J V Ortiz

List of Publications by Year in descending order

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183	5,561	81743	118652
papers	citations	39 h-index	62 g-index

194	194	194	2206
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.	1.2	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.	1.2	278
3	Semidirect algorithms for third-order electron propagator calculations. International Journal of Quantum Chemistry, 1995, 53, 583-590.	1.0	247
4	Comparison of perturbative and multiconfigurational electron propagator methods. International Journal of Quantum Chemistry, 1996, 60, 29-36.	1.0	200
5	Semidirect algorithms in electron propagator calculations. International Journal of Quantum Chemistry, 1994, 52, 23-27.	1.0	115
6	A nondiagonal, renormalized extension of partial third-order quasiparticle theory: Comparisons for closed-shell ionization energies. Journal of Chemical Physics, 1998, 108, 1008-1014.	1.2	114
7	Ionization energies of anthracene, phenanthrene, and naphthacene. Journal of Chemical Physics, 1996, 105, 8748-8753.	1.2	82
8	Anionic and Neutral Complexes of Uracil and Water. Journal of Physical Chemistry A, 1999, 103, 7912-7917.	1.1	81
9	Electron Propagator Theory of Guanine and Its Cations:Â Tautomerism and Photoelectron Spectra. Journal of the American Chemical Society, 2000, 122, 12304-12309.	6.6	78
10	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.	1.0	76
11	Electron binding energies of TCNQ and TCNE. Journal of Chemical Physics, 1996, 105, 5872-5877.	1.2	73
12	The Electron Propagator Picture of Molecular Electronic Structure. Computational Chemistry - Reviews of Current Trends, 1997, , 1-61.	0.4	70
13	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.	2.3	69
14	One-Electron Pictures of Electronic Structure: Propagator Calculations on Photoelectron Spectra of Aromatic Molecules. , 1997, , 465-517.		68
15	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. Helvetica Chimica Acta, 1984, 67, 1-17.	1.0	67
16	Dyson-orbital concepts for description of electrons in molecules. Journal of Chemical Physics, 2020, 153, 070902.	1.2	66
17	Hydride bridges between LnCp2 centers. Inorganic Chemistry, 1985, 24, 2095-2104.	1.9	65
18	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	2.3	61

#	Article	IF	Citations
19	Efficient evaluation of analytic Fukui functions. Journal of Chemical Physics, 2008, 129, 224105.	1.2	60
20	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.	1.2	59
21	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. Journal of Chemical Theory and Computation, 2016, 12, 627-637.	2.3	56
22	Ground states and ionization energies of Si2H6, Si3H8, Si4H10, and Si5H12. Journal of the American Chemical Society, 1988, 110, 4522-4527.	6.6	54
23	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.	1.1	53
24	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.	6.6	51
25	Electron propagator theory of BO2and BOâ¯2electronic structure. Journal of Chemical Physics, 1993, 99, 6727-6731.	1.2	51
26	Ionization Energies and Dyson Orbitals of Thymine and Other Methylated Uracilsâ€. Journal of Physical Chemistry A, 2002, 106, 8411-8416.	1.1	49
27	Electron propagator theory calculations of molecular photoionization cross sections: The first-row hydrides. Journal of Chemical Physics, 2004, 121, 4143-4155.	1.2	49
28	Ground and excited states of CaCH3, CaNH2, CaOH, and CaF through electron propagator calculations. Journal of Chemical Physics, 1990, 92, 6728-6731.	1.2	47
29	Vertical Electron Detachment Energies for Octahedral Closed-Shell Multiply-Charged Anions. Journal of the American Chemical Society, 1994, 116, 9262-9268.	6.6	47
30	Electron propagator calculations on uracil and adenine ionization energies. International Journal of Quantum Chemistry, 2000, 80, 831-835.	1.0	47
31	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.	1.1	47
32	Siliconâ¯Nitrogen Bonding in Silatranes:Â Assignment of Photoelectron Spectra. Journal of the American Chemical Society, 2005, 127, 986-995.	6.6	46
33	Electronic Structure of Al3On and Al3On- (n = 1â¯3) Clusters. Journal of Physical Chemistry A, 2001, 105, 8787-8793.	1.1	45
34	Diffuse-Bound and Valence-Bound Anions of Cytosine. Journal of Physical Chemistry A, 2001, 105, 8782-8786.	1.1	44
35	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.	1.2	42
36	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.	1.2	42

