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	Partial thirdâ€order quasiparticle theory: Comparisons for closedâ€shell ionization energies and an application to the Borazine photoelectron spectrum. Journal of Chemical Physics, 1996, 104, 7599-7605.	3.0	291
2	Electron binding energies of anionic alkali metal atoms from partial fourth order electron propagator theory calculations. Journal of Chemical Physics, 1988, 89, 6348-6352.	3.0	278
3	Semidirect algorithms for third-order electron propagator calculations. International Journal of Quantum Chemistry, 1995, 53, 583-590.	2.0	247
4	Comparison of perturbative and multiconfigurational electron propagator methods. International Journal of Quantum Chemistry, 1996, 60, 29-36.	2.0	200
5	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
6	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
7	Semidirect algorithms in electron propagator calculations. International Journal of Quantum Chemistry, 1994, 52, 23-27.	2.0	115
8	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
9	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
10	Role of d and f orbitals in the geometries of low-valent actinide compounds. Ab initio studies of U(CH3)3, Np(CH3)3, and Pu(CH3)3. Journal of the American Chemical Society, 1992, 114, 2736-2737.	13.7	103
11	Ionization energies of anthracene, phenanthrene, and naphthacene. Journal of Chemical Physics, 1996, 105, 8748-8753.	3.0	82
12	Anionic and Neutral Complexes of Uracil and Water. Journal of Physical Chemistry A, 1999, 103, 7912-7917.	2.5	81
13	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
14	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
15	Electron binding energies of TCNQ and TCNE. Journal of Chemical Physics, 1996, 105, 5872-5877.	3.0	73
16	The Electron Propagator Picture of Molecular Electronic Structure. Computational Chemistry - Reviews of Current Trends, 1997, , 1-61.	0.4	70
17	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
18	One-Electron Pictures of Electronic Structure: Propagator Calculations on Photoelectron Spectra of Aromatic Molecules. , 1997, , 465-517.		68

#	Article	IF	Citations
19	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. Helvetica Chimica Acta, 1984, 67, 1-17.	1.6	67
20	Dyson-orbital concepts for description of electrons in molecules. Journal of Chemical Physics, 2020, 153, 070902.	3.0	66
21	Hydride bridges between LnCp2 centers. Inorganic Chemistry, 1985, 24, 2095-2104.	4.0	65
22	Structures and electron detachment energies of uracil anions. Chemical Physics Letters, 1999, 307, 220-226.	2.6	63
23	Base and Phosphate Electron Detachment Energies of Deoxyribonucleotide Anions. Journal of the American Chemical Society, 2006, 128, 13350-13351.	13.7	62
24	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61
25	Efficient evaluation of analytic Fukui functions. Journal of Chemical Physics, 2008, 129, 224105.	3.0	60
26	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
27	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
28	Ground states and ionization energies of Si2H6, Si3H8, Si4H10, and Si5H12. Journal of the American Chemical Society, 1988, 110, 4522-4527.	13.7	54
29	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
30	Preparation and characterization of the first organoactinide polysulfide (.eta.5-C5Me5)2ThS5. A unique example of the twist-boat conformation of the MS5 ring. Journal of the American Chemical Society, 1986, 108, 174-175.	13.7	51
31	Synthesis and structure of a metallophosphenium-borane(3) complex containing a bridging BH3 group. Organometallics, 1986, 5, 380-383.	2.3	51
32	Electron propagator theory of BO2and BOâ¯2electronic structure. Journal of Chemical Physics, 1993, 99, 6727-6731.	3.0	51
33	Ionization Energies and Dyson Orbitals of Thymine and Other Methylated Uracilsâ€. Journal of Physical Chemistry A, 2002, 106, 8411-8416.	2.5	49
34	Electron propagator theory calculations of molecular photoionization cross sections: The first-row hydrides. Journal of Chemical Physics, 2004, 121, 4143-4155.	3.0	49
35	Ground and excited states of CaCH3, CaNH2, CaOH, and CaF through electron propagator calculations. Journal of Chemical Physics, 1990, 92, 6728-6731.	3.0	47
36	Vertical Electron Detachment Energies for Octahedral Closed-Shell Multiply-Charged Anions. Journal of the American Chemical Society, 1994, 116, 9262-9268.	13.7	47

