Peter R SurjÃ¡n

List of Publications by Year
in descending order

173	4,579	109321	128289
papers	citations	35 h-index	60 g-index

183	183	183	2218
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stability analysis of the Lippmannâ€“Schwinger equation. Molecular Physics, 2023, 121, .	1.7	1
2	The $$gamma$$ function in quantum theory II. Mathematical challenges and paradoxa. Journal of Mathematical Chemistry, 2022, 60, 267-282.	1.5	0
3	Editorial: In memoriam IstvÃ¡n Mayer. International Journal of Quantum Chemistry, 2022, 122, .	2.0	0
4	A note on perturbation-adapted perturbation theory. Journal of Chemical Physics, 2022, 156, 116102.	3.0	0
5	Many-Body Perturbation Theory with Localized Orbitals: Accounting for Localization Diagrams as Integral Dressing. Journal of Chemical Theory and Computation, 2022, , .	5.3	0
6	Comment on â€œImproved many-body expansions from eigenvector continuationâ€• Physical Review C, 2021, 103, .	2.9	0
7	Symmetry-Adapted Perturbation with Half-Projection for Spin Unrestricted Geminals. Journal of Chemical Theory and Computation, 2021, 17, 4122-4143.	5.3	4
8	Improving half-projected spin-contaminated wave functions by multi-configuration perturbation theory. Journal of Chemical Physics, 2021, 154, 234110.	3.0	5
9	On the variational principle for the non-linear SchrÃ¶dinger equation. Journal of Mathematical Chemistry, 2020, 58, 340-351.	1.5	0
10	Introducing the Î³ function in quantum theory. International Journal of Quantum Chemistry, 2020, 120, e26221.	2.0	4
11	Half-Projection of the Strongly Orthogonal Unrestricted Geminalsâ€™ Product Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 892-903.	5.3	14
12	Application of the Cauchy integral formula as a tool of analytic continuation for the resummation of divergent perturbation series. Journal of Chemical Physics, 2019, 150, 031101.	3.0	8
13	Geminal perturbation theory based on the unrestricted Hartreeâ€“Fock wavefunction. Journal of Chemical Physics, 2019, 150, 034103.	3.0	10
14	Editorial: in memoriam JÃ¡nos G. Ãngyán (1956â€“2017). Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
15	The inverse boundary value problem: application in many-body perturbation theory. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
16	Effect of partitioning on the convergence properties of the Rayleigh-SchrÃ¶dinger perturbation series. Journal of Chemical Physics, 2017, 146, 124121.	3.0	6
17	Analytic-continuation approach to the resummation of divergent series in Rayleigh-SchrÃ¶dinger perturbation theory. Physical Review A, 2017, 96, .	2.5	10
18	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. Journal of Physical Chemistry A, 2016, 120, 5527-5538.	2.5	9

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19	Spin Symmetry and Size Consistency of Strongly Orthogonal Geminals. Journal of Chemical Theory and Computation, 2015, 11, 3096-3103.	5.3	15
20	Role of triplet states in geminal-based perturbation theory. Molecular Physics, 2015, 113, 2960-2963.	1.7	13
21	Local spin from strongly orthogonal geminal wavefunctions. Molecular Physics, 2015, 113, 249-259.	1.7	23
22	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized Ï€-electron method. Journal of Chemical Physics, 2014, 140, 044112.	3.0	5
23	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. Physica Status Solidi (B): Basic Research, 2014, 251, 2451-2456.	1.5	6
24	Perspectives of APSGâ€based multireference perturbation theories. International Journal of Quantum Chemistry, 2014, 114, 1048-1052.	2.0	39
25	Composite particles in quantum chemistry: From twoâ€electron bonds to cold atoms. International Journal of Quantum Chemistry, 2013, 113, 185-189.	2.0	1
26	Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: Role of Dispersive Interactions. Journal of Chemical Theory and Computation, 2013, 9, 2602-2608.	5.3	42
27	Spin-adaptation and redundancy in state-specific multireference perturbation theory. Journal of Chemical Physics, 2013, 138, 124110.	3.0	14
28	Efficient iterative diagonalization of the Boseâ€“Hubbard model for ultracold bosons in a periodic optical trap. Chemical Physics, 2012, 401, 208-216.	1.9	6
29	Mayerâ€™s orthogonalization: relation to the Gram-Schmidt and LÃ¶wdinâ€™s symmetrical scheme. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	12
30	Strongly orthogonal geminals: size-extensive and variational reference states. Journal of Mathematical Chemistry, 2012, 50, 534-551.	1.5	68
31	A stationary property of the APSG wave function. Journal of Mathematical Chemistry, 2011, 49, 1217-1225.	1.5	2
32	Perturbative Approximations to Avoid Matrix Diagonalization. Challenges and Advances in Computational Chemistry and Physics, 2011, , 83-95.	0.6	1
33	Zero-field-splitting in triplet-state nanotubes. Chemical Physics Letters, 2010, 498, 292-295.	2.6	4
34	Jahnâ€“Teller distortion of ionized and excited carbon nanotubes. Journal of Chemical Physics, 2010, 132, 034309.	3.0	9
35	Generalized MÃ¸llerâ€“Plesset Partitioning in Multiconfiguration Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 2024-2033.	5.3	53
36	On The Coupled-Cluster Equations. Stability Analysis And Nonstandard Correction Schemes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 513-534.	0.6	1