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37	Improved electron propagator methods: An investigation of C4, Câ¯4, and C+4. Journal of Chemical Physics, 1993, 99, 6716-6726.	1.2	42
38	Brueckner orbitals, Dyson orbitals, and correlation potentials. International Journal of Quantum Chemistry, 2004, 100, 1131-1135.	1.0	42
39	Electronic Structure of AlO2, AlO2-, Al3O5, and Al3O5-Clusters. Journal of Physical Chemistry A, 2001, 105, 11291-11294.	1.1	40
40	Partial fourth order electron propagator theory. International Journal of Quantum Chemistry, 1988, 34, 431-436.	1.0	39
41	Ab initio conformation and ionization potentials of polysilane oligomers. Macromolecules, 1988, 21, 1189-1191.	2.2	39
42	A test of partial third order electron propagator theory: Vertical ionization energies of azabenzenes. Journal of Chemical Physics, 1996, 105, 2762-2769.	1.2	39
43	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. Journal of Physical Chemistry A, 2000, 104, 11786-11795.	1.1	39
44	Electron Propagator Calculations Show that Alkyl Substituents Alter Porphyrin Ionization Energies. Journal of the American Chemical Society, 2005, 127, 8240-8241.	6.6	39
45	Assessment of transition operator reference states in electron propagator calculations. Journal of Chemical Physics, 2007, 127, 134106.	1.2	39
46	Oneâ€electron density matrices and energy gradients in secondâ€order electron propagator theory. Journal of Chemical Physics, 1992, 96, 8379-8389.	1.2	38
47	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.	1.2	38
48	Orbital and shakeup operator renormalizations in electron propagator theory. Journal of Chemical Physics, 1998, 109, 5741-5746.	1.2	37
49	Ab initioelectron propagator theory of molecular wires: I. Formalism. Journal of Chemical Physics, 2005, 123, 184711.	1.2	37
50	Ground state and vertical electron detachment energies of icosahedral and D5h Al13â¯. Journal of Chemical Physics, 1999, 111, 10762-10765.	1.2	36
51	A simplified model of oligosilane ionization energies. Journal of Chemical Physics, 1991, 94, 6064-6072.	1.2	33
52	Al3O4 and Al3O4- Clusters:â€‰ Structure, Bonding, and Electron Binding Energies. Journal of Physical Chemistry A, 2003, 107, 2589-2595.	1.1	33
53	The electron-propagator approach to conceptual density-functional theory. Journal of Chemical Sciences, 2005, 117, 387-400.	0.7	33
54	Electron propagator calculations on linear and branched carbon cluster dianions. Journal of Chemical Physics, 1995, 102, 294-300.	1.2	32