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37	Electron propagator calculations on uracil and adenine ionization energies. International Journal of Quantum Chemistry, 2000, 80, 831-835.	2.0	47
38	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
39	Siliconâ^'Nitrogen Bonding in Silatranes:Â Assignment of Photoelectron Spectra. Journal of the American Chemical Society, 2005, 127, 986-995.	13.7	46
40	Electron detachment energies of closed-shell anions calculated with a renormalized electron propagator. Chemical Physics Letters, 1998, 296, 494-498.	2.6	45
41	Electronic Structure of Al3On and Al3On- (n = 1â^'3) Clusters. Journal of Physical Chemistry A, 2001, 105, 8787-8793.	2.5	45
42	Diffuse-Bound and Valence-Bound Anions of Cytosine. Journal of Physical Chemistry A, 2001, 105, 8782-8786.	2.5	44
43	Vertical and adiabatic ionization energies of NHâ^'4isomers via electron propagator theory and many body perturbation theory calculations with large basis sets. Journal of Chemical Physics, 1987, 87, 3557-3562.	3.0	42
44	Electron affinity calculations on NHâ^'2, PHâ^'2, CNâ^', SHâ^', OHâ^', Clâ^', and Fâ^': Basis sets and direct vs indirect methods. Journal of Chemical Physics, 1987, 86, 308-312.	3.0	42
45	Electron propagator calculations on the ionization energies of CrHâ^', MnHâ^' and FeHâ^'. Chemical Physics Letters, 1990, 171, 197-200.	2.6	42
46	Improved electron propagator methods: An investigation of C4, Câ^'4, and C+4. Journal of Chemical Physics, 1993, 99, 6716-6726.	3.0	42
47	Brueckner orbitals, Dyson orbitals, and correlation potentials. International Journal of Quantum Chemistry, 2004, 100, 1131-1135.	2.0	42
48	Electron propagator theory of BS2 and BSâ^'2 electronic structure. Chemical Physics Letters, 1993, 214, 467-472.	2.6	41
49	Electronic Structure of AlO2, AlO2-, Al3O5, and Al3O5-Clusters. Journal of Physical Chemistry A, 2001, 105, 11291-11294.	2.5	40
50	Electron Propagator Theory. Advances in Quantum Chemistry, 2017, 74, 267-298.	0.8	40
51	Partial fourth order electron propagator theory. International Journal of Quantum Chemistry, 1988, 34, 431-436.	2.0	39
52	Ab initio conformation and ionization potentials of polysilane oligomers. Macromolecules, 1988, 21, 1189-1191.	4.8	39
53	A test of partial third order electron propagator theory: Vertical ionization energies of azabenzenes. Journal of Chemical Physics, 1996, 105, 2762-2769.	3.0	39
54	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. Journal of Physical Chemistry A, 2000, 104, 11786-11795.	2.5	39

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55	Electron Propagator Calculations Show that Alkyl Substituents Alter Porphyrin Ionization Energies. Journal of the American Chemical Society, 2005, 127, 8240-8241.	13.7	39
56	Assessment of transition operator reference states in electron propagator calculations. Journal of Chemical Physics, 2007, 127, 134106.	3.0	39
57	Oneâ€electron density matrices and energy gradients in secondâ€order electron propagator theory. Journal of Chemical Physics, 1992, 96, 8379-8389.	3.0	38
58	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
59	Orbital and shakeup operator renormalizations in electron propagator theory. Journal of Chemical Physics, 1998, 109, 5741-5746.	3.0	37
60	Ab initioelectron propagator theory of molecular wires: I. Formalism. Journal of Chemical Physics, 2005, 123, 184711.	3.0	37
61	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
62	Ground state and vertical electron detachment energies of icosahedral and D5h Al13â¯. Journal of Chemical Physics, 1999, 111, 10762-10765.	3.0	36
63	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
64	Ab Initio Calculations on some Antiepileptic Drugs such as Phenytoin, Phenbarbital, Ethosuximide and Carbamazepine. Structural Chemistry, 2017, 28, 957-964.	2.0	34
65	A simplified model of oligosilane ionization energies. Journal of Chemical Physics, 1991, 94, 6064-6072.	3.0	33
66	Al3O4 and Al3O4- Clusters:â€‰ Structure, Bonding, and Electron Binding Energies. Journal of Physical Chemistry A, 2003, 107, 2589-2595.	2.5	33
67	The electron-propagator approach to conceptual density-functional theory. Journal of Chemical Sciences, 2005, 117, 387-400.	1.5	33
68	Electron propagator calculations on linear and branched carbon cluster dianions. Journal of Chemical Physics, 1995, 102, 294-300.	3.0	32
69	Electron binding energies of nucleobases and nucleotides. International Journal of Quantum Chemistry, 2002, 90, 1547-1554.	2.0	32
70	Ionization Energies and Dyson Orbitals of Cytosine and 1-Methylcytosine. Journal of Physical Chemistry A, 2003, 107, 822-828.	2.5	31
71	Single-reference electron propagator calculations on vertical ionization energies of ozone. Chemical Physics Letters, 1998, 297, 193-199.	2.6	30
72	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

