Michael S Deleuze

List of Publications by Year
in descending order

119	3,834	109321	155660
papers	citations	35 h-index	55 g-index

122	122	122	2692
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nucleation of organic semiconductors on inert substrates. Physical Review B, 2003, 68, .	3.2	231
2	A benchmark theoretical study of the electronic ground state and of the singlet-triplet split of benzene and linear acenes. Journal of Chemical Physics, 2009, 131, 224321.	3.0	187
3	Benchmark theoretical study of the ionization threshold of benzene and oligoacenes. Journal of Chemical Physics, 2003, 119, 3106-3119.	3.0	108
4	Valence one-electron and shake-up ionization bands of polycyclic aromatic hydrocarbons. II. Azulene, phenanthrene, pyrene, chrysene, triphenylene, and perylene. Journal of Chemical Physics, 2002, 116, 7012-7026.	3.0	105
5	Valence one-electron and shake-up ionization bands of polycyclic aromatic hydrocarbons. I. Benzene, naphthalene, anthracene, naphthacene, and pentacene. Journal of Chemical Physics, 2001, 115, 5859-5882.	3.0	103
6	High level theoretical study of the structure and rotational barriers of trans-stilbene. Journal of Chemical Physics, 2003, 118, 7823-7836.	3.0	98
7	A benchmark theoretical study of the electron affinities of benzene and linear acenes. Journal of Chemical Physics, 2008, 129, 084308.	3.0	97
8	Focal Point Analysis of the Singletâ€“Triplet Energy Gap of Octacene and Larger Acenes. Journal of Physical Chemistry A, 2011, 115, 9282-9293.	2.5	95
9	Controlling the Frequency of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes. Journal of the American Chemical Society, 1998, 120, 6458-6467.	13.7	92
10	High resolution electron momentum spectroscopy of the valence orbitals of water. Chemical Physics, 2008, 343, 19-30.	1.9	70
11	How Do Benzylic Amide [2]Catenane Rings Rotate?. Journal of the American Chemical Society, 1999, 121, 2364-2379.	13.7	69
12	High-level theoretical study of the conformational equilibrium of n-pentane. Journal of Chemical Physics, 2002, 116, 1296-1302.	3.0	67
13	Probing Molecular Conformations with Electron Momentum Spectroscopy: The Case ofn-Butane. Journal of the American Chemical Society, 2001, 123, 4049-4061.	13.7	66
14	Theoretical Study of the Oxidation Mechanisms of Naphthalene Initiated by Hydroxyl Radicals: The OH-Addition Pathway. Journal of Physical Chemistry A, 2014, 118, 4593-4610.	2.5	65
15	Plane wave and orthogonalized plane wave many-body Green's function calculations of photoionization intensities. Molecular Physics, 1994, 83, 655-686.	1.7	63
16	Valence One-Electron and Shake-Up Ionization Bands of Polycyclic Aromatic Hydrocarbons. III. Coronene, 1.2,6.7-Dibenzopyrene, 1.12-Benzoperylene, Anthanthrene. Journal of Physical Chemistry A, 2004, 108, 9244-9259.	2.5	61
17	Half-metallicity and spin-contamination of the electronic ground state of graphene nanoribbons and related systems: An impossible compromise?. Journal of Chemical Physics, 2011, 135, 104704.	3.0	61
18	Study of the molecular structure, ionization spectrum, and electronic wave function of 1,3-butadiene using electron momentum spectroscopy and benchmark Dyson orbital theories. Journal of Chemical Physics, 2006, 125, 104309.	3.0	56