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37	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
38	Fermi-Vacuum Invariance in Multiconfiguration Perturbation Theory. Progress in Theoretical Chemistry and Physics, 2009, , 257-268.	0.2	4
39	Distorted s-type orbitals: the $${m H}^{+}_{2}$$ problem revisited. Journal of Mathematical Chemistry, 2008, 43, 227-236.	1.5	3
40	Iterative solution of Bloch-type equations: stability conditions and chaotic behavior. Journal of Mathematical Chemistry, 2008, 43, 314-327.	1.5	11
41	Stability conditions for the coupled cluster equations. International Journal of Quantum Chemistry, 2008, 108, 2043-2052.	2.0	13
42	Frozen localized molecular orbitals in electron correlation calculations â€“ Exploiting the Hartreeâ€“Fock density matrix. Chemical Physics Letters, 2008, 450, 400-403.	2.6	6
43	A sparse matrix based full-configuration interaction algorithm. Journal of Chemical Physics, 2008, 128, 144101.	3.0	26
44	Intershell interaction in double walled carbon nanotubes: Charge transfer and orbital mixing. Physical Review B, 2008, 77, .	3.2	61
45	EffectiveÏ€-electron Hamiltonian for small-radius nanotubes: Interpretation of curvature-induced conductivity. Physical Review B, 2008, 77, .	3.2	3
46	A Note on the Symmetry Properties of LÃ¶wdin's Orthogonalization Schemes. Collection of Czechoslovak Chemical Communications, 2008, 73, 937-944.	1.0	2
47	Natural orbitals in CIS and singular-value decomposition. Chemical Physics Letters, 2007, 439, 393-394.	2.6	38
48	Semiconductor-to-metal transition of double walled carbon nanotubes induced by inter-shell interaction. Physica Status Solidi (B): Basic Research, 2006, 243, 3476-3479.	1.5	30
49	Diagonalization-free initial guess to SCF calculations for large molecules. Chemical Physics Letters, 2006, 424, 420-424.	2.6	25
50	Coupled-cluster theory and the method of moments. Computational and Theoretical Chemistry, 2006, 768, 17-23.	1.5	6
51	Intertube interactions in carbon nanotube bundles. Physical Review B, 2006, 73, .	3.2	41
52	The high-rank Hartreeâ€“Fock method as an averaging procedure. Molecular Physics, 2006, 104, 2037-2046.	1.7	0
53	The MP2 energy as a functional of the Hartreeâ€“Fock density matrix. Chemical Physics Letters, 2005, 406, 318-320.	2.6	53
54	Stability and Properties of Polyhelicenes and Anellated Fused-Ring Carbon Helices: Models Toward Helical Graphites.. ChemInform, 2005, 36, no.	0.0	0

