Joseph Ortiz

List of Publications by Year
in descending order

245	7,069	66343	95266
papers	citations	42 h-index	68 g-index

258	258	258	2946
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron Propagator Self-Energies versus Improved GW100 Vertical Ionization Energies. Journal of Chemical Theory and Computation, 2022, 18, 4927-4944.	5.3	8
2	Ionization Energies and Dyson Orbitals of the Iso-electronic SO2, O3, and S3 Molecules from Electron Propagator Calculations. Journal of Physical Chemistry A, 2021, 125, 3664-3680.	2.5	3
3	Electron binding energies and Dyson orbitals of OnH2n+1+,0,â^' clusters: Double Rydberg anions, Rydberg radicals, and micro-solvated hydronium cations. Journal of Chemical Physics, 2021, 154, 234304.	3.0	6
4	Complete-active-space extended Koopmans theorem method. Journal of Chemical Physics, 2021, 155, 051102.	3.0	7
5	Tribute to Alexander I. Boldyrev. Journal of Physical Chemistry A, 2021, 125, 9261-9263.	2.5	0
6	A new generation of diagonal self-energies for the calculation of electron removal energies. Journal of Chemical Physics, 2021, 155, 204107.	3.0	17
7	Aufbau Principle for Diffuse Electrons of Double-Shell Metal Ammonia Complexes: The Case of M(NH₃)₄@12NH₃, M = Li, Be⁺, B²⁺. Journal of Physical Chemistry A, 2020, 124, 505-512.	2.5	23
8	Eigenvalues of uncorrelated, density-difference matrices and the interpretation of Î”-self-consistent-field calculations. Journal of Chemical Physics, 2020, 153, 114122.	3.0	3
9	Dyson-orbital concepts for description of electrons in molecules. Journal of Chemical Physics, 2020, 153, 070902.	3.0	66
10	Relativistic electron detachment energies and spinâ€“orbit splittings from quasiparticle electron propagator calculations. Molecular Physics, 2020, 118, e1700314.	1.7	2
11	Excess electrons bound to H₂S trimer and tetramer clusters. Physical Chemistry Chemical Physics, 2020, 22, 3273-3280.	2.8	4
12	Double Rydberg anions with solvated ammonium kernels: Electron binding energies and Dyson orbitals. Journal of Chemical Physics, 2019, 151, .	3.0	9
13	Carborane superhalide bases and their conjugate BrÃ¸nsted-Lowry Superacids: Electron binding energies and Dyson orbitals. Chemical Physics, 2019, 521, 77-84.	1.9	9
14	Transition-metal solvated-electron precursors: diffuse and 3d electrons in V(NH₃)0,Â±6. Physical Chemistry Chemical Physics, 2019, 21, 7090-7097.	2.8	19
15	Dyson Orbitals and Double Rydberg Anions: Methylated, Annulated, and Paramagnetic. Journal of Physical Chemistry A, 2019, 123, 10961-10967.	2.5	5
16	Do Dyson Orbitals resemble canonical Hartreeâ€“Fock orbitals?. Molecular Physics, 2019, 117, 2275-2283.	1.7	23
17	Aufbau Rules for Solvated Electron Precursors: Be(NH₃)₄^{0,Â±} Complexes and Beyond. Journal of Physical Chemistry Letters, 2018, 9, 84-88.	4.6	37
18	MgH Rydberg series: Transition energies from electron propagator theory and oscillator strengths from the molecular quantum defect orbital method. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 206, 323-327.	2.3	6

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19	Electron Propagator Methods for Vertical Electron Detachment Energies of Anions: Benchmarks and Case Studies. Journal of Chemical Theory and Computation, 2018, 14, 5881-5895.	5.3	19
20	Molecules mimicking atoms: monomers and dimers of alkali metal solvated electron precursors. Physical Chemistry Chemical Physics, 2018, 20, 24186-24191.	2.8	29
21	Electron Propagator Theory. Advances in Quantum Chemistry, 2017, 74, 267-298.	0.8	40
22	Assessment of Electron Propagator Methods for the Simulation of Vibrationally Resolved Valence and Core Photoionization Spectra. Journal of Chemical Theory and Computation, 2017, 13, 3120-3135.	5.3	10
23	Ab Initio Calculations on some Antiepileptic Drugs such as Phenytoin, Phenbarbital, Ethosuximide and Carbamazepine. Structural Chemistry, 2017, 28, 957-964.	2.0	34
