Vincent Liegeois

List of Publications by Year
in descending order

51	992	430874 18	454955 30
papers	citations	h-index	g-index

51	51	51	1063
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Basis Set and Density Functional Dependence of Vibrational Raman Optical Activity Calculations. Journal of Physical Chemistry A, 2005, 109, 7567-7574.	2.5	105
2	An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra. Journal of Chemical Physics, 2007, 127, 204105.	3.0	79
3	On the Aromatic Character of 1,2-Dihydro-1,2-azaborine According to Magnetic Criteria. Journal of Physical Chemistry Letters, 2010, 1, 1563-1568.	4.6	51
4	Evaluation of the molecular static and dynamic first hyperpolarizabilities. International Journal of Quantum Chemistry, 2014, 114, 900-910.	2.0	51
5	Nonlinear Optical Switching Behavior in the Solid State: A Theoretical Investigation on Anils. Chemistry of Materials, 2011, 23, 3993-4001.	6.7	47
6	Time-dependent density functional theory investigation of the absorption and emission spectra of a cyanine dye. Chemical Physics Letters, 2007, 446, 165-169.	2.6	46
7	TDHF Evaluation of the Dipoleâ^'Quadrupole Polarizability and Its Geometrical Derivatives. Journal of Chemical Theory and Computation, 2005, 1, 444-452.	5.3	45
8	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. Physical Chemistry Chemical Physics, 2017, 19, 7124-7131.	2.8	43
9	Theoretical Determination of the Vibrational Raman Optical Activity Signatures of Helical Polypropylene Chains. ChemPhysChem, 2006, 7, 2366-2376.	2.1	37
10	Vibrational Raman optical activity of Ï€â€conjugated helical systems: Hexahelicene and heterohelicenes. Journal of Computational Chemistry, 2009, 30, 1261-1278.	3.3	34
11	Analyzing the Vibrational Signatures of Thiophenol Adsorbed on Small Gold Clusters by DFT Calculations. ChemPhysChem, 2013, 14, 1633-1645.	2.1	33
12	Enhanced open-circuit voltage in polymer solar cells by dithieno[3,2-b:2â€²,3â€²-d]pyrrole N-acylation. Journal of Materials Chemistry A, 2014, 2, 7535-7545.	10.3	33
13	Vibrational Raman optical activity as a mean for revealing the helicity of oligosilanes: A quantum chemical investigation. Journal of Chemical Physics, 2005, 122, 214304.	3.0	23
14	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	22
15	Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models. ChemPhotoChem, 2017, 1, 281-296.	3.0	22
16	Analysis of Vibrational Raman Optical Activity Signatures of the (TG)N and (GG)N Conformations of Isotactic Polypropylene Chains in Terms of Localized Modes. Journal of Physical Chemistry A, 2010, 114, 7198-7212.	2.5	21
17	Investigation of the Electronic Excited-State Equilibrium Geometries of Three Molecules Undergoing ESIPT: A RI-CC2 and TDDFT Study. Journal of Physical Chemistry A, 2018, 122, 972-984.	2.5	20
18	Resonant Raman spectra of molecules with diradical character: multiconfigurational wavefunction investigation of neutral viologens. Physical Chemistry Chemical Physics, 2014, 16, 21721-21731.	2.8	19

