Takashi Kawakami

List of Publications by Year
in descending order

125 papers	2,073 citations	394421 19 h-index	289244 40 g-index
125 all docs	125 docs citations	125 times ranked	2453 citing authors

#	Article	IF	Citations
1	Over 8% efficient CsSnI₃-based mesoporous perovskite solar cells enabled by two-step thermal annealing and surface cationic coordination dual treatment. Journal of Materials Chemistry A, 2022, 10, 3642-3649.	10.3	35
2	Relative energies among S3 intermediates in the photosystem II revealed by DLPNO coupled cluster and hybrid DFT calculations. Possible pathways of water insertion in the S2 to S3 transition. Chemical Physics Letters, 2022, 793, 139439.	2.6	8
3	Higher-order transition state approximation. Journal of Chemical Physics, 2022, 156, 114112.	3.0	6
4	Modeling the Conformational Preference of the Lignocellulose Interface and Its Interaction with Weak Acids. Journal of Physical Chemistry A, 2022, 126, 2119-2126.	2.5	8
5	Searching for a Reliable Density Functional for Moleculeâ€“Environment Interactions, Found B97M-V/def2-mTZVP. Journal of Physical Chemistry A, 2022, 126, 2397-2406.	2.5	10
6	Mechanism of Water Oxidation in Photosynthesis Elucidated by Interplay Between Experiment and Theory. Advances in Photosynthesis and Respiration, 2021, , 39-80.	1.0	0
7	Electron Density-based Estimation of Diradical Character: An Easy Scheme for DFT/Plane-wave Calculations. Chemistry Letters, 2021, 50, 392-396.	1.3	6
8	Magnetic Properties of a Mixed Spin-((1/2,5/2)) Chain in (4-Cl-o-MePy-V)FeCl₄. Journal of the Physical Society of Japan, 2021, 90, 064707.	1.6	4
9	Gibbs Energy of Hydrogen Adsorption on Pt Surface by Machine Learning Potential and Metadynamics. Chemistry Letters, 2021, 50, 1329-1332.	1.3	1
10	An improved Slaterâ€™s transition state approximation. Journal of Chemical Physics, 2021, 155, 034101.	3.0	12
11	Extension of the Linear Response Function of Electron Density to a Plane-wave Basis and the First Application to Periodic Surface Systems. Chemistry Letters, 2021, 50, 1801-1805.	1.3	2
12	Theoretical Study of Proton Tunneling in the Imidazoleâ€“Imidazolium Complex. Journal of Physical Chemistry A, 2021, 125, 6902-6912.	2.5	3
13	Spin-Crossover-Triggered Linkage Isomerization by the Pedal-like Motion of the Azobenzene Ligand in a Neutral Heteroleptic Iron(III) Complex. Inorganic Chemistry, 2021, 60, 12735-12739.	4.0	8
14	DFT Study of Î±-Keggin-type Iso-polyoxotungstate Anions [H_nW₁₂O₄₀]^{(8â€“n)â€“} (n =1â€“4): Can [H₄W₁₂O₄₀]^{4â€“} Exist?. Inorganic Chemistry, 2021, 60, 15336-15342.	4.0	1
15	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	7.4	54
16	On the question of steric repulsionversusnoncovalent attractive interactions in chiral phosphoric acid catalyzed asymmetric reactions. Physical Chemistry Chemical Physics, 2021, 23, 18936-18950.	2.8	10
17	Can we enhance diradical character using interaction with stoichiometric surfaces of ionic oxides? A theoretical investigation using chemical indices. Physical Chemistry Chemical Physics, 2021, 23, 25024-25028.	2.8	8
18	Dynamic Symmetry Conversion in Mixed-Halide Hybrid Perovskite upon Illumination. ACS Energy Letters, 2021, 6, 3858-3863.	17.4	5