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19	Valence one-electron and shake-up ionization bands of carbon clusters. I. The Cn (n=3,5,7,9) chains. Journal of Chemical Physics, 1999, 111, 5851-5865.	3.0	53
20	Surface Molecular Structure of Self-Assembled Alkanethiols Evidenced by UPS and Photoemission with Synchrotron Radiation. Journal of Physical Chemistry B, 1997, 101, 884-890.	2.6	52
21	Structural, Rotational, Vibrational, and Electronic Properties of Ionized Carbon Clusters Cn+ (n =) Tj ETQq1 1 0.784314 rgBT /Overloc	2.5	52
22	Theoretical study of spectral differences in the XPS valence bands of polyethylene lamellae and films. The Journal of Physical Chemistry, 1993, 97, 5115-5123.	2.9	47
23	Aromaticity of Giant Polycyclic Aromatic Hydrocarbons with Hollow Sites: Super Ring Currents in Super-Rings. Chemistry - A European Journal, 2006, 12, 5757-5769.	3.3	47
24	Size-consistency aspects and physical interpretation of many-body Greenâ€™s-function calculations on extended chains. Physical Review B, 1992, 46, 15668-15682.	3.2	45
25	Probing Dyson orbitals with Greenâ€™s Function theory and Electron Momentum Spectroscopy. Chemical Physics Letters, 2006, 421, 52-57.	2.6	45
26	Evidence for a partial breakdown of the molecular orbital picture in the ionization spectra of large saturated hydrocarbons. Journal of Chemical Physics, 1996, 105, 7583-7596.	3.0	43
27	Norbornane: An investigation into its valence electronic structure using electron momentum spectroscopy, and density functional and Greenâ€™s function theories. Journal of Chemical Physics, 2004, 121, 10525-10541.	3.0	43
28	Valence one-electron and shake-up ionisation bands of polycyclic aromatic hydrocarbons. IV. The dibenzanthracene species. Chemical Physics, 2006, 329, 22-38.	1.9	43
29	Valence correlation bands of model oligomers of polyethylene: A Greenâ€™s function study by the band-Lanczos approach. Journal of Chemical Physics, 1999, 110, 6014-6024.	3.0	41
30	Valence one-electron and shake-up ionization bands of carbon clusters. II. The Cnâ€,(n=4,6,8,10) rings. Journal of Chemical Physics, 2000, 112, 5325-5338.	3.0	41
31	On the sizeâ€dependence of the static selfâ€energy in propagator calculations. Journal of Chemical Physics, 1995, 103, 3578-3588.	3.0	40
32	Correlation effects in the valence x-ray photoionization spectra of ethylene, butadiene, and hexatriene. International Journal of Quantum Chemistry, 1997, 63, 465-481.	2.0	39
33	The New Challenges of the Theory of Ionization for Polymers and Solids. Advances in Quantum Chemistry, 1999, 35, 77-94.	0.8	39
34	Imaging Momentum Orbital Densities of Conformationally Versatile Molecules:Â A Benchmark Theoretical Study of the Molecular and Electronic Structures of Dimethoxymethane. Journal of Physical Chemistry A, 2007, 111, 5879-5897.	2.5	39
35	Probing Nuclear Dynamics in Momentum Space: A New Interpretation of (e, 2e) Electron Impact Ionization Experiments on Ethanol. Journal of Physical Chemistry A, 2009, 113, 7138-7154.	2.5	37
36	Probing the Molecular Primary and Secondary Structures of Saturated Hydrocarbons by X-ray Photoionization Spectroscopy. Journal of the American Chemical Society, 1994, 116, 10715-10724.	13.7	35

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37	The issues of size and charge consistency and the implications of translation symmetry in advanced Green's function theories. International Journal of Quantum Chemistry, 2003, 93, 191-211.	2.0	35
38	Evidence in the XPS valence band of the fold structure at the surface of polyethylene lamellae. Chemical Physics Letters, 1993, 210, 21-24.	2.6	34
39	Size-Consistency and Size-Intensivity Aspects of Many-Body Green's Function Calculations on Polymers : Characterization of the Convergence of Direct Lattice Self-energy Summations. Advances in Quantum Chemistry, 1995, , 35-98.	0.8	34
40	Formation of satellite bands in the ionization spectra of extended systems. Physical Review B, 1996, 53, 13326-13339.	3.2	34
41	Benchmark Dyson Orbital Study of the Ionization Spectrum and Electron Momentum Distributions of Ethanol in Conformational Equilibrium. Journal of Physical Chemistry A, 2008, 112, 9083-9096.	2.5	33
42	Investigation of the molecular conformations of ethanol using electron momentum spectroscopy. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 175103.	1.5	33
43	Quantum Chemical Study of Conformational Fingerprints in the Photoelectron Spectra and (e, 2e) Electron Momentum Distributions ofn-Hexane. Journal of Physical Chemistry A, 2010, 114, 4400-4417.	2.5	33
44	Insights into the molecular structure and chemical bonding of regular oligomers and polymers from their XPS valence spectra. Computational and Theoretical Chemistry, 1992, 261, 187-202.	1.5	31
45	Theoretical study of the oxidation mechanisms of naphthalene initiated by hydroxyl radicals: the O₂ addition reaction pathways. Physical Chemistry Chemical Physics, 2015, 17, 13719-13732.	2.8	31
46	Valence One-Electron and Shake-Up Ionization Bands of Carbon Clusters. III. The Cn(n = 5,7,9,11) Rings. Journal of Physical Chemistry A, 2002, 106, 5626-5637.	2.5	29
47	Diagonal Two-Particle-Hole Tamm-Dankoff Approximation Green's Function Simulation of the Valence X-ray Photoelectron Spectra of Cycloalkanes: Theoretical Search for Signatures of the Molecular Structure. The Journal of Physical Chemistry, 1994, 98, 2382-2396.	2.9	28
48	Probing the Shape and Stereochemistry of Molecular Orbitals in Locally Flexible Aromatic Chains:â€‰ A Penning Ionization Electron Spectroscopy and Green's Function Study of the Electronic Structure of Biphenyl. Journal of Physical Chemistry A, 2005, 109, 10535-10546.	2.5	28
49	Investigation into the Valence Electronic Structure of Norbornene Using Electron Momentum Spectroscopy, Green's Function, and Density Functional Theories. Journal of Physical Chemistry A, 2005, 109, 9324-9340.	2.5	28
50	Theoretical study of molecular vibrations in electron momentum spectroscopy experiments on furan: An analytical versus a molecular dynamical approach. Journal of Chemical Physics, 2015, 142, 094308.	3.0	28
51	Computational study of the structural and vibrational properties of ten and twelve vertex closo-carboranes. Chemical Physics, 2003, 286, 45-61.	1.9	26
52	Theoretical Study of the Conversion of Sulfonyl Precursors into Chains of Poly(p-phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 142 T	13.7	26
53	Comparison of Geant4-DNA simulation of S-values with other Monte Carlo codes. Nuclear Instruments & Methods in Physics Research B, 2014, 319, 87-94.	1.4	26
54	Theoretical Study of the Oxidation Mechanisms of Naphthalene Initiated by Hydroxyl Radicals: The H Abstraction Pathway. Journal of Physical Chemistry A, 2014, 118, 3625-3636.	2.5	26