24	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101.	3.0	13
25	One-particle many-body Greenâ€™s function theory: Algebraic recursive definitions, linked-diagram theorem, irreducible-diagram theorem, and general-order algorithms. Journal of Chemical Physics, 2017, 147, 044108.	3.0	59
26	Electron propagators based on generalised density operators. Molecular Physics, 2017, 115, 545-551.	1.7	4
27	CaH Rydberg series, oscillator strengths and photoionization cross sections from Molecular Quantum Defect and Dyson Orbital theories. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 187, 161-166.	2.3	8
28	Comment on: â€œProbing the Properties of Polynuclear Superhalogens without Halogen Ligand via abâ€…Initio Calculations: A Case Study on Double-Bridged [Mg2(CN)5]â^'1Anionsâ€•by Li etâ€…al.. ChemPhysChem, 2016, 17, 2945-2946.	2.1	9
29	Comment on â€œAre polynuclear superhalogens without halogen atoms probable? A high-level ab initio case study on triple-bridged binuclear anions with cyanide ligandsâ€•[J. Chem. Phys. 140, 094301 (2014)]. Journal of Chemical Physics, 2016, 145, 147101.	3.0	9
30	Composite electron propagator methods for calculating ionization energies. Journal of Chemical Physics, 2016, 144, 224110.	3.0	24
31	Comment on â€œIs the regulation of the electronic properties of organic molecules by polynuclear superhalogens more effective than that by mononuclear superhalogens? A high-level ab initio case studyâ€•by M.-M. Li, J.-F. Li, H.-C. Bai, Y.-Y. Sun, J.-L. Li and B. Yin, Phys. Chem. Chem. Phys., 2015, 17, 20338. Physical Chemistry Chemical Physics, 2016, 18, 15456-15457.	2.8	9
32	Numerical test of SAC-CI methods for calculating vertical ionization energies. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	7
33	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit. Journal of Chemical Theory and Computation, 2016, 12, 595-604.	5.3	69
34	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. Journal of Chemical Theory and Computation, 2016, 12, 627-637.	5.3	56
35	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626.	5.3	154
36	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61

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37	NR2 and P3+: Accurate, Efficient Electron-Propagator Methods for Calculating Valence, Vertical Ionization Energies of Closed-Shell Molecules. Journal of Physical Chemistry A, 2015, 119, 8813-8821.	2.5	53
38	Excitation energies, photoionization cross sections, and asymmetry parameters of the methyl and silyl radicals. Journal of Chemical Physics, 2014, 141, 074308.	3.0	6
39	Computational Tests of Quantum Chemical Models for Excited and Ionized States of Molecules with Phosphorus and Sulfur Atoms. Journal of Physical Chemistry A, 2014, 118, 3514-3524.	2.5	5
40	Microsolvation effects on the electron binding energies of halide anions. Molecular Physics, 2014, 112, 332-339.	1.7	2
41	Vertical Ionization Energies of Free Radicals and Electron Detachment Energies of Their Anions: A Comparison of Direct and Indirect Methods Versus Experiment. Journal of Physical Chemistry A, 2014, 118, 6125-6131.	2.5	20
42	Electron Propagator Calculations on the Ground and Excited States of C₆₀^{â€“}. Journal of Physical Chemistry A, 2014, 118, 7424-7429.	2.5	25
43	Valence-Bound and Diffuse-Bound Anions of 5-Azauracil. Journal of Physical Chemistry A, 2014, 118, 6908-6913.	2.5	5
44	Electron propagator theory: an approach to prediction and interpretation in quantum chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 123-142.	14.6	164
45	Photoelectron Spectroscopy of the 6-Azauracil Anion. Journal of Physical Chemistry A, 2013, 117, 1079-1082.	2.5	4