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55	Electron binding energies of nucleobases and nucleotides. International Journal of Quantum Chemistry, 2002, 90, 1547-1554.	1.0	32
56	Ionization Energies and Dyson Orbitals of Cytosine and 1-Methylcytosine. Journal of Physical Chemistry A, 2003, 107, 822-828.	1.1	31
57	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.	1.1	30
58	Ionization energies of OHâˆ’3 isomers. Journal of Chemical Physics, 1989, 91, 7024-7029.	1.2	29
59	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.	1.1	29
60	Ab initioelectron propagator theory of molecular wires. II. Multiorbital terminal description. Journal of Chemical Physics, 2006, 124, 144114.	1.2	29
61	Conformational Effects on Glycine Ionization Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2004, 108, 11703-11708.	1.1	28
62	Three approximations to the nonlocal and energyâ€dependent correlation potential in electron propagator theory. International Journal of Quantum Chemistry, 2010, 110, 706-715.	1.0	28
63	A generalized any-particle propagator theory: Prediction of proton affinities and acidity properties with the proton propagator. Journal of Chemical Physics, 2013, 138, 194108.	1.2	28
64	Many-body theory of the ionization energies of CH3-, SiH3-, and GeH3-. Journal of the American Chemical Society, 1987, 109, 5072-5076.	6.6	27
65	Electron binding energies of linear C3, C5, C7, and C9 clusters. Journal of Chemical Physics, 1994, 100, 6614-6619.	1.2	27
66	Interpretation of the photoelectron spectra of superalkali species: Li3O and Li3Oâˆ’. Journal of Chemical Physics, 2011, 135, 164307.	1.2	27
67	Qualitative propagator theory of AX4 Auger spectra. Journal of Chemical Physics, 1984, 81, 5873-5888.	1.2	26
68	Electron binding energies of anionic alkali metal triatomics from partial fourth order electron propagator theory calculations. Journal of Chemical Physics, 1988, 89, 6353-6356.	1.2	26
69	Structures and properties of double-Rydberg anions. The Journal of Physical Chemistry, 1990, 94, 4762-4763.	2.9	26
70	Electron Propagator Calculations on the Ground and Excited States of C₆₀^{â€“}. Journal of Physical Chemistry A, 2014, 118, 7424-7429.	1.1	25
71	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.	1.2	24
72	Oneâ€electron density matrices and energy gradients in the random phase approximation. Journal of Chemical Physics, 1994, 101, 6743-6749.	1.2	24

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73	Composite electron propagator methods for calculating ionization energies. Journal of Chemical Physics, 2016, 144, 224110.	1.2	24
74	Application and Testing of Diagonal, Partial Third-Order Electron Propagator Approximations. , 2001, , 131-160.		24
75	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.	6.6	23
76	Dichlorobenzene Ionization Energies. The Journal of Physical Chemistry, 1996, 100, 13979-13984.	2.9	23
77	Nondipole bound anions: Be2â^' and Be3â^'. Journal of Chemical Physics, 2002, 117, 3687-3693.	1.2	23
78	Electron propagator studies of vertical electron detachment energies and isomerism in purinic deoxyribonucleotides. International Journal of Quantum Chemistry, 2007, 107, 2266-2273.	1.0	23
79	Do Dyson Orbitals resemble canonical Hartreeâ€“Fock orbitals?. Molecular Physics, 2019, 117, 2275-2283.	0.8	23
80	Qualitative propagator theory of CH3CN, CH3NC, and CH3CCH Auger spectra. Journal of Chemical Physics, 1985, 83, 4604-4617.	1.2	22
81	Total energies and energy gradients in electron propagator theory. International Journal of Quantum Chemistry, 1992, 44, 1-11.	1.0	22
82	Quasiparticle virtual orbitals in electron propagator calculations. Journal of Chemical Physics, 2008, 128, 164105.	1.2	22
83	Addition of water, methanol, and ammonia to Al3O3â^' clusters: Reaction products, transition states, and electron detachment energies. Journal of Chemical Physics, 2005, 122, 214309.	1.2	21
84	Vertical Ionization Energies of Adenine and 9-Methyl Adenine. Journal of Physical Chemistry A, 2009, 113, 14630-14635.	1.1	21
85	Ionization Energies of Acridine, Phenazine, and Diazaphenanthrenes. Journal of Physical Chemistry A, 1997, 101, 8554-8564.	1.1	20
86	Approximate Brueckner orbitals in electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 615-621.	1.0	20
87	Molecular photoionization cross sections in electron propagator theory: Angular distributions beyond the dipole approximation. Journal of Chemical Physics, 2005, 123, 114105.	1.2	20
88	Correlated Ab initio electron propagators in the study of molecular wires. International Journal of Quantum Chemistry, 2006, 106, 3387-3392.	1.0	20
89	Integral approximations in ab initio, electron propagator calculations. Journal of Chemical Physics, 2009, 131, 124110.	1.2	20
90	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.	1.1	20