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73	Ionization energies of OHâˆ’3 isomers. Journal of Chemical Physics, 1989, 91, 7024-7029.	3.0	29
74	Theoretical Study of the Structure and Bonding of a Metalâˆ’DNA Base Complex:Â Alâˆ’Guanine. Journal of Physical Chemistry A, 2003, 107, 9415-9421.	2.5	29
75	Ab initioelectron propagator theory of molecular wires. II. Multiorbital terminal description. Journal of Chemical Physics, 2006, 124, 144114.	3.0	29
76	Molecules mimicking atoms: monomers and dimers of alkali metal solvated electron precursors. Physical Chemistry Chemical Physics, 2018, 20, 24186-24191.	2.8	29
77	Conformational Effects on Glycine Ionization Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2004, 108, 11703-11708.	2.5	28
78	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
79	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
80	Many-body theory of the ionization energies of CH3-, SiH3-, and GeH3-. Journal of the American Chemical Society, 1987, 109, 5072-5076.	13.7	27
81	Electron binding energies of linear C3, C5, C7, and C9 clusters. Journal of Chemical Physics, 1994, 100, 6614-6619.	3.0	27
82	Interpretation of the photoelectron spectra of superalkali species: Li3O and Li3Oâˆ’. Journal of Chemical Physics, 2011, 135, 164307.	3.0	27
83	Qualitative propagator theory of AX4 Auger spectra. Journal of Chemical Physics, 1984, 81, 5873-5888.	3.0	26
84	Direct versus indirect many-body methods for calculating vertical electron affinities: applications to Fâˆ’, OHâˆ’ , NH2âˆ’, CNâˆ’, Clâˆ’, SHâˆ’ and PH2âˆ’. Chemical Physics Letters, 1987, 136, 387-391.	2.6	26
85	Electron binding energies of anionic alkali metal triatomics from partial fourth order electron propagator theory calculations. Journal of Chemical Physics, 1988, 89, 6353-6356.	3.0	26
86	Structures and properties of double-Rydberg anions. The Journal of Physical Chemistry, 1990, 94, 4762-4763.	2.9	26
87	Ab Initio Electron Propagator Methods: Applications to Fullerenes and Nucleic Acid Fragments. Annual Reports in Computational Chemistry, 2010, 6, 79-94.	1.7	26
88	Electron Propagator Calculations on the Ground and Excited States of C₆₀^{â€“}. Journal of Physical Chemistry A, 2014, 118, 7424-7429.	2.5	25
89	Electron-propagator calculations with a transition-operator reference. Chemical Physics Letters, 1983, 103, 29-34.	2.6	24
90	Applications of electron propagator theory to the electron affinities of AsH2, SeH, Br, SbH2, TeH, and I. Journal of Chemical Physics, 1987, 87, 1701-1704.	3.0	24