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55	Size dependence of Feenberg scaling. International Journal of Quantum Chemistry, 2005, 101, 287-290.	2.0	6
56	Multiconfiguration perturbation theory: Size consistency at second order. Journal of Chemical Physics, 2005, 122, 114104.	3.0	54
57	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
58	Idempotency-Conserving Iteration Scheme for the One-Electron Density Matrix. Physical Review Letters, 2005, 95, 013002.	7.8	14
59	Stability and Properties of Polyhelicenes and Annelated Fused-Ring Carbon Helices:Â Models Toward Helical Graphites. Journal of Chemical Information and Modeling, 2005, 45, 850-855.	5.4	11
60	Convergence Enhancement in Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2004, 69, 105-120.	1.0	8
61	Partitioning in multiconfiguration perturbation theory. Annalen Der Physik, 2004, 13, 223-231.	2.4	45
62	Appendix to â€œStudies in Perturbation Theoryâ€• The Problem of Partitioning. , 2004, , 129-185.		13
63	Direct determination of fragment localized molecular orbitals and the orthogonality constraint. Chemical Physics Letters, 2003, 369, 125-130.	2.6	26
64	Optimized partitioning in PT: Application for the equation of motion describing ionization processes. International Journal of Quantum Chemistry, 2003, 92, 160-167.	2.0	4
65	On the perturbation of multiconfiguration wave functions. Journal of Chemical Physics, 2003, 119, 1922-1928.	3.0	82
66	Optimized Quasiparticle Energies in Many-Body Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2003, 68, 331-339.	1.0	7
67	Laplace-transformed denominators in perturbation theory: Linear-scaling second-order treatment of weakly interacting nanostructures. Physical Review A, 2003, 68, .	2.5	13
68	Two-body zeroth order Hamiltonians in multireference perturbation theory: The APSG reference state. Journal of Chemical Physics, 2002, 116, 878-890.	3.0	100
69	A general state-selective multireference coupled-cluster algorithm. Journal of Chemical Physics, 2002, 117, 980-990.	3.0	237
70	On the Use of Connected Moments Expansion with Coupled Cluster Reference. International Journal of Molecular Sciences, 2002, 3, 508-521.	4.1	9
71	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. Chirality, 2002, 14, 377-385.	2.6	12
72	Constant denominator perturbative schemes and the partitioning technique. International Journal of Quantum Chemistry, 2002, 90, 20-26.	2.0	12

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73	Nonsymmetrical perturbation theory for improving coupled-cluster wave functions. International Journal of Quantum Chemistry, 2002, 90, 1309-1320.	2.0	14
74	On the â€œkiller conditionâ€™' in the equation-of-motion method: ionization potentials from multi-reference wave functions. Physical Chemistry Chemical Physics, 2001, 3, 696-701.	2.8	15
75	Near-degeneracy corrections for second-order perturbation theory: comparison of two approaches. Theoretical Chemistry Accounts, 2001, 105, 408-412.	1.4	5
76	An effective hopping model for weakly interacting Ï€ systems: Electronic structure of stacked polyaromatic hydrocarbons. International Journal of Quantum Chemistry, 2001, 84, 216-225.	2.0	18
77	Circular dichroism of host-guest complexes of achiral pyridino- and phenazino-18-crown-6 ligands with the enantiomers of chiral aralkyl ammonium salts. Chirality, 2001, 13, 109-117.	2.6	11
78	On the convergence of the coupled-cluster sequence: the H8 model. Computational and Theoretical Chemistry, 2001, 547, 145-151.	1.5	15
79	Higher excitations in coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 2945-2954.	3.0	666
80	Interaction of chemical bonds. V. Perturbative corrections to geminal-type wave functions. International Journal of Quantum Chemistry, 2000, 80, 96-104.	2.0	35
81	Orthogonality constrained excited states. Chemical Physics Letters, 2000, 325, 120-126.	2.6	14
82	The nature of electronic excitations in singly bonded C 60 dimer. Computational and Theoretical Chemistry, 2000, 501-502, 369-377.	1.5	1
83	Optimized partitioning in perturbation theory: Comparison to related approaches. Journal of Chemical Physics, 2000, 112, 4438-4446.	3.0	43
84	Computing coupled-cluster wave functions with arbitrary excitations. Journal of Chemical Physics, 2000, 113, 1359-1365.	3.0	127
85	Covalent bond orders and atomic valences from correlated wavefunctions. Chemical Physics Letters, 1999, 299, 1-8.	2.6	60
86	Optimized partitioning in Rayleighâ€“SchrÃ¶dinger perturbation theory. Chemical Physics Letters, 1999, 308, 303-309.	2.6	34
87	Improving CISD calculations by geminal-type reference states. Chemical Physics Letters, 1999, 312, 221-228.	2.6	16
88	An Introduction to the Theory of Geminals. Topics in Current Chemistry, 1999, , 63-88.	4.0	115
89	Scanning tunnelling microscopy (STM) imaging of carbon nanotubes. Carbon, 1998, 36, 689-696.	10.3	54
90	Hybridization effects in localized wave functions. Computational and Theoretical Chemistry, 1998, 455, 175-182.	1.5	1