46	A generalized any-particle propagator theory: Prediction of proton affinities and acidity properties with the proton propagator. Journal of Chemical Physics, 2013, 138, 194108.	3.0	28
47	Assignment of photoelectron spectra of halideâ€“water clusters: Contrasting patterns of delocalization in Dyson orbitals. Journal of Chemical Physics, 2013, 138, 164317.	3.0	9
48	Direct Î”MBPT(2) method for ionization potentials, electron affinities, and excitation energies using fractional occupation numbers. Journal of Chemical Physics, 2013, 138, 074101.	3.0	15
49	Concepts of chemical bonding from electron propagator theory. , 2012, , .		3
50	Valence and diffuse-bound anions of noble-gas complexes with uracil. Journal of Chemical Physics, 2012, 137, 194310.	3.0	5
51	Valence XPS, IR, and C13 NMR spectral analysis of 6 polymers by quantum chemical calculations. Journal of Molecular Structure, 2012, 1027, 20-30.	3.6	8
52	Ab initio electron propagator calculations on electron detachment energies of nickel phthalocyanine tetrasulfonate tetraanions. International Journal of Quantum Chemistry, 2012, 112, 184-194.	2.0	4
53	Electronic structure of a beryllium halfâ€sandwich complex, Be(Î·⁵â€C₅H₅). International Journal of Quantum Chemistry, 2012, 112, 2981-2985.	2.0	1
54	Electron detachment energies of aqueous and cluster halide anions from electron propagator calculations with the polarizable continuum model. International Journal of Quantum Chemistry, 2012, 112, 3840-3848.	2.0	5

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55	Interpretation of the photoelectron spectra of superalkali species: Na3O and Na3Oâ˜. Journal of Chemical Physics, 2012, 136, 224305.	3.0	11
56	Electron propagator and coupled-cluster calculations on the photoelectron spectra of thiouracil and dithiouracil anions. Journal of Chemical Physics, 2011, 134, 074305.	3.0	17
57	Computational Tests of Models for Kinetic Parameters of Unimolecular Reactions of Organophosphorus and Organosulfur Compounds. Journal of Physical Chemistry A, 2011, 115, 14143-14152.	2.5	6
58	Simulant Molecules with Trivalent or Pentavalent Phosphorus Atoms: Bond Dissociation Energies and Other Thermodynamic and Structural Properties from Quantum Chemical Models. Journal of Physical Chemistry A, 2011, 115, 8532-8539.	2.5	5
59	The arrested Agulhas retroflection. Journal of Marine Research, 2011, 69, 659-691.	0.3	6
60	Delocalization of Dyson orbitals in F^{â˜}(H₂O) and Cl^{â˜}(H₂O). International Journal of Quantum Chemistry, 2011, 111, 1701-1708.	2.0	7
61	Ab initio Electron Propagator Calculations on Electron Detachment Energies of Fullerenes, Macrocyclic Molecules, and Nucleotide Fragments. Advances in Quantum Chemistry, 2011, 62, 105-136.	0.8	34
62	Interpretation of the photoelectron spectra of superalkali species: Li3O and Li3Oâ˜. Journal of Chemical Physics, 2011, 135, 164307.	3.0	27
63	Tautomeric forms of adenine: Vertical ionization energies and Dyson orbitals. International Journal of Quantum Chemistry, 2010, 110, 1901-1915.	2.0	12
64	Three approximations to the nonlocal and energyâ€dependent correlation potential in electron propagator theory. International Journal of Quantum Chemistry, 2010, 110, 706-715.	2.0	28
65	Ab initio electron propagator methods: Applications to nucleic acids fragments and metallophthalocyanines. International Journal of Quantum Chemistry, 2010, 110, 2918-2930.	2.0	18
66	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. Journal of Chemical Physics, 2010, 132, 214507.	3.0	11
67	The electron propagator. Molecular Physics, 2010, 108, 2871-2875.	1.7	8
68	Computational Tests of Quantum Chemical Models for Structures, Vibrational Frequencies, and Heats of Formation of Molecules with Phosphorus and Sulfur Atoms. Journal of Physical Chemistry A, 2010, 114, 8142-8155.	2.5	12