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91	Molecular similarity indices in electron propagator theory. Chemical Physics Letters, 1991, 185, 270-275.	2.6	24
92	Oneâ€electron density matrices and energy gradients in the random phase approximation. Journal of Chemical Physics, 1994, 101, 6743-6749.	3.0	24
93	Composite electron propagator methods for calculating ionization energies. Journal of Chemical Physics, 2016, 144, 224110.	3.0	24
94	Application and Testing of Diagonal, Partial Third-Order Electron Propagator Approximations. , 2001, , 131-160.		24
95	Molecular orbital calculations on the thorium-nickel interaction in Th(.eta.5-C5H5)2(.mu.-PH2)2Ni(CO)2. Journal of the American Chemical Society, 1986, 108, 550-551.	13.7	23
96	Dichlorobenzene Ionization Energies. The Journal of Physical Chemistry, 1996, 100, 13979-13984.	2.9	23
97	Nondipole bound anions: Be2â^' and Be3â^'. Journal of Chemical Physics, 2002, 117, 3687-3693.	3.0	23
98	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
99	Do Dyson Orbitals resemble canonical Hartreeâ€“Fock orbitals?. Molecular Physics, 2019, 117, 2275-2283.	1.7	23
100	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
101	Qualitative propagator theory of CH3CN, CH3NC, and CH3CCH Auger spectra. Journal of Chemical Physics, 1985, 83, 4604-4617.	3.0	22
102	Total energies and energy gradients in electron propagator theory. International Journal of Quantum Chemistry, 1992, 44, 1-11.	2.0	22
103	Quasiparticle virtual orbitals in electron propagator calculations. Journal of Chemical Physics, 2008, 128, 164105.	3.0	22
104	Ground and excited states of CaSH through electron propagator calculations. Chemical Physics Letters, 1990, 169, 116-120.	2.6	21
105	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
106	Vertical Ionization Energies of Adenine and 9-Methyl Adenine. Journal of Physical Chemistry A, 2009, 113, 14630-14635.	2.5	21
107	Correlation and polarization effects in the thermochemical properties of small boron hydrides. Chemical Physics Letters, 1983, 103, 59-62.	2.6	20
108	Ionization Energies of Acridine, Phenazine, and Diazaphenanthrenes. Journal of Physical Chemistry A, 1997, 101, 8554-8564.	2.5	20

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109	Approximate Brueckner orbitals in electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 615-621.	2.0	20
110	Molecular photoionization cross sections in electron propagator theory: Angular distributions beyond the dipole approximation. Journal of Chemical Physics, 2005, 123, 114105.	3.0	20
111	Correlated Ab initio electron propagators in the study of molecular wires. International Journal of Quantum Chemistry, 2006, 106, 3387-3392.	2.0	20
112	Integral approximations in ab initio, electron propagator calculations. Journal of Chemical Physics, 2009, 131, 124110.	3.0	20
113	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
114	Calculations on species relevant to the photoionization of the van der Waals molecule (H2S)2. Journal of Chemical Physics, 1986, 84, 1653-1658.	3.0	19
115	Electron propagator theory of the ground and excited states of CaC5H5. Journal of the American Chemical Society, 1991, 113, 3593-3595.	13.7	19
116	Electron propagator calculations on the adiabatic electron binding energies of C3. Journal of Chemical Physics, 1992, 97, 7531-7536.	3.0	19
117	Comparison of electron propagator methods for calculating electron detachment energies of anions. International Journal of Quantum Chemistry, 1997, 65, 463-469.	2.0	19
118	Improved algorithms for renormalized electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 607-614.	2.0	19
119	Energy gradients and effective density differences in electron propagator theory. Journal of Chemical Physics, 2000, 112, 56-68.	3.0	19
120	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
121	Ground and excited states of NH4: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2004, 120, 7949-7954.	3.0	19
122	New insights in the photochromic spiro-dihydroindolizine/betaine-system. Photochemical and Photobiological Sciences, 2008, 7, 1449-1456.	2.9	19
123	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
124	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
125	Electron propagator theory of bonding in saturated silicon chains. Polyhedron, 1991, 10, 1285-1297.	2.2	18
126	Double-Rydberg Anions:Â Predictions on NH3AHn-and OH2AHn-Structures. Journal of the American Chemical Society, 2000, 122, 12813-12818.	13.7	18

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127	Electron-propagator calculations on the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2001, 114, 130.	3.0	18
128	Electron propagator calculations on C60 and C70 photoelectron spectra. Journal of Chemical Physics, 2008, 129, 104306.	3.0	18
129	Ab initio electron propagator methods: Applications to nucleic acids fragments and metallophthalocyanines. International Journal of Quantum Chemistry, 2010, 110, 2918-2930.	2.0	18
130	Molecular orbital theory of alkylideneoxirane-cyclopropanone rearrangements. Journal of Organic Chemistry, 1983, 48, 4744-4749.	3.2	17
131	Coupled-cluster reference electron propagator calculations on the ionization energies of O2. Chemical Physics Letters, 1992, 199, 530-534.	2.6	17
132	Ionization energies of benzo[a]pyrene and benzo[e]pyrene. Journal of Chemical Physics, 1997, 107, 7906-7911.	3.0	17
133	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
134	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
135	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
136	A new generation of diagonal self-energies for the calculation of electron removal energies. Journal of Chemical Physics, 2021, 155, 204107.	3.0	17
137	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
138	Quasiparticle approximations and electron propagator theory. International Journal of Quantum Chemistry, 2003, 95, 593-599.	2.0	16
139	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
140	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
141	Partial photoionization cross sections of NH4 and H3O Rydberg radicals. Journal of Chemical Physics, 2009, 131, 024104.	3.0	16
142	Conformationally induced localization in the electronic structure of polysilanes. Macromolecules, 1993, 26, 7282-7287.	4.8	15
143	Electron propagator theory of conformational effects on anisole and thioanisole photoelectron spectra. International Journal of Quantum Chemistry, 1998, 70, 1037-1043.	2.0	15
144	Structure, bonding, and energetics of C72â^' isomers. Journal of Chemical Physics, 1998, 109, 87-93.	3.0	15