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19	Controlling Quantum-Well Width Distribution and Crystal Orientation in Two-Dimensional Tin Halide Perovskites via a Strong Interlayer Electrostatic Interaction. ACS Applied Materials & Interfaces, 2021, 13, 49907-49915.	8.0	13
20	Isolobal and isospin analogy between organic and inorganic open-shell moleculesâ€"Application to oxygenation reactions by active oxygen and oxy-radicals and water oxidation in the native and artificial photosynthesis. Advances in Quantum Chemistry, 2021, , 425-564.	0.8	1
21	Taking Advantage of a Systematic Energy Non-linearity Error in Density Functional Theory for the Calculation of Electronic Energy Levels. Journal of Physical Chemistry A, 2021, 125, 10507-10513.	2.5	5
22	Electron dynamics method using a locally projected group diabatic Fock matrix for molecules and aggregates. Chemical Physics, 2020, 528, 110508.	1.9	1
23	Theoretical Investigation of the Heterojunction Effect on the Catalytic Activity and Selectivity of an Au@NiO Coreâ€"Shell Catalyst in Aerobic Oxidation. Journal of Physical Chemistry C, 2020, 124, 17039-17047.	3.1	7
24	Development of broken-symmetry (BS) methods in chemical reactions. A theoretical view of water oxidation in photosystem II and related systems. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 402, 112791.	3.9	3
25	Core-Level Excitation Energies of Nucleic Acid Bases Expressed as Orbital Energies of the Kohnâ€"Sham Density Functional Theory with Long-Range Corrected Functionals. Journal of Physical Chemistry A, 2020, 124, 10482-10494.	2.5	9
26	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
27	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	3.0	60
28	Clarification of the Relationship between the Magnetic and Conductive Properties of Infinite Chains in Trioxotriangulene Radical Crystals by Spinâ€Projected DFT/Planeâ€Wave Calculations. Advanced Theory and Simulations, 2020, 3, 2000050.	2.8	10
29	Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding. Journal of Chemical Theory and Computation, 2020, 16, 2952-2964.	5.3	19
30	Experimental realization of Lieb-Mattis plateau in a quantum spin chain. Scientific Reports, 2020, 10, 9193.	3.3	13
31	UNO(ULO) active space for multireference calculations on classical and quantum computers. Revisit to the iron-sulfur complexes. Chemical Physics Letters, 2020, 746, 137252.	2.6	2
32	Quantum mechanical/molecular mechanical trajectory surface hopping molecular dynamics simulation by spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2020, 152, 024119.	3.0	8
33	Theory of chemical bonds in metalloenzymes XXIV electronic and spin structures of FeMoco and Fe-S clusters by classical and quantum computing. Molecular Physics, 2020, 118, e1760388.	1.7	5
34	Electronic transport investigation of redox-switching of azulenequinones/hydroquinones via first-principles studies. Physical Chemistry Chemical Physics, 2019, 21, 17859-17867.	2.8	2
35	Comparison of the Hydrogen Bond Interaction Dynamics in the Guanine and Cytosine Crystals: Ab Initio Molecular Dynamics and Spectroscopic Study. Journal of Physical Chemistry A, 2019, 123, 10757-10763.	2.5	8
36	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. Journal of Physical Chemistry B, 2019, 123, 10001-10013.	2.6	18