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91	Dyson-corrected orbital energies for the perturbative treatment of electron correlation. International Journal of Quantum Chemistry, 1998, 69, 713-719.	2.0	9
92	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. International Journal of Quantum Chemistry, 1998, 70, 571-581.	2.0	12
93	Triplet State Characteristics of Higher Fullerenes. Journal of Physical Chemistry A, 1998, 102, 1261-1273.	2.5	26
94	Electronic structure of the singly bonded(C60)xfullerene polymer. Physical Review B, 1998, 58, 3490-3493.	3.2	22
95	Highly symmetric borane clusters as fullerene analogs. , 1998, , .		0
96	Triplet State Characteristics of Smaller Fullerenes. Fullerenes, Nanotubes, and Carbon Nanostructures, 1997, 5, 355-373.	0.6	2
97	Energetics and zero-field-splitting in triplet states of C70. Computational and Theoretical Chemistry, 1997, 398-399, 293-300.	1.5	7
98	The phase diagram of charge- and spin-density waves in polymeric C 60. Applied Physics A: Materials Science and Processing, 1997, 64, 315-319.	2.3	7
99	Calculation of correlation-corrected band structures of polymers in the case of quasi-degeneracy. Solid State Communications, 1997, 103, 639-644.	1.9	4
100	Charge vs. spin density waves in the fullerene polymer. , 1997, 63, 425-435.		5
101	Third-order many-body perturbation theory for intermolecular interactions. I. Hartree-Fock level. , 1997, 64, 43-51.		12
102	Perturbative calculation of intermolecular interactions in orthogonalized or biorthogonal basis sets. Theoretica Chimica Acta, 1996, 94, 333-344.	0.8	4
103	Excited states of the C60 dimer. Synthetic Metals, 1996, 77, 107-110.	3.9	9
104	Zero-field-splitting in the lowest triplet state of C60. Chemical Physics Letters, 1996, 251, 115-118.	2.6	37
105	Zeroâ€fieldâ€splitting and Ï€â€electron spin densities in the lowest excited triplet state of oligothiophenes. Journal of Chemical Physics, 1996, 105, 4441-4447.	3.0	34
106	Damping of perturbation corrections in quasidegenerate situations. Journal of Chemical Physics, 1996, 104, 3320-3324.	3.0	16
107	The interaction of chemical bonds. IV. Interbond charge transfer by a coupled-cluster-type formalism. International Journal of Quantum Chemistry, 1995, 55, 109-116.	2.0	22
108	sp3 Hybridized carbons on buckminsterfullerene. Computational and Theoretical Chemistry, 1995, 338, 215-223.	1.5	15

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109	Optical spectra of diels-alder adducts of C60. Synthetic Metals, 1995, 70, 1377-1378.	3.9	5
110	Electronic excitations in fullerenes: Jahn-Teller distorted structures of C60. Journal of Molecular Structure, 1994, 311, 55-68.	3.6	10
111	The interaction of chemical bonds. III. Perturbed strictly localized geminals inLMObasis. International Journal of Quantum Chemistry, 1994, 52, 563-574.	2.0	26
112	The reliability of the point charge model representing intermolecular effects in ab initio calculations. Chemical Physics Letters, 1994, 225, 258-264.	2.6	21
113	Band structures of neutral and doped (C60)x polymers. Solid State Communications, 1994, 92, 407-411.	1.9	34
114	Ab initio Hartree- Fock calculations of the interaction energy of bimolecular complexes. Computational and Theoretical Chemistry, 1994, 307, 239-259.	1.5	9
115	Electronic excitations in fullerenes: Jahnâ€"Teller distorted structures of C60. Computational and Theoretical Chemistry, 1994, 311, 55-68.	1.5	27
116	Localization maps by orbital partitioning of the electron density. Theoretica Chimica Acta, 1993, 86, 379-389.	0.8	4
117	Design of small gap conjugated polymers. Synthetic Metals, 1993, 57, 4338-4343.	3.9	36
118	Quinoid-aromatic competition as a tool for band structure design for conjugated polymers. Synthetic Metals, 1993, 57, 4260-4265.	3.9	3
119	Jahn-Teller Distorted Excited States of C60. Springer Series in Solid-state Sciences, 1993, , 126-130.	0.3	6
120	Searching for low-band-gap conjugated polymers by LHS calculations. Synthetic Metals, 1992, 50, 537-542.	3.9	4
121	Embedded units in conjugated polymers. Journal of Mathematical Chemistry, 1992, 10, 313-327.	1.5	7
122	An observable-based interpretation of electronic wavefunctions: application to â€œhypervalentâ€• molecules. Computational and Theoretical Chemistry, 1992, 255, 9-33.	1.5	137
123	Monomer geometry relaxation and the basis set superposition error. Chemical Physics Letters, 1992, 191, 497-499.	2.6	113
124	NDDO fragment self-consistent field approximation for large electronic systems. Journal of Computational Chemistry, 1992, 13, 830-837.	3.3	85
125	An ab initio study of the H2O-mediated 1,3-hydrogen rearrangement in the isoelectric series: X, Yâ€,=â€,CH2, NH, or O. Canadian Journal of Chemistry, 1991, 69, 1589-1599.	1.1	15
126	Electronic structure and optical absorption of poly(biisothianaphthene-methine) and poly(isonaphthothiophene-thiophene): two low-band-gap polymers. Journal of the American Chemical Society, 1991, 113, 9865-9867.	13.7	77