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19	Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity. International Journal of Quantum Chemistry, 2006, 106, 3097-3107.	2.0	17
20	Intramolecular [3 + 2] Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET). Journal of Physical Chemistry A, 2018, 122, 7472-7481.	2.5	17
21	Beta Sheets with a Twist: The Conformation of Helical Polyisocyanopeptides Determined by Using Vibrational Circular Dichroism. Chemistry - A European Journal, 2013, 19, 13168-13174.	3.3	15
22	Analysis of the Resonant Raman Spectra of Viologens and of Their Radical Cations Using Range-Separated Hybrid Density Functionals. Journal of Physical Chemistry C, 2014, 118, 12469-12484.	3.1	15
23	Spiro-Based Thermally Activated Delayed Fluorescence Emitters with Reduced Nonradiative Decay for High-Quantum-Efficiency, Low-Roll-Off, Organic Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2021, 13, 44628-44640.	8.0	15
24	Pigment violet 19 â€" a test case to define a simple method to simulate the vibronic structure of absorption spectra of organic pigments and dyes in solution. Photochemical and Photobiological Sciences, 2015, 14, 444-456.	2.9	14
25	Evaluation of Aromaticity for Openâ€Shell Singlet Dicyclopentaâ€Fused Acenes and Polyacenes Based on a Magnetically Induced Current. Chemistry - A European Journal, 2018, 24, 13457-13466.	3.3	14
26	Faraday Effect in Stacks of Aromatic Molecules. Journal of Physical Chemistry C, 2017, 121, 15348-15352.	3.1	13
27	Analysis of the VROA signals of helical heptasilanes using an atomistic approach. Vibrational Spectroscopy, 2006, 42, 309-316.	2.2	12
28	Combined Experimental and Theoretical Study on the Raman and Raman Optical Activity Signatures of Pentamethylundecane Diastereoisomers. Journal of Physical Chemistry B, 2010, 114, 11753-11760.	2.6	12
29	Functionalized Dithienylthiazolo[5,4â€d]thiazoles For Solutionâ€Processable Organic Fieldâ€Effect Transistors. ChemPlusChem, 2012, 77, 923-930.	2.8	12
30	Density Functional Theory Investigation of the Binding of ThioTEPA to Purine Bases: Thermodynamics and Bond Evolution Theory Analysis. Journal of Physical Chemistry A, 2020, 124, 4068-4080.	2.5	12
31	Topological investigation of the reaction mechanism of glycerol carbonate decomposition by bond evolution theory. RSC Advances, 2021, 11, 10083-10093.	3.6	12
32	The ring current model of the pentaprismane molecule. Journal of Computational Chemistry, 2011, 32, 1599-1611.	3.3	11
33	Magnetically-induced current density investigation in carbohelicenes and azahelicenes. Physical Chemistry Chemical Physics, 2019, 21, 14678-14691.	2.8	11
34	A Vibrational Raman Optical Activity Study of 1,1â€²â€Binaphthyl Derivatives. ChemPhysChem, 2009, 10, 2017-2025.	2.1	10
35	Theoretical Investigation of Vibrational Sum-Frequency Generation Signatures of Functionalized Hâ€"Si(111). Journal of Physical Chemistry C, 2015, 119, 3180-3191.	3.1	9
36	Theoretical Investigation of Raman Optical Activity Signatures of TrÃ¶gerâ€™s Base. Journal of Physical Chemistry A, 2011, 115, 13706-13713.	2.5	6

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37	Towards modelling the vibrational signatures of functionalized surfaces: carboxylic acids on Hâ€“Si(111) surfaces. Journal of Physics Condensed Matter, 2012, 24, 124111.	1.8	5
38	Coupled-cluster sum-frequency generation nonlinear susceptibilities of methyl (CH₃) and methylene (CH₂) groups. Physical Chemistry Chemical Physics, 2017, 19, 29822-29832.	2.8	5
39	Theoretical Insight into the Inelastic Electron Tunneling Spectra of an Anil Derivative. Journal of Physical Chemistry A, 2013, 117, 12783-12795.	2.5	4
40	Effects of the basis set and of the exchangeâ€“correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 34-41.	3.9	4
41	TDDFT Investigation of the Raman and Resonant Raman Spectra of Fluorescent Protein Chromophore Models. Journal of Physical Chemistry B, 2022, 126, 3414-3424.	2.6	4
42	Numerical differentiation method to calculate molecular properties at ground and excited states â€“ Application to Julolidinemalononitrile. Chemical Physics Letters, 2015, 634, 249-254.	2.6	3
43	Inelastic Electron Tunneling of C₆₀ on Gold Surfaces from First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 803-818.	3.1	3
44	Rototranslational sum rules for electromagnetic hypershielding at the nuclei and related atomic Cartesian derivatives of the optical rotatory power. Journal of Chemical Physics, 2008, 128, 244107.	3.0	2
45	Probing alkylsilane molecular structure on amorphous silica surfaces by sum frequency generation vibrational spectroscopy: First-principles calculations. Journal of Chemical Physics, 2019, 150, 074703.	3.0	2
46	Raman Optical Activity Study of the Signatures Associated to (TG)[sub N] and (GG)[sub N] Conformations of Isotactic Polypropylene Chains using Mode Localization Method. , 2010, , .		1
47	Electronic Band Structure of Helical Polyisocyanides. Journal of Physical Chemistry A, 2017, 121, 7993-8002.	2.5	1
48	Methods for Simulating and Interpreting Vibrational Spectra of Molecules. , 2009, , .		0
49	Frontispiece: Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. Chemistry - A European Journal, 2018, 24, .	3.3	0
50	Analytical Time-Dependent Hartree-Fock Scheme to Evaluate the Vibrational (Hyper)Polarizabilities. , 2009, , .		0
51	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Highlights in Theoretical Chemistry, 2014, , 225-239.	0.0	0