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91	Electron propagator theory of the ground and excited states of CaC5H5. Journal of the American Chemical Society, 1991, 113, 3593-3595.	6.6	19
92	Electron propagator calculations on the adiabatic electron binding energies of C3. Journal of Chemical Physics, 1992, 97, 7531-7536.	1.2	19
93	Comparison of electron propagator methods for calculating electron detachment energies of anions. International Journal of Quantum Chemistry, 1997, 65, 463-469.	1.0	19
94	Improved algorithms for renormalized electron propagator calculations. International Journal of Quantum Chemistry, 1999, 75, 607-614.	1.0	19
95	Energy gradients and effective density differences in electron propagator theory. Journal of Chemical Physics, 2000, 112, 56-68.	1.2	19
96	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.	1.2	19
97	Ground and excited states of NH4: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2004, 120, 7949-7954.	1.2	19
98	Electron Propagator Methods for Vertical Electron Detachment Energies of Anions: Benchmarks and Case Studies. Journal of Chemical Theory and Computation, 2018, 14, 5881-5895.	2.3	19
99	Double-Rydberg Anions:Â Predictions on NH3AHn-and OH2AHn-Structures. Journal of the American Chemical Society, 2000, 122, 12813-12818.	6.6	18
100	Electron-propagator calculations on the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2001, 114, 130.	1.2	18
101	Electron propagator calculations on C60 and C70 photoelectron spectra. Journal of Chemical Physics, 2008, 129, 104306.	1.2	18
102	Ab initio electron propagator methods: Applications to nucleic acids fragments and metallophthalocyanines. International Journal of Quantum Chemistry, 2010, 110, 2918-2930.	1.0	18
103	Molecular orbital theory of alkylideneoxirane-cyclopropanone rearrangements. Journal of Organic Chemistry, 1983, 48, 4744-4749.	1.7	17
104	Ionization energies of benzo[a]pyrene and benzo[e]pyrene. Journal of Chemical Physics, 1997, 107, 7906-7911.	1.2	17
105	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.	1.2	17
106	Electronic Structure of ScC6H6-and ScC6H6:Â Geometries, Electron Binding Energies, and Dyson Orbitalsâ€. Journal of Physical Chemistry A, 2004, 108, 2988-2992.	1.1	17
107	Electron propagator and coupled-cluster calculations on the photoelectron spectra of thiouracil and dithiouracil anions. Journal of Chemical Physics, 2011, 134, 074305.	1.2	17
108	A new generation of diagonal self-energies for the calculation of electron removal energies. Journal of Chemical Physics, 2021, 155, 204107.	1.2	17