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55	Diagonal 2ph-TDA Green's function simulation of the valence X-ray photoelectron spectra of n-alkane compounds: a theoretical search for conformational signatures. Chemical Physics, 1993, 175, 427-446.	1.9	25
56	An XPS valence band study of alkane chains secondary structure. Surface and Interface Analysis, 1994, 22, 507-510.	1.8	25
57	Effect of Thermal Motions on the Structure and UVâ^'Visible Electronic Spectra of Stilbene and Model Oligomers of Poly(p-Phenylene Vinylene). Journal of Physical Chemistry A, 2003, 107, 5168-5180.	2.5	25
58	Photoelectron and Electron Momentum Spectroscopy of Tetrahydrofuran from a Molecular Dynamical Perspective. Journal of Physical Chemistry A, 2013, 117, 1918-1929.	2.5	23
59	Application of the Green's function theory to the calculation of ionization potentials of model oligomeric systems. International Journal of Quantum Chemistry, 1992, 41, 243-255.	2.0	22
60	Valence electron momentum spectroscopy of n-butane. Journal of Chemical Physics, 2000, 112, 8043-8052.	3.0	22
61	Can Benzylic Amide [2]Catenane Rings Rotate on Graphite?. Journal of the American Chemical Society, 2000, 122, 1130-1143.	13.7	22
62	Green's function study of the one-electron and shake-up ionization spectra of unsaturated hydrocarbon cage compounds. Journal of Computational Chemistry, 2006, 27, 1703-1722.	3.3	21
63	Ionization Bands and Electron Affinities of Mixed Boronâ^'Nitrogen BnNn Clusters (n = 3,4,5). Journal of Physical Chemistry A, 2000, 104, 1588-1596.	2.5	20
64	Quenching of magnetism in hexagonal graphene nanoflakes by non-local electron correlation. Chemical Physics Letters, 2012, 553, 6-10.	2.6	20
65	The Band 12 Issue in the Electron Momentum Spectra of Norbornane: A Comparison with Additional Green's Function Calculations and Ultraviolet Photoemission Measurements. Journal of Physical Chemistry A, 2005, 109, 4267-4273.	2.5	19
66	Study of the photoelectron and electron momentum spectra of cyclopentene using benchmark Dyson orbital theories. Physical Chemistry Chemical Physics, 2008, 10, 2374.	2.8	19
67	Electron momentum spectroscopy of metal carbonyls: a reinvestigation of the role of nuclear dynamics. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	19
68	Electron momentum spectroscopy of dimethyl ether taking account of nuclear dynamics in the electronic ground state. Journal of Chemical Physics, 2015, 143, 134309.	3.0	19
69	Inelastic neutron scattering of large molecular systems: The case of the original benzylic amide [2]catenane. Journal of Chemical Physics, 1998, 109, 11094-11100.	3.0	18
70	Modeling Buckminsterfullerene Spinning in (C60)nClusters. Journal of the American Chemical Society, 1999, 121, 5281-5286.	13.7	18
71	Ab initio and density functional theory calculation of the structure and vibrational properties of n-vertex closo-carboranes, n=5, 6 and 7. Chemical Physics, 2001, 271, 17-30.	1.9	18
72	Temperature effects on the UV-Vis electronic spectrum of trans-stilbene. International Journal of Quantum Chemistry, 2001, 85, 557-568.	2.0	18