69	Ab Initio Electron Propagator Methods: Applications to Fullerenes and Nucleic Acid Fragments. Annual Reports in Computational Chemistry, 2010, 6, 79-94.	1.7	26
70	Integral approximations in ab initio, electron propagator calculations. Journal of Chemical Physics, 2009, 131, 124110.	3.0	20
71	Vertical Ionization Energies of Adenine and 9-Methyl Adenine. Journal of Physical Chemistry A, 2009, 113, 14630-14635.	2.5	21
72	Partial photoionization cross sections of NH4 and H3O Rydberg radicals. Journal of Chemical Physics, 2009, 131, 024104.	3.0	16

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73	Strong correlation effects in the electron binding energies of phthalocyanine. International Journal of Quantum Chemistry, 2009, 109, 3619-3625.	2.0	5
74	Efficient and Accurate Electron Propagator Methods and Algorithms. , 2009, , 1-17.		8
75	Virtual space reduction in quasiâ€particle electron propagator calculations: Applications to polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 2008, 108, 2862-2869.	2.0	11
76	Efficient evaluation of analytic Fukui functions. Journal of Chemical Physics, 2008, 129, 224105.	3.0	60
77	Quasiparticle virtual orbitals in electron propagator calculations. Journal of Chemical Physics, 2008, 128, 164105.	3.0	22
78	Second-order, two-electron Dyson propagator theory: Comparisons for vertical double ionization potentials. Journal of Chemical Physics, 2008, 129, 084105.	3.0	10
79	New insights in the photochromic spiro-dihydroindolizine/betaine-system. Photochemical and Photobiological Sciences, 2008, 7, 1449-1456.	2.9	19
80	Nonconventional Hydrogen Bonds: A Theoretical Study of [uracil-L]^{â^'}(L = F, Cl, Br, I, Al, Ga,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	16
81	Electron propagator calculations on C60 and C70 photoelectron spectra. Journal of Chemical Physics, 2008, 129, 104306.	3.0	18
82	Chapter 6 Electronic structure and reactivity in double Rydberg anions: characterization of a novel kind of electron pair. Theoretical and Computational Chemistry, 2007, 19, 87-100.	0.4	10
83	O H 3 â^' and O2H5â^' double Rydberg anions: Predictions and comparisons with NH4â^' and N2H7â^'. Journal of Chemical Physics, 2007, 127, 014307.	3.0	16
84	Electron binding energies and Dyson orbitals of Al5Omâ^' (m=3,4,5) and Al5O5H2â^'. Journal of Chemical Physics, 2007, 127, 234302.	3.0	9
85	Surface Greenâ€™s function calculations: A nonrecursive scheme with an infinite number of principal layers. Journal of Chemical Physics, 2007, 126, 134105.	3.0	10
86	Removing Electrons Can Increase the Electron Density:Â A Computational Study of Negative Fukui Functions. Journal of Physical Chemistry A, 2007, 111, 10017-10019.	2.5	105
87	Electron Propagator Theory and the Development of Chemical Intuition. AIP Conference Proceedings, 2007, , .	0.4	1
88	Tautomeric Forms of Azolide Anions:Â Vertical Electron Detachment Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2007, 111, 13069-13074.	2.5	10
89	Assessment of transition operator reference states in electron propagator calculations. Journal of Chemical Physics, 2007, 127, 134106.	3.0	39
90	Sequential addition of H2O, CH3OH, and NH3 to Al3O3â^': A theoretical study. Journal of Chemical Physics, 2007, 126, 024309.	3.0	7

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91	Electron propagator studies of vertical electron detachment energies and isomerism in purinic deoxyribonucleotides. International Journal of Quantum Chemistry, 2007, 107, 2266-2273.	2.0	23
92	Correlated, ab initio electron propagators in the study of molecular wires: Application to a single molecular bridge placed between two model leads. International Journal of Quantum Chemistry, 2007, 107, 3228-3235.	2.0	12
93	Deprotonated Cytosine Anions:Â A Theoretical Prediction of Photoelectron Spectra. Journal of Physical Chemistry A, 2006, 110, 11174-11177.	2.5	10