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109	Approximate Brueckner orbitals and shakeup operators in electron propagator calculations: Applications to F? And OH?. International Journal of Quantum Chemistry, 1998, 70, 651-658.	1.0	16
110	Quasiparticle approximations and electron propagator theory. International Journal of Quantum Chemistry, 2003, 95, 593-599.	1.0	16
111	O H 3 â^' and O2H5â^' double Rydberg anions: Predictions and comparisons with NH4â^' and N2H7â^'. Journal of Chemical Physics, 2007, 127, 014307.	1.2	16
112	Nonconventional Hydrogen Bonds: A Theoretical Study of [uracil-L]^{â^'}(L = F, Cl, Br, I, Al, Ga,) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	16
113	Partial photoionization cross sections of NH4 and H3O Rydberg radicals. Journal of Chemical Physics, 2009, 131, 024104.	1.2	16
114	Conformationally induced localization in the electronic structure of polysilanes. Macromolecules, 1993, 26, 7282-7287.	2.2	15
115	Electron propagator theory of conformational effects on anisole and thioanisole photoelectron spectra. International Journal of Quantum Chemistry, 1998, 70, 1037-1043.	1.0	15
116	Structure, bonding, and energetics of C72â^' isomers. Journal of Chemical Physics, 1998, 109, 87-93.	1.2	15
117	Are structures with Alâ€“H bonds represented in the photoelectron spectrum of Al3O4H2â^'?. Journal of Chemical Physics, 2006, 124, 214304.	1.2	15
118	Direct Î”MBPT(2) method for ionization potentials, electron affinities, and excitation energies using fractional occupation numbers. Journal of Chemical Physics, 2013, 138, 074101.	1.2	15
119	Calculation and interpretation of total energies in electron propagator theory. Journal of Chemical Physics, 1995, 103, 5630-5639.	1.2	14
120	Vertical Ionization Energies of Naphthalene. Journal of Physical Chemistry A, 2000, 104, 10032-10034.	1.1	14
121	Aromatic Carboxylate Superhalogens and Multiply Charged Anions. Journal of Physical Chemistry A, 2002, 106, 5373-5379.	1.1	14
122	Ground and excited states of the Rydberg radical H3O: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2005, 122, 234317.	1.2	14
123	Electron propagator theory of ZnCH3, Zn(CH3)2, and related ions. Journal of Chemical Physics, 1994, 100, 6508-6513.	1.2	13
124	Electron propagator calculations with Kohn-Sham reference states. International Journal of Quantum Chemistry, 2001, 85, 411-420.	1.0	13
125	Solvated Succinate Dianion:â€‰ Structures, Electron Binding Energies, and Dyson Orbitals. Journal of Physical Chemistry A, 2003, 107, 10360-10369.	1.1	13
126	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101.	1.2	13

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127	Efficient electron propagator algorithms for shakeup final states: Anthracene and acridine. International Journal of Quantum Chemistry, 2000, 80, 836-841.	1.0	12
128	Ionization Energies and Dyson Orbitals of 1,2-Dithiin. Journal of Physical Chemistry A, 2002, 106, 5924-5927.	1.1	12
129	Electronic Structure Analysis and Electron Detachment Energies of Polynitrogen Pentagonal Aromatic Anions. Journal of Physical Chemistry A, 2006, 110, 12231-12235.	1.1	12
130	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.	1.0	12
131	Tautomeric forms of adenine: Vertical ionization energies and Dyson orbitals. International Journal of Quantum Chemistry, 2010, 110, 1901-1915.	1.0	12
132	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.	1.1	12
133	Virtual space reduction in quasiâ€particle electron propagator calculations: Applications to polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 2008, 108, 2862-2869.	1.0	11
134	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.	1.0	11
135	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. Journal of Chemical Physics, 2010, 132, 214507.	1.2	11
136	Interpretation of the photoelectron spectra of superalkali species: Na3O and Na3Oâ˙. Journal of Chemical Physics, 2012, 136, 224305.	1.2	11
137	Applying electron propagator theory to electron affinities. International Journal of Quantum Chemistry, 1987, 32, 469-473.	1.0	10
138	Electron propagator theory of the ground and excited states of calcium borohydride. Journal of the American Chemical Society, 1991, 113, 1102-1108.	6.6	10
139	Deprotonated Cytosine Anions:Â A Theoretical Prediction of Photoelectron Spectra. Journal of Physical Chemistry A, 2006, 110, 11174-11177.	1.1	10
140	Surface Greenâ€™s function calculations: A nonrecursive scheme with an infinite number of principal layers. Journal of Chemical Physics, 2007, 126, 134105.	1.2	10
141	Tautomeric Forms of Azolide Anions:Â Vertical Electron Detachment Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2007, 111, 13069-13074.	1.1	10
142	Second-order, two-electron Dyson propagator theory: Comparisons for vertical double ionization potentials. Journal of Chemical Physics, 2008, 129, 084105.	1.2	10
143	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.	2.3	10
144	Renormalized ground states in electron propagator theory. International Journal of Quantum Chemistry, 1991, 40, 35-42.	1.0	9