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127	Impurity-induced tetramerization in Peierls-distorted polymers: Reducing the band gap. Solid State Communications, 1991, 77, 875-877.	1.9	2
128	On the perturbation operator in ab initio theories of intermolecular interactions. Computational and Theoretical Chemistry, 1991, 226, 39-46.	1.5	5
129	Intermolecular interactions: biorthogonal perturbation theory revisited. Computational and Theoretical Chemistry, 1991, 226, 47-58.	1.5	17
130	Second quantization and exchange perturbation theory for intermolecular interactions. the basis set superposition error problem. Computational and Theoretical Chemistry, 1991, 232, 51-63.	1.5	4
131	Interaction energies between H2O and HXâ€”CH=Y/X=CHâ€”YH for X, Y=CH2, NH or O â€” the chemical Hamiltonian approach. Chemical Physics Letters, 1991, 183, 25-30.	2.6	2
132	Nonlinear schrï¿½dinger equations and intermolecular interactions. Journal of Mathematical Chemistry, 1991, 8, 151-160.	1.5	4
133	Normalization corrections to perturbation theory for the time-independent nonlinear SchrÃ¶dinger equation. Physical Review A, 1991, 44, 2188-2191.	2.5	13
134	Perturbation theoretical vs supermolecule calculations on intermolecular interactions. Acta Physica Hungarica, 1990, 67, 387-400.	0.1	6
135	Computational chemistry on a PC. International Journal of Quantum Chemistry, 1990, 38, 163-171.	2.0	3
136	Quinoid vs aromatic structure of polyisothianaphthene. Journal of Chemical Physics, 1990, 92, 3247-3248.	3.0	49
137	The Two-Electron Bond as a Molecular Building Block. , 1990, , 205-256.		4
138	Improved intermolecularSCFtheory and theBSSEproblem. International Journal of Quantum Chemistry, 1989, 36, 225-240.	2.0	68
139	BSSE-free SCF methods for intermolecular interactions. International Journal of Quantum Chemistry, 1989, 36, 281-290.	2.0	0
140	Second Quantized Approach to Quantum Chemistry. , 1989, , .		94
141	Quinoid-Aromatic Transition in Polythiophene-like Systems. Springer Series in Solid-state Sciences, 1989, , 69-72.	0.3	13
142	Second quantization and the Hellmannâ€”Feynman Theorem: A unified view on energy derivatives. Computational and Theoretical Chemistry, 1988, 170, 1-7.	1.5	6
143	A preliminary ab initio investigation of retinal analogs. Computational and Theoretical Chemistry, 1988, 167, 321-329.	1.5	9
144	The role of hybridization in perturbative bond theories: The existence of exact strictly localized orbitals in small molecules. Computational and Theoretical Chemistry, 1988, 169, 95-104.	1.5	3