94	Electronic Structure Analysis and Electron Detachment Energies of Polynitrogen Pentagonal Aromatic Anions. Journal of Physical Chemistry A, 2006, 110, 12231-12235.	2.5	12
95	Base and Phosphate Electron Detachment Energies of Deoxyribonucleotide Anions. Journal of the American Chemical Society, 2006, 128, 13350-13351.	13.7	62
96	Ab initioelectron propagator theory of molecular wires. II. Multiorbital terminal description. Journal of Chemical Physics, 2006, 124, 144114.	3.0	29
97	Correlated Ab initio electron propagators in the study of molecular wires. International Journal of Quantum Chemistry, 2006, 106, 3387-3392.	2.0	20
98	Are structures with Alâ€“H bonds represented in the photoelectron spectrum of Al3O4H2â¯?. Journal of Chemical Physics, 2006, 124, 214304.	3.0	15
99	The electron-propagator approach to conceptual density-functional theory. Journal of Chemical Sciences, 2005, 117, 387-400.	1.5	33
100	Correlated one-electron wave functions. International Journal of Quantum Chemistry, 2005, 104, 299-327.	2.0	4
101	An efficient, renormalized self-energy for calculating the electron binding energies of closed-shell molecules and anions. International Journal of Quantum Chemistry, 2005, 105, 803-808.	2.0	76
102	Molecular photoionization cross sections in electron propagator theory: Angular distributions beyond the dipole approximation. Journal of Chemical Physics, 2005, 123, 114105.	3.0	20
103	Ground and excited states of the Rydberg radical H3O: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2005, 122, 234317.	3.0	14
104	Addition of water, methanol, and ammonia to Al3O3â¯ clusters: Reaction products, transition states, and electron detachment energies. Journal of Chemical Physics, 2005, 122, 214309.	3.0	21
105	Siliconâ¯Nitrogen Bonding in Silatranes:Â Assignment of Photoelectron Spectra. Journal of the American Chemical Society, 2005, 127, 986-995.	13.7	46
106	Ab Initio Electron Propagator Calculations on the Ionization Energies of Free Base Porphine, Magnesium Porphyrin, and Zinc Porphyrinâ€. Journal of Physical Chemistry A, 2005, 109, 11596-11601.	2.5	30
107	Ab initioelectron propagator theory of molecular wires: I. Formalism. Journal of Chemical Physics, 2005, 123, 184711.	3.0	37
108	Pseudopotential and electron propagator methods for the calculation of the photoelectron spectra of anionic silicon clusters: Predictions on Si10â¯. Journal of Chemical Physics, 2005, 123, 144314.	3.0	5

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109	Electron Propagator Calculations Show that Alkyl Substituents Alter Porphyrin Ionization Energies. Journal of the American Chemical Society, 2005, 127, 8240-8241.	13.7	39
110	Electron propagator theory calculations of molecular photoionization cross sections: The first-row hydrides. Journal of Chemical Physics, 2004, 121, 4143-4155.	3.0	49
111	Construction of unique canonical coefficients for antisymmeterized geminal power states. International Journal of Quantum Chemistry, 2004, 97, 896-907.	2.0	7
112	Brueckner orbitals, Dyson orbitals, and correlation potentials. International Journal of Quantum Chemistry, 2004, 100, 1131-1135.	2.0	42
113	Products of the addition of water molecules to Al3O3â^' clusters:â€ƒ Structure, bonding, and electron binding energies in Al3O4H2â^', Al3O5H4â^', Al3O4H2, and Al3O5H4. Journal of Chemical Physics, 2004, 120, 7955-7962.	3.0	17
114	Solvation of Alâ^'Guanine Complexes with NH3:Â A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 5845-5850.	2.5	8
115	Electronic Structure of ScC6H6-and ScC6H6:Â Geometries, Electron Binding Energies, and Dyson Orbitalsâ€. Journal of Physical Chemistry A, 2004, 108, 2988-2992.	2.5	17
116	Ground and excited states of NH4: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2004, 120, 7949-7954.	3.0	19
