i>European Journal of Soil Science</i> , 2020, 71, 845-855.	3.9	11
54	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. <i>Journal of Chemical Physics</i> , 2021, 154, 044306.	3.0	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. <i>ChemPhysChem</i> , 2014, 15, 3334-3341.	2.1	10
56	The characterization of electronic defect states of single and double carbon vacancies in graphene sheets using molecular density functional theory. <i>Molecular Physics</i> , 2019, 117, 1519-1531.	1.7	10
57	Chromophores inspired by the colors of fruit, flowers and wine. <i>Pure and Applied Chemistry</i> , 2020, 92, 255-263.	1.9	10
58	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorization via valence bond theory and high-level computational approaches. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22003-22015.	2.8	10
59	Triple-Columned and Multiple-Layered 3D Polymers: Design, Synthesis, Aggregation-Induced Emission (AIE), and Computational Study. <i>Research</i> , 2021, 2021, 3565791.	5.7	10
60	Molecular Dynamics Simulation of the Excited-State Proton Transfer Mechanism in 3-Hydroxyflavone Using Explicit Hydration Models. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5765-5778.	2.5	10
61	Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1152-1165.	2.5	10
62	Anab initio study of the molecules P2O and P2O+. <i>Theoretica Chimica Acta</i> , 1991, 79, 105-114.	0.8	9
63	Electronic Structure and Vibrational Mode Study of Nafion Membrane Interfacial Water Interactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1754-1764.	2.5	9
64	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. <i>Journal of Chemical Physics</i> , 2017, 147, 194702.	3.0	9
65	Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10954-10966.	2.5	9
66	A computational study of the ground and excited state acidities of synthetic analogs of red wine pyranoanthocyanins. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	9
67	Effect of Hydration on Promoting Oxidative Reactions with Aluminum Oxide and Oxyhydroxide Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15017-15026.	3.1	8
68	Cycloaddition of Strained Cyclic Alkenes and <i>Ortho</i> -Quinones: A Distortion/Interaction Analysis. <i>Journal of Organic Chemistry</i> , 2020, 85, 13557-13566.	3.2	8
69	Theoretical C-H bond dissociation enthalpies of selected aromatic and non-aromatic molecules. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	8
70	Pathways to fluorescence via restriction of intramolecular motion in substituted tetraphenylethylenes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1722-1735.	2.8	8
71	Characterization of Charge Transfer in Excited States of Extended Clusters of π -Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4532-4542.	2.5	7
72	Quantum chemical evidence for the origin of the red/blue colors of <i>Hydrangea macrophylla</i> sepals. <i>New Journal of Chemistry</i> , 2019, 43, 7532-7540.	2.8	7

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73	Stress-altered aluminum powder dust combustion. <i>Journal of Applied Physics</i> , 2020, 127, .	2.5	7
74	Regulating magnesium combustion using surface chemistry and heating rate. <i>Combustion and Flame</i> , 2021, 226, 419-429.	5.2	7
75	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9464-9473.	2.5	6
76	Photoacidity of the 7â€“Hydroxyflavylium Cation. <i>Photochemistry and Photobiology</i> , 2019, 95, 1339-1344.	2.5	6
77	Theoretical Study of O-CH₃ Bond Dissociation Enthalpy in Anisole Systems. <i>ACS Omega</i> , 2021, 6, 21952-21959.	3.5	6
78	Fluorescence and Phosphorescence of Flavylum Cation Analogues of Anthocyanins. <i>Photochem</i> , 2022, 2, 423-434.	2.2	6
79	Ab Initio Molecular Dynamics Simulations on the Hydrated Structures of Na+â€“Nafion Models. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11215-11225.	3.1	5
80	Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	5
81	Benchmark ab initio calculations on intermolecular structures and the exciton character of poly(p-phenylenevinylene) dimers. <i>Journal of Chemical Physics</i> , 2020, 152, 044306.	3.0	5
82	Highâ€“level <i>Ab Initio</i> Absorption Spectra Simulations of Neutral, Anionic and Neutral+ Chromophore of Green Fluorescence Protein Chromophore Models in Gas Phase and Solution. <i>Photochemistry and Photobiology</i> , 2017, 93, 1356-1367.	2.5	4
83	A quantum dynamical study of the rotation of the dihydrogen ligand in the Fe(H)2(H2)(PEtPh)3 coordination complex. <i>Journal of Chemical Physics</i> , 2018, 148, 154303.	3.0	4
84	Structures and binding energies for complexations of different spin states of Ni⁺ and Ni²⁺ to aromatic molecules. <i>Molecular Physics</i> , 2019, 117, 1392-1403.	1.7	4
85	Synthesis and characterization of polymeric films with stress-altered aluminum particle fillers. <i>Journal of Materials Science</i> , 2020, 55, 14229-14242.	3.7	4
86	Microhydration of Polymer Electrolyte Membranes: A Comparison of Hydrogen-Bonding Networks and Spectral Properties of Nafion and Bis[(perfluoroalkyl)sulfonyl] Imide. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9899-9911.	2.6	3
87	Conical intersections and the weak fluorescence of betalains. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1972-1981.	2.9	3
88	Influence of water molecule bridges on sequestration of phenol in soil organic matter of sapric histosol. <i>Environmental Chemistry</i> , 2019, 16, 541.	1.5	3
89	A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. <i>International Journal of Mass Spectrometry</i> , 2021, 461, 116495.	1.5	3
90	Spin-density calculation via the graphical unitary group approach. <i>Molecular Physics</i> , 2023, 121, .	1.7	3

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91	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. <i>Journal of Chemical Physics</i> , 2021, 154, 104308.	3.0	2
92	Quantum chemical investigation of the ground- and excited-state acidities of a dihydroxyfuranoflavylium cation. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	2
93	Ab initio calculation of the excited states of nitropyrenes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	2
94	Adsorption and exchange reactions of iodine molecules at the alumina surface: modelling alumina-iodine reaction mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	0