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37	A Simple Model for Relative Energies of All Fullerenes Reveals the Interplay between Intrinsic Resonance and Structural Deformation Effects in Medium-Sized Fullerenes. Journal of Chemical Theory and Computation, 2019, 15, 1255-1264.	5.3	15
38	Trajectory surface hopping molecular dynamics simulation by spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2019, 150, 204120.	3.0	13
39	Theoretical and computational investigations of geometrical, electronic and spin structures of the CaMn 4 O X (Xâ€‰=â€‰5, 6) cluster in the Kok cycle S i (iâ€‰=â€‰0â€“3) of oxygen evolving complex of photosystem II. Physiologia Plantarum, 2019, 166, 44-59.	5.2	14
40	Theoretical study of correlations between the coordination structures and catalytic activities in polymerâ€stabilized au nanocluster catalysts. Journal of Computational Chemistry, 2019, 40, 222-228.	3.3	9
41	UNO DMRG CAS CI calculations of binuclear manganese complex Mn(IV) 2 O 2 (NHCHCO 2) 4 : Scope and applicability of Heisenberg model. Journal of Computational Chemistry, 2019, 40, 333-341.	3.3	16
42	Free energy reaction root mapping of alanine tripeptide in water. Molecular Physics, 2019, 117, 2284-2292.	1.7	4
43	A path integral molecular dynamics study on intermolecular hydrogen bond of acetic acidâ€“arsenic acid anion and acetic acidâ€“phosphoric acid anion clusters. Journal of Computational Chemistry, 2019, 40, 172-180.	3.3	3
44	Au Atom Diffusions on Reduced and Cl-Adsorbed Rutile TiO₂(110) Surfaces: A DFT + <i>U</i> Study. E-Journal of Surface Science and Nanotechnology, 2018, 16, 267-273.	0.4	3
45	High-throughput screening of perovskite oxynitride and oxide materials for visible-light photocatalysis. APL Materials, 2018, 6, .	5.1	14
46	Theoretical Investigation of Surface Oxidation of NiO/Au Core-Shell Catalyst. E-Journal of Surface Science and Nanotechnology, 2018, 16, 242-246.	0.4	5
47	Theoretical study on mesoscopic-size impurity effects in the charge separation process of organic photocells. Physical Chemistry Chemical Physics, 2018, 20, 14846-14854.	2.8	1
48	Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in PhotosystemÂII. Journal of Physical Chemistry B, 2018, 122, 6491-6502.	2.6	21
49	MPI/OpenMP hybrid parallel algorithm for resolution of identity secondâ€order MÃ¸llerâ€“Plesset perturbation calculation of analytical energy gradient for massively parallel multicore supercomputers. Journal of Computational Chemistry, 2017, 38, 489-507.	3.3	1
50	Theoretical Clarification of the Coexistence of Cl Effects on Au/TiO2: The Interaction between Au Clusters and the TiO2 Surface, and the Aggregation of Au Clusters on the TiO2 Surface. Bulletin of the Chemical Society of Japan, 2017, 90, 506-519.	3.2	18
51	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. Molecular Physics, 2017, 115, 2154-2167.	1.7	2
52	Discovery of Pb-Free Perovskite Solar Cells via High-Throughput Simulation on the K Computer. Journal of Physical Chemistry Letters, 2017, 8, 4826-4831.	4.6	134
53	Can Electron-Rich Oxygen (O^{2â€“}) Withdraw Electrons from Metal Centers? A DFT Study on Oxoanion-Caged Polyoxometalates. Journal of Physical Chemistry A, 2017, 121, 7684-7689.	2.5	2
54	Correlation effects beyond coupled cluster singles and doubles approximation through Fock matrix dressing. Journal of Chemical Physics, 2017, 147, 204108.	3.0	7

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55	Theoretical Investigation for Heterojunction Effects in Polymer-stabilized Au Nanocluster Catalysis: Difference in Catalytic Activity between Au:PVP and Au:PAA. Chemistry Letters, 2016, 45, 344-346.	1.3	10
56	Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers. Journal of Computational Chemistry, 2016, 37, 2623-2633.	3.3	22
57	Theoretical study on spin-forbidden transitions of osmium complexes by two-component relativistic time-dependent density functional theory. Chemical Physics Letters, 2016, 648, 60-65.	2.6	9
58	Theoretical Study of Electronic Properties of Phenalenyl Radical and Zethrene Diradical Species: Possibility of Triplet Oxygen Adsorption onto Graphene Surface. Bulletin of the Chemical Society of Japan, 2015, 88, 149-161.	3.2	8
59	Theoretical Investigation on the Au-Anchor Site in Phosphate-Doped Au/Al₂O₃Catalysts. E-Journal of Surface Science and Nanotechnology, 2015, 13, 380-384.	0.4	6
60	First principle calculations of effective exchange integrals: Comparison between SR (BS) and MR computational results. , 2