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145	Are structures with Alâ€“H bonds represented in the photoelectron spectrum of Al3O4H2â¯? Journal of Chemical Physics, 2006, 124, 214304.	3.0	15
146	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
147	Calculation and interpretation of total energies in electron propagator theory. Journal of Chemical Physics, 1995, 103, 5630-5639.	3.0	14
148	Direct algorithm for the random-phase approximation. International Journal of Quantum Chemistry, 1996, 60, 1241-1247.	2.0	14
149	Vertical Ionization Energies of Naphthalene. Journal of Physical Chemistry A, 2000, 104, 10032-10034.	2.5	14
150	Aromatic Carboxylate Superhalogens and Multiply Charged Anions. Journal of Physical Chemistry A, 2002, 106, 5373-5379.	2.5	14
151	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
152	An electron propagator study of bonding in aminoborane. Chemical Physics Letters, 1989, 156, 489-493.	2.6	13
153	Electron propagator calculations on the electron affinity of C5. Chemical Physics Letters, 1993, 216, 319-323.	2.6	13
154	Electron propagator theory of ZnCH3, Zn(CH3)2, and related ions. Journal of Chemical Physics, 1994, 100, 6508-6513.	3.0	13
155	Electron propagator calculations with Kohn-Sham reference states. International Journal of Quantum Chemistry, 2001, 85, 411-420.	2.0	13
156	Solvated Succinate Dianion:â€‰ Structures, Electron Binding Energies, and Dyson Orbitals. Journal of Physical Chemistry A, 2003, 107, 10360-10369.	2.5	13
157	The AGP wavefunction and its relation to other descriptions of electronic structure. International Journal of Quantum Chemistry, 1981, 20, 113-128.	2.0	13
158	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101.	3.0	13
159	Efficient electron propagator algorithms for shakeup final states: Anthracene and acridine. International Journal of Quantum Chemistry, 2000, 80, 836-841.	2.0	12
160	Ionization Energies and Dyson Orbitals of 1,2-Dithiin. Journal of Physical Chemistry A, 2002, 106, 5924-5927.	2.5	12
161	Electronic Structure Analysis and Electron Detachment Energies of Polynitrogen Pentagonal Aromatic Anions. Journal of Physical Chemistry A, 2006, 110, 12231-12235.	2.5	12
162	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

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163	Tautomeric forms of adenine: Vertical ionization energies and Dyson orbitals. International Journal of Quantum Chemistry, 2010, 110, 1901-1915.	2.0	12
164	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
165	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
166	Electron propagator calculations with nondiagonal partial fourth-order self-energies and unrestricted hartree-fock reference states. International Journal of Quantum Chemistry, 1989, 36, 321-332.	2.0	11
167	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
168	Interpretation of the photoelectron spectra of superalkali species: Na3O and Na3Oâˆ’. Journal of Chemical Physics, 2012, 136, 224305.	3.0	11
169	Applying electron propagator theory to electron affinities. International Journal of Quantum Chemistry, 1987, 32, 469-473.	2.0	10
170	Electron propagator theory of the ground and excited states of calcium borohydride. Journal of the American Chemical Society, 1991, 113, 1102-1108.	13.7	10
171	Vertical ionization energies of cubane. Chemical Physics Letters, 1994, 230, 313-316.	2.6	10
172	Deprotonated Cytosine Anions:Â A Theoretical Prediction of Photoelectron Spectra. Journal of Physical Chemistry A, 2006, 110, 11174-11177.	2.5	10
173	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
174	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
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