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73	From Sulfoxide Precursors to Model Oligomers of Conducting Polymers. Journal of the American Chemical Society, 2002, 124, 7563-7572.	13.7	18
74	The Fate of Dicationic States in Molecular Clusters of Benzene and Related Compounds. Journal of the American Chemical Society, 2005, 127, 16824-16834.	13.7	17
75	Benchmark theoretical study of the electric polarizabilities of naphthalene, anthracene, and tetracene. Journal of Chemical Physics, 2013, 138, 024319.	3.0	17
76	Many-body Green's function study of the valence band formation of polyoxymethylene. Physica Scripta, 1995, 51, 111-125.	2.5	16
77	Study of the Valence Wave Function of Thiophene with High Resolution Electron Momentum Spectroscopy and Advanced Dyson Orbital Theories. Journal of Physical Chemistry A, 2008, 112, 2339-2354.	2.5	16
78	Theoretical study of the oxidation mechanisms of thiophene initiated by hydroxyl radicals. Journal of Molecular Modeling, 2015, 21, 301.	1.8	16
79	Structural, Rotational, and Vibrational Properties of Mixed Ionized Boronâ^'Nitrogen Clusters BnNn+ (n = 3â^'10). Journal of Physical Chemistry A, 2000, 104, 5855-5860.	2.5	15
80	Molecular packing of oligomer chains of poly(p-phenylene vinylene). Chemical Physics Letters, 2001, 339, 216-222.	2.6	15
81	Comparative study of the molecular structure of stilbene using molecular mechanics, Hartreeâ€"Fock and density functional theories. Computational and Theoretical Chemistry, 2001, 549, 63-67.	1.5	15
82	Structural, Rotational, Vibrational, and Electronic Properties of Carbon Cluster Anions Cn-(n= 3â^'13). Journal of Physical Chemistry A, 2002, 106, 8569-8582.	2.5	15
83	Theoretical study of the internal elimination reactions of xanthate precursors. Journal of Computational Chemistry, 2003, 24, 2023-2031.	3.3	15
84	Electron Momentum Spectroscopy of 1-Butene: A Theoretical Analysis Using Molecular Dynamics and Molecular Quantum Similarity. Journal of Physical Chemistry A, 2013, 117, 8388-8398.	2.5	15
85	Investigation of the valence electronic structure of n-butane using (e,2e) spectroscopy. Chemical Physics Letters, 1998, 296, 605-610.	2.6	14
86	Nuclear Motions of an Inclusion Complex of Calix[4]arene. Journal of Physical Chemistry A, 1998, 102, 6910-6915.	2.5	13
87	Theoretical Study of the Fragmentation Pathways of Norbornane in Its Doubly Ionized Ground State. Journal of Physical Chemistry A, 2007, 111, 10834-10848.	2.5	13
88	Electron Momentum Spectroscopy of pyrimidine at the benchmark ADC(3) level. Chemical Physics Letters, 2010, 498, 45-51.	2.6	13
89	Many-body calculations of molecular electric polarizabilities in asymptotically complete basis sets. Molecular Physics, 2011, 109, 2317-2339.	1.7	13
90	Benchmark theoretical study of the ionization energies, electron affinities and singletâ€"triplet energy gaps of azulene, phenanthrene, pyrene, chrysene and perylene. Chemical Physics, 2012, 406, 55-64.	1.9	13