117	Conformational Effects on Glycine Ionization Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2004, 108, 11703-11708.	2.5	28
118	Al3O4 and Al3O4- Clusters: Structure, Bonding, and Electron Binding Energies. ChemInform, 2003, 34, no.	0.0	0
119	Quasiparticle approximations and electron propagator theory. International Journal of Quantum Chemistry, 2003, 95, 593-599.	2.0	16
120	Solvated Succinate Dianion:â€‰ Structures, Electron Binding Energies, and Dyson Orbitals. Journal of Physical Chemistry A, 2003, 107, 10360-10369.	2.5	13
121	Ionization Energies and Dyson Orbitals of Cytosine and 1-Methylcytosine. Journal of Physical Chemistry A, 2003, 107, 822-828.	2.5	31
122	Theoretical Study of the Structure and Bonding of a Metalâ^'DNA Base Complex:Â Alâ^'Guanine. Journal of Physical Chemistry A, 2003, 107, 9415-9421.	2.5	29
123	Al3O4 and Al3O4- Clusters:â€‰ Structure, Bonding, and Electron Binding Energies. Journal of Physical Chemistry A, 2003, 107, 2589-2595.	2.5	33
124	Electron Propagator Calculations on the Ionization Energies of Nucleic Acid Bases, Base-Water Complexes and Base Dimers. , 2003, , 1199-1229.		1
125	Effective procedure for energy optimizing antisymmetrized geminal power states. Journal of Chemical Physics, 2002, 117, 5135-5154.	3.0	9
126	Nondipole bound anions: Be2â^' and Be3â^'. Journal of Chemical Physics, 2002, 117, 3687-3693.	3.0	23

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127	A double Rydberg anion with a hydrogen bond and a solvated double Rydberg anion: Interpretation of the photoelectron spectrum of N2H7â¯. Journal of Chemical Physics, 2002, 117, 5748-5756.	3.0	19
128	Ionization Energies and Dyson Orbitals of Thymine and Other Methylated Uracilsâ€. Journal of Physical Chemistry A, 2002, 106, 8411-8416.	2.5	49
129	Aromatic Carboxylate Superhalogens and Multiply Charged Anions. Journal of Physical Chemistry A, 2002, 106, 5373-5379.	2.5	14
130	Al3Onand Al3On-(n= 1â¯3) Clusters:Â Structures, Photoelectron Spectra, Harmonic Vibrational Frequencies, and Atomic Charges. Journal of Physical Chemistry A, 2002, 106, 10630-10635.	2.5	47
131	Ionization Energies and Dyson Orbitals of 1,2-Dithiin. Journal of Physical Chemistry A, 2002, 106, 5924-5927.	2.5	12
132	Electron binding energies of nucleobases and nucleotides. International Journal of Quantum Chemistry, 2002, 90, 1547-1554.	2.0	32
133	Electronic Structure of AlO2, AlO2-, Al3O5, and Al3O5-Clusters. Journal of Physical Chemistry A, 2001, 105, 11291-11294.	2.5	40
134	Diffuse-Bound and Valence-Bound Anions of Cytosine. Journal of Physical Chemistry A, 2001, 105, 8782-8786.	2.5	44
135	Electronic Structure of Al3On and Al3On- (n = 1â¯3) Clusters. Journal of Physical Chemistry A, 2001, 105, 8787-8793.	2.5	45
136	Electron propagator calculations with Kohn-Sham reference states. International Journal of Quantum Chemistry, 2001, 85, 411-420.	2.0	13
137	Electron-propagator calculations on the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2001, 114, 130.	3.0	18
138	Application and Testing of Diagonal, Partial Third-Order Electron Propagator Approximations. , 2001, , 131-160.		24
139	Electron propagator calculations on uracil and adenine ionization energies. International Journal of Quantum Chemistry, 2000, 80, 831-835.	2.0	47
140	Efficient electron propagator algorithms for shakeup final states: Anthracene and acridine. International Journal of Quantum Chemistry, 2000, 80, 836-841.	2.0	12
141	Energy gradients and effective density differences in electron propagator theory. Journal of Chemical Physics, 2000, 112, 56-68.	3.0	19
142	Electron Propagator Theory of Guanine and Its Cations:Â Tautomerism and Photoelectron Spectra. Journal of the American Chemical Society, 2000, 122, 12304-12309.	13.7	78
143	Double-Rydberg Anions:Â Predictions on NH3AHn-and OH2AHn-Structures. Journal of the American Chemical Society, 2000, 122, 12813-12818.	13.7	18
