Javier Segarra-MartÃ-

List of Publications by Year
in descending order

52 papers	2,698 citations	304743 22 h-index	182427 51 g-index
55 all docs	55 docs citations	55 times ranked	3039 citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
2	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
3	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in trans-Azobenzene. Journal of Physical Chemistry Letters, 2018, 9, 1534-1541.	4.6	96
4	Photophysics of Deoxycytidine and 5-Methyldeoxycytidine in Solution: A Comprehensive Picture by Quantum Mechanical Calculations and Femtosecond Fluorescence Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7780-7791.	13.7	76
5	Excitation of Nucleobases from a Computational Perspective I: Reaction Paths. Topics in Current Chemistry, 2013, 355, 57-97.	4.0	66
6	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. Journal of Physical Chemistry Letters, 2017, 8, 1777-1783.	4.6	60
7	COBRAMM 2.0 â€" A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. Journal of Molecular Modeling, 2018, 24, 271.	1.8	55
8	From White to Red: Electricâ€Field Dependent Chromaticity of Lightâ€Emitting Electrochemical Cells based on Archetypal Porphyrins. Advanced Functional Materials, 2016, 26, 6737-6750.	14.9	49
9	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. Physical Chemistry Chemical Physics, 2018, 20, 6877-6890.	2.8	46
10	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. Journal of Chemical Physics, 2015, 142, 212443.	3.0	44
11	Multiconfigurational Second-Order Perturbation Theory with Frozen Natural Orbitals Extended to the Treatment of Photochemical Problems. Journal of Chemical Theory and Computation, 2015, 11, 3772-3784.	5.3	41
12	Computing the Absorption and Emission Spectra of 5-Methylcytidine in Different Solvents: A Test-Case for Different Solvation Models. Journal of Chemical Theory and Computation, 2016, 12, 4430-4439.	5.3	41
13	Ab initio determination of the ionization potentials of water clusters (H2O)n (n =) Tj ETQq1 1 0.784314 rgBT /Ov	3.0	36
14	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. Frontiers in Chemistry, 2015, 3, 29.	3.6	31
15	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	3.3	31
16	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. Faraday Discussions, 2015, 177, 345-362.	3.2	29
17	Assessment of the Potential Energy Hypersurfaces in Thymine within Multiconfigurational Theory: CASSCF vs. CASPT2. Molecules, 2016, 21, 1666.	3.8	28
18	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	28

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19	On the photophysics and photochemistry of the water dimer. Journal of Chemical Physics, 2012, 137, 244309.	3.0	24
20	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. Faraday Discussions, 2019, 221, 219-244.	3.2	24
21	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry, 2018, 376, 24.	5.8	23
22	On the N₁â€“H and N₃â€“H Bond Dissociation in Uracil by Low Energy Electrons: A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2012, 8, 2769-2776.	5.3	22
23	Theoretical study on the excited-state Ï€-stacking versus intermolecular hydrogen-transfer processes in the guanineâ€“cytosine/cytosine trimer. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	20
24	Complete-active-space second-order perturbation theory (CASPT2//CASSCF) study of the dissociative electron attachment in canonical DNA nucleobases caused by low-energy electrons (0-3 eV). Journal of Chemical Physics, 2015, 143, 215101.	3.0	19
25	Ultrafast and radiationless electronic excited state decay of uracil and thymine cations: computing the effects of dynamic electron correlation. Physical Chemistry Chemical Physics, 2019, 21, 14322-14330.	2.8	19
26	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 2570-2585.	5.3	16
27	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14
28	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. Faraday Discussions, 2018, 207, 233-250.	3.2	14
29	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. Physical Chemistry Chemical Physics, 2020, 22, 15496-15508.	2.8	14
30	Can the Hexagonal Ice-like Model Render the Spectroscopic Fingerprints of Structured Water? Feedback from Quantum-Chemical Computations. Entropy, 2014, 16, 4101-4120.	2.2	12
31	Computing the Ultrafast and Radiationless Electronic Excited State Decay of Cytosine and 5â€methylâ€cytosine Cations: Uncovering the Role of Dynamic Electron Correlation. ChemPhotoChem, 2019, 3, 856-865.	3.0	12
32	Excitedâ€State Dynamics of Thienoguanosine, an Isomorphic Highly Fluorescent Analogue of Guanosine. Chemistry - A European Journal, 2019, 25, 7375-7386.	3.3	11
33	Towards the understanding at the molecular level of the structured-water absorption and fluorescence spectra: a fingerprint of Ï€-stacked water. Molecular Physics, 2013, 111, 1308-1315.	1.7	10
34	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	2.9	10
35	Molecular excited state calculations with adaptive wavefunctions on a quantum eigensolver emulation: reducing circuit depth and separating spin states. Physical Chemistry Chemical Physics, 2021, 23, 26438-26450.	2.8	10
36	Converging many-body correlation energies by means of sequence extrapolation. Journal of Chemical Physics, 2018, 148, 034107.	3.0	8

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37	A theoretical study of the intramolecular charge transfer in 4-(dimethylamino)benzethyne. Physical Chemistry Chemical Physics, 2014, 16, 25642-25648.	2.8	7
38	Molecular Vertical Excitation Energies Studied with First-Order RASSCF (RAS[1,1]): Balancing Covalent and Ionic Excited States. Journal of Physical Chemistry A, 2019, 123, 5223-5230.	2.5	7
39	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	5
40	Electroluminescence: From White to Red: Electricâ€Field Dependent Chromaticity of Lightâ€Emitting Electrochemical Cells based on Archetypal Porphyrins (Adv. Funct. Mater. 37/2016). Advanced Functional Materials, 2016, 26, 6736-6736.	14.9	5
41	Photocrosslinking between nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 283-306.	3.2	5
42	Quantum coherence in complex environments: general discussion. Faraday Discussions, 2019, 221, 168-201.	3.2	5
43	Modelling Photoionisation in Isocytosine: Potential Formation of Longerâ€Lived Excited State Cations in its Keto Form. ChemPhysChem, 2021, 22, 2172-2181.	2.1	5
44	Quantum chemistry of the excited state: recent trends in methods developments and applications. Photochemistry, 2018, , 28-77.	0.2	5
45	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry Collections, 2019, , 63-112.	0.5	4
46	Modelling Photoionisations in Tautomeric DNA Nucleobase Derivatives 7H-Adenine and 7H-Guanine: Ultrafast Decay and Photostability. Photochem, 2021, 1, 287-301.	2.2	4
47	On the hexagonal ice-like model of structured water: Theoretical analysis of the low-lying excited states. Computational and Theoretical Chemistry, 2014, 1040-1041, 266-273.	2.5	3
48	Highlights from the Faraday discussion on photoinduced processes in nucleic acids and proteins. Chemical Communications, 2018, 54, 4207-4215.	4.1	2
49	Spectroscopic signatures of quantum effects: general discussion. Faraday Discussions, 2019, 221, 322-349.	3.2	2
50	Light induced charge and energy transport in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 153-180.	3.2	1
51	Modelling Photoionisation in Isocytosine: Potential Formation of Longerâ€Lived Excited State Cations in its Keto Form. ChemPhysChem, 2021, 22, 2140-2140.	2.1	1
52	Light induced damage and repair in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 389-408.	3.2	0