

# Adelia J A Aquino

## List of Publications by Year in descending order

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94  
papers

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	Spin-density calculation via the graphical unitary group approach. <i>Molecular Physics</i> , 2023, 121, .	1.7	3
2	Pathways to fluorescence <i>via</i> restriction of intramolecular motion in substituted tetraphenylethylenes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1722-1735.	2.8	8
3	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
4	Fluorescence and Phosphorescence of Flavylum Cation Analogues of Anthocyanins. <i>Photochem</i> , 2022, 2, 423-434.	2.2	6
5	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. <i>Journal of Chemical Physics</i> , 2021, 154, 044306.	3.0	11
6	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
7	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
8	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
9	Regulating magnesium combustion using surface chemistry and heating rate. <i>Combustion and Flame</i> , 2021, 226, 419-429.	5.2	7
10	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
11	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
12	Ab initio calculation of the excited states of nitropyrenes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	2
13	Theoretical Study of O-CH <sub>3</sub> Bond Dissociation Enthalpy in Anisole Systems. <i>ACS Omega</i> , 2021, 6, 21952-21959.	3.5	6
14	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
15	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
16	Chromophores inspired by the colors of fruit, flowers and wine. <i>Pure and Applied Chemistry</i> , 2020, 92, 255-263.	1.9	10
17	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
18	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

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19	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
20	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
21	Stress-altered aluminum powder dust combustion. <i>Journal of Applied Physics</i> , 2020, 127, .	2.5	7
22	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
23	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
24	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
25	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
26	Theoretical C-H bond dissociation enthalpies of selected aromatic and non-aromatic molecules. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	8
27	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for cis-trans-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
28	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
29	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
30	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
31	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
32	Photoacidity of the 7-Hydroxyflavylium Cation. <i>Photochemistry and Photobiology</i> , 2019, 95, 1339-1344.	2.5	6
33	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
34	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
35	The electronic transitions of analogs of red wine pyranoanthocyanin pigments. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 45-53.	2.9	16
36	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

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37	Dynamics of benzene excimer formation from the parallel-displaced dimer. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13916-13924.	2.8	23
38	Conical intersections and the weak fluorescence of betalains. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1972-1981.	2.9	3
39	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
40	Characterization of Charge Transfer in Excited States of Extended Clusters of $\pi$ -Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4532-4542.	2.5	7
41	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
42	Lewis acid base chemistry of Bestmann's ylide, Ph <sub>3</sub> PCCO, and its bulkier analogue, (cyclohexyl) <sub>3</sub> PCCO. <i>Chemical Communications</i> , 2019, 55, 3513-3516.	4.1	14
43	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
44	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
45	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
46	Structures and binding energies for complexations of different spin states of Ni <sup>+</sup> and Ni <sup>2+</sup> to aromatic molecules. <i>Molecular Physics</i> , 2019, 117, 1392-1403.	1.7	4
47	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
48	Analysis of charge transfer transitions in stacked $\pi$ -electron donor-acceptor complexes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26957-26967.	2.8	19
49	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
50	Multireference Approaches for Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7293-7361.	47.7	287
51	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
52	A quantum dynamical study of the rotation of the dihydrogen ligand in the Fe(H) <sub>2</sub> (H <sub>2</sub> )(PEtPh <sub>2</sub> ) <sub>3</sub> coordination complex. <i>Journal of Chemical Physics</i> , 2018, 148, 154303.	3.0	4
53	Isomeric Separation of Permethylated Glycans by Porous Graphitic Carbon (PGC)-LC-MS/MS at High Temperatures. <i>Analytical Chemistry</i> , 2017, 89, 6590-6597.	6.5	96
54	Ab Initio Molecular Dynamics Simulations on the Hydrated Structures of Na <sup>+</sup> -Nafion Models. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11215-11225.	3.1	5

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55	High-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
56	Post-transition state dynamics and product energy partitioning following thermal excitation of the $\tilde{F}^{\leftarrow}HCH_2CN$ transition state: Disagreement with experiment. <i>Journal of Chemical Physics</i> , 2017, 147, 144301.	3.0	14
57	Singlet $L_{a\leftarrow b}$ and $L_{b\leftarrow a}$ Bands for N-Acenes ( $\langle N \rangle = 2\text{--}7$ ): A CASSCF/CASPT2 Study. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4297-4306.	5.3	30
58	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
59	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
60	Fluorination of an Alumina Surface: Modeling Aluminum-Fluorine Reaction Mechanisms. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 24290-24297.	8.0	49
61	Effect of Polar Environments on the Aluminum Oxide Shell Surrounding Aluminum Particles: Simulations of Surface Hydroxyl Bonding and Charge. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 13926-13933.	8.0	17
62	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
63	$\pi\text{--}\pi$ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22300-22310.	2.8	57
64	Intramolecular Charge-Transfer Excited-State Processes in 4-( <i>N,N</i> -Dimethylamino)benzonitrile: The Role of Twisting and the $\tilde{I}^{\leftarrow f^*}$ State. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6232-6243.	2.5	60
65	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
66	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
67	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
68	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
69	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
70	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
71	<i>Ab Initio</i> Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. <i>Journal of the American Chemical Society</i> , 2013, 135, 18252-18255.	13.7	59
72	Electronically Excited States in Poly( <i>p</i> -phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level <i>Ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2181-2189.	2.5	65

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73	Water-Ionomer Interfacial Interactions Investigated by Infrared Spectroscopy and Computational Methods. <i>Langmuir</i> , 2013, 29, 13890-13897.	3.5	17
74	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
75	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
76	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9016.	2.8	69
77	Electronically excited states and photodynamics: a continuing challenge. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	77
78	Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. <i>Environmental Science &amp; Technology</i> , 2011, 45, 8411-8419.	10.0	54
79	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6145.	2.8	84
80	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5247-5255.	2.5	84
81	The decay mechanism of photoexcited guanine - A nonadiabatic dynamics study. <i>Journal of Chemical Physics</i> , 2011, 134, 014304.	3.0	70
82	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
83	The charge-transfer states in a stacked nucleobase dimer complex: A benchmark study. <i>Journal of Computational Chemistry</i> , 2011, 32, 1217-1227.	3.3	73
84	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 21453-21458.	7.1	362
85	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4959.	2.8	208
86	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
87	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
88	Ultrafast internal conversion pathway and mechanism in 2-(2-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1406.	2.8	174
89	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
90	Ultrafast two-step process in the non-adiabatic relaxation of the CH <sub>2</sub> molecule. <i>Molecular Physics</i> , 2006, 104, 1053-1060.	1.7	64

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91	Excited-State Properties and Environmental Effects for Protonated Schiff Bases: A Theoretical Study. ChemPhysChem, 2006, 7, 2089-2096.	2.1	43
92	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
93	Solvent Effects on Hydrogen Bonds A Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871.	2.5	167
94	Anab initio study of the molecules P2O and P2O+. Theoretica Chimica Acta, 1991, 79, 105-114.	0.8	9