144	Electron Propagator Theory of the Photoelectron Spectrum of Methanesulfenic Acid. Journal of Physical Chemistry A, 2000, 104, 11433-11438.	2.5	4

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145	Vertical Ionization Energies of Naphthalene. Journal of Physical Chemistry A, 2000, 104, 10032-10034.	2.5	14
146	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. Journal of Physical Chemistry A, 2000, 104, 11786-11795.	2.5	39
147	Ground state and vertical electron detachment energies of icosahedral and D5h Al13â^'. Journal of Chemical Physics, 1999, 111, 10762-10765.	3.0	36
148	Structures and electron detachment energies of uracil anions. Chemical Physics Letters, 1999, 307, 220-226.	2.6	63
149	Improved algorithms for renormalized electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 607-614.	2.0	19
150	Approximate Brueckner orbitals in electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 615-621.	2.0	20
151	Anionic and Neutral Complexes of Uracil and Water. Journal of Physical Chemistry A, 1999, 103, 7912-7917.	2.5	81
152	Approximate Brueckner orbitals in electron propagator calculations. , 1999, 75, 615.		1
153	Electron detachment energies of closed-shell anions calculated with a renormalized electron propagator. Chemical Physics Letters, 1998, 296, 494-498.	2.6	45
154	Single-reference electron propagator calculations on vertical ionization energies of ozone. Chemical Physics Letters, 1998, 297, 193-199.	2.6	30
155	Second-order shakeup terms in electron propagator calculations on F2 and H2O2. International Journal of Quantum Chemistry, 1998, 69, 175-182.	2.0	7
156	Electron propagator theory of conformational effects on anisole and thioanisole photoelectron spectra. International Journal of Quantum Chemistry, 1998, 70, 1037-1043.	2.0	15
157	Approximate Brueckner orbitals and shakeup operators in electron propagator calculations: Applications to F? And OH?. International Journal of Quantum Chemistry, 1998, 70, 651-658.	2.0	16
158	A nondiagonal, renormalized extension of partial third-order quasiparticle theory: Comparisons for closed-shell ionization energies. Journal of Chemical Physics, 1998, 108, 1008-1014.	3.0	114
159	Orbital and shakeup operator renormalizations in electron propagator theory. Journal of Chemical Physics, 1998, 109, 5741-5746.	3.0	37
160	Structure, bonding, and energetics of C72â^' isomers. Journal of Chemical Physics, 1998, 109, 87-93.	3.0	15
161	Ionization energies of benzo[a]pyrene and benzo[e]pyrene. Journal of Chemical Physics, 1997, 107, 7906-7911.	3.0	17
162	The Electron Propagator Picture of Molecular Electronic Structure. Computational Chemistry - Reviews of Current Trends, 1997, , 1-61.	0.4	70

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163	Hydroxide Attack on Acetylene:Â Theoretical Structures and Energies. Journal of Physical Chemistry A, 1997, 101, 1758-1762.	2.5	3
164	One-Electron Pictures of Electronic Structure: Propagator Calculations on Photoelectron Spectra of Aromatic Molecules. , 1997, , 465-517.		68
165	Ionization Energies of Acridine, Phenazine, and Diazaphenanthrenes. Journal of Physical Chemistry A, 1997, 101, 8554-8564.	2.5	20
166	Theoretical study of the valence ionization energies and electron affinities of linear C2n+1 (n=1â€“6) clusters. Journal of Chemical Physics, 1997, 106, 3258-3269.	3.0	38
167	Partial third-order quasiparticle theory: An application to the photoelectron spectrum of S-tetrazine. International Journal of Quantum Chemistry, 1997, 63, 291-299.	2.0	9
168	Comparison of electron propagator methods for calculating electron detachment energies of anions. International Journal of Quantum Chemistry, 1997, 65, 463-469.	2.0	19
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