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145	Energy, geometry and valence: The influence of sulfur d-orbital exponent. Computational and Theoretical Chemistry, 1988, 165, 297-307.	1.5	16
146	Theoretical estimation of static charge fluctuation in amorphous silicon. Physical Review B, 1988, 37, 9069-9071.	3.2	27
147	Effect of protonation on the ground state properties of retinal analogs: an ab-initio study. Canadian Journal of Chemistry, 1987, 65, 892-897.	1.1	14
148	Connected moments expansion calculations of the correlation energy in small molecules. Chemical Physics Letters, 1987, 138, 516-519.	2.6	22
149	The application of strictly localized geminals to the description of chemical bonds. Journal of Computational Chemistry, 1987, 8, 436-441.	3.3	16
150	Interruption of conjugations of polyacetylene chains. Physical Review B, 1986, 33, 2615-2624.	3.2	63
151	Intermolecular interactions using small basis sets: Perturbation theory calculations avoiding basis set superposition error. Chemical Physics Letters, 1986, 128, 358-362.	2.6	37
152	The use of the mulliken approximation in bond-bond pair potentials describing rotational barriers. Chemical Physics Letters, 1985, 117, 386-388.	2.6	4
153	Second-quantization-based perturbation theory for intermolecular interactions without basis set superposition error. Chemical Physics Letters, 1985, 119, 538-542.	2.6	43
154	Interaction of chemical bonds. II.Ab initiotheory for overlap, delocalization, and dispersion interactions. Physical Review A, 1985, 32, 748-755.	2.5	42
155	Quantum chemical conformational analysis of the catalytic triad in Î±-chymotrypsin. Computational and Theoretical Chemistry, 1985, 123, 85-95.	1.5	14
156	Nitrogen bridgehead compounds. 48. Synthesis and stereochemistry of 4-oxo-1,6,7,8,9,9a-hexahydro-4H-pyrido[1,2-a]pyrimidine-3-carboxamides. Journal of Organic Chemistry, 1985, 50, 2918-2925.	3.2	12
157	Quantum chemical conformational analysis of the catalytic triad in Î±-chymotrypsin. Computational and Theoretical Chemistry, 1985, 24, 85-95.	1.5	0
158	Localization and delocalization. II. Role of overlap in interbond interactions. Journal of Chemical Physics, 1984, 80, 5649-5658.	3.0	40
159	Interaction of chemical bonds: Strictly localized wave functions in orthogonal basis. Physical Review A, 1984, 30, 43-50.	2.5	40
160	Bond orbital approach for optical rotatory strength calculations. Theoretica Chimica Acta, 1983, 63, 43-54.	0.8	7
161	Bond orbital framework for rapid calculation of environmental effects on molecular potential surfaces. Chemical Physics Letters, 1983, 96, 499-501.	2.6	42
162	Electronic transition moments and optical absorption for trans-polyacetylene. Solid State Communications, 1983, 48, 243-247.	1.9	16

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163	Nitrogen bridgehead compounds. Part 32. Absolute configuration and circular dichroism of 6-methyl-tetrahydro-4H-pyrido[1,2-a]pyrimidin-4-ones. Journal of the Chemical Society Perkin Transactions II, 1983, , 1413-1420.	0.9	10
164	Perturbation theory for nonlinear time-independent SchrÃ¶dinger equations. Physical Review A, 1983, 28, 45-48.	2.5	35
165	Ab initionumerical studies on density-matrix asymptotics in extended systems. Physical Review B, 1983, 27, 7583-7588.	3.2	14
166	Localization and delocalization: Distinction between through space and through bond interactions. Journal of Chemical Physics, 1982, 77, 2454-2459.	3.0	55
167	Bondâ€"bond pair potentials describing barrier to rotations around single bonds. Chemical Physics Letters, 1982, 92, 483-485.	2.6	10
168	Conformational analysis by bond orbitals with delocalization corrections: Rotation of the ser-195 side chain in Î±-chymotrypsin. International Journal of Quantum Chemistry, 1982, 22, 929-938.	2.0	13
169	Strictly localized molecular orbitals. Journal of the Chemical Society, Faraday Transactions 2, 1981, 77, 1129-1131.	1.1	28
170	Delocalization corrections to the strictly localized molecular orbitals: A linearized SCF approximation. Theoretica Chimica Acta, 1981, 59, 603-607.	0.8	28
171	Trapping of phase kinks in polyacetylene. Solid State Communications, 1981, 39, 611-614.	1.9	36
172	On Trapping of Phase Kinks in Polyacetylene. Molecular Crystals and Liquid Crystals, 1981, 77, 341-348.	0.8	2
173	Optical rotatory strength calculation by evaluating the gradient matrix through the equation of motion. Theoretica Chimica Acta, 1980, 55, 103-115.	0.8	3