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91	Reaction mechanisms and kinetics of the isomerization processes of naphthalene peroxy radicals. Computational and Theoretical Chemistry, 2015, 1074, 26-35.	2.5	12
92	Second-order Green's function calculations of the ionization potential of a (H2)7 chain embedded in a homogeneous electric field. Theoretica Chimica Acta, 1992, 82, 309-319.	0.8	11
93	The coupled perturbed electron propagator in the two-particle-hole and extended two-particle-hole Tamm-Dancoff approximations. International Journal of Quantum Chemistry, 1997, 63, 483-509.	2.0	11
94	Correlation effects in the valence ionization spectra of large conjugated molecules: p-Benzoquinone, anthracenequinone and pentacenequinone. Journal of Electron Spectroscopy and Related Phenomena, 2010, 178-179, 61-79.	1.7	10
95	Half-metallicity of graphene nanoribbons and related systems: a new quantum mechanical El Dorado for nanotechnologies â€¦ or a hype for materials scientists?. Journal of Molecular Modeling, 2013, 19, 2699-2714.	1.8	10
96	Electron Momentum Spectroscopy of Norbornadiene at the Benchmark ADC(3) Level. Journal of Physical Chemistry A, 2010, 114, 9374-9387.	2.5	9
97	Collision-energy-resolved Penning ionization electron spectroscopy of bromomethanes (CH3Br,) Tj ETQq1 1 0.784314 rgBT /Overlock 1 3074-3086.	3.0	8
98	Probing electron correlation and nuclear dynamics in Momentum Space. Journal of Physics: Conference Series, 2010, 212, 012020.	0.4	8
99	Bonding in negative ions: the role of d orbitals in the heavy analogues of pyridine and furanradical anions. Physical Chemistry Chemical Physics, 2011, 13, 1663-1668.	2.8	8
100	Understanding the kinetics and mechanism of thermal cheletropic elimination of N2 from (2,5-dihydro-1H-pyrrol-1-ium-1-ylidene) amide using RRKM and ELF theories. Research on Chemical Intermediates, 2017, 43, 1575-1590.	2.7	8
101	Size consistency and size extensivity of linear response properties using the perturbed electron propagator. Journal of Chemical Physics, 1995, 102, 8967-8977.	3.0	7
102	Gauge invariance of linear response properties using the perturbed electron propagator. Journal of Chemical Physics, 1995, 102, 6128-6144.	3.0	7
103	Outer-Valence Green's Function Study of Cycloalkane and Cycloalkylâ"Alkane Compounds. Journal of Physical Chemistry A, 2001, 105, 6695-6702.	2.5	7
104	Photoelectron and electron momentum spectroscopy of 1-butene at benchmark theoretical levels. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 235101.	1.5	7
105	Kinetic and mechanistic study on the pyrolysis of 1,3-dihydroisothianaphthene-2,2-dioxide toward benzocyclobutene using RRKM and BET theories. Chemical Physics, 2017, 483-484, 12-25.	1.9	7
106	Theoretical study of the vertical electron excitation of linear carbon clusters C3, C5, and C7. International Journal of Quantum Chemistry, 2001, 85, 475-491.	2.0	5
107	Momentum space analysis of the electronic structure of biphenyl. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 225102.	1.5	5
108	Electron momentum spectroscopy of aniline taking account of nuclear dynamics in the initial electronic ground state. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 075102.	1.5	5

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109	Calculation of molecular response properties with the second-order coupled perturbed electron propagator. International Journal of Quantum Chemistry, 2000, 77, 625-640.	2.0	4
110	Reaction Mechanisms and Kinetics of the O2 Addition Pathways to the Main Thiophene-OH Adduct: A Theoretical Study. Progress in Reaction Kinetics and Mechanism, 2016, 41, 398-417.	2.1	4
111	Theoretical study on the elimination kinetics in the gas phase of allyl methyl compounds. Monatshefte FÃ¼r Chemie, 2018, 149, 1389-1400.	1.8	4
112	Evidences from electron momentum spectroscopy for ultra-fast charge transfers and structural reorganizations in a floppy molecule: Ethanol. Journal of Physics: Conference Series, 2009, 194, 052004.	0.4	3
113	Theoretical chemistry in Belgium. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	3
114	Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories. Chemical Physics, 2017, 485-486, 140-148.	1.9	3
115	Valence one-electron and shake-up ionization bands of fluorene, carbazole and dibenzofuran. Chemical Physics, 2013, 417, 17-25.	1.9	2
116	On the wetting of saturated hydrocarbon surfaces. An exploratory molecular investigation. Computational and Theoretical Chemistry, 2000, 501-502, 535-538.	1.5	1
117	Theoretical study of the internal conversion of sulfoxide precursors of poly-isothianaphthene and related polymers. Journal of Computational Chemistry, 2004, 25, 40-50.	3.3	1
118	Electron momentum spectroscopy of metal carbonyls: a reinvestigation of the role of nuclear dynamics. Highlights in Theoretical Chemistry, 2014, , 95-109.	0.0	1
119	Analytical and molecular dynamical investigations of the influence of molecular vibrations upon the (e,2e) electron momentum distributions of furan. Journal of Physics: Conference Series, 2015, 635, 072010.	0.4	0