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145	Partial third-order quasiparticle theory: An application to the photoelectron spectrum of S-tetrazine. International Journal of Quantum Chemistry, 1997, 63, 291-299.	1.0	9
146	Effective procedure for energy optimizing antisymmetrized geminal power states. Journal of Chemical Physics, 2002, 117, 5135-5154.	1.2	9
147	Electron binding energies and Dyson orbitals of Al5Omâ˜ (m=3,4,5) and Al5O5H2â˜. Journal of Chemical Physics, 2007, 127, 234302.	1.2	9
148	Assignment of photoelectron spectra of halideâ€“water clusters: Contrasting patterns of delocalization in Dyson orbitals. Journal of Chemical Physics, 2013, 138, 164317.	1.2	9
149	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.	1.2	9
150	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.	1.3	9
151	Double Rydberg anions with solvated ammonium kernels: Electron binding energies and Dyson orbitals. Journal of Chemical Physics, 2019, 151, .	1.2	9
152	Ground-state and vertical ionization energies versus silicon-silicon-silicon and carbon-carbon-carbon bond angles in trisilane and propane. The Journal of Physical Chemistry, 1991, 95, 8609-8613.	2.9	8
153	Solvation of Alâ˜Guanine Complexes with NH3:Â A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 5845-5850.	1.1	8
154	Efficient and Accurate Electron Propagator Methods and Algorithms. , 2009, , 1-17.		8
155	Electron Propagator Self-Energies versus Improved GW100 Vertical Ionization Energies. Journal of Chemical Theory and Computation, 2022, 18, 4927-4944.	2.3	8
156	Second-order shakeup terms in electron propagator calculations on F2 and H2O2. International Journal of Quantum Chemistry, 1998, 69, 175-182.	1.0	7
157	Construction of unique canonical coefficients for antisymmeterized geminal power states. International Journal of Quantum Chemistry, 2004, 97, 896-907.	1.0	7
158	Sequential addition of H2O, CH3OH, and NH3 to Al3O3â˜: A theoretical study. Journal of Chemical Physics, 2007, 126, 024309.	1.2	7
159	Delocalization of Dyson orbitals in F^{â˜}(H₂O) and Cl^{â˜}(H₂O). International Journal of Quantum Chemistry, 2011, 111, 1701-1708.	1.0	7
160	Numerical test of SAC-CI methods for calculating vertical ionization energies. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
161	Bond rotations and localization in the electronic structure of polysilanes. Macromolecules, 1993, 26, 2989-2991.	2.2	6
162	Electron Propagator Theory of ZnC5H5, Zn(C5H5)2, and Related Ions. The Journal of Physical Chemistry, 1994, 98, 13198-13202.	2.9	6

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163	Contour integrals in electron propagator theory. International Journal of Quantum Chemistry, 1995, 56, 331-337.	1.0	6
164	Computational Tests of Models for Kinetic Parameters of Unimolecular Reactions of Organophosphorus and Organosulfur Compounds. Journal of Physical Chemistry A, 2011, 115, 14143-14152.	1.1	6
165	Excitation energies, photoionization cross sections, and asymmetry parameters of the methyl and silyl radicals. Journal of Chemical Physics, 2014, 141, 074308.	1.2	6
166	Strong correlation effects in the electron binding energies of phthalocyanine. International Journal of Quantum Chemistry, 2009, 109, 3619-3625.	1.0	5
167	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.	1.1	5
168	Valence and diffuse-bound anions of noble-gas complexes with uracil. Journal of Chemical Physics, 2012, 137, 194310.	1.2	5
169	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.	1.1	5
170	Valence-Bound and Diffuse-Bound Anions of 5-Azauracil. Journal of Physical Chemistry A, 2014, 118, 6908-6913.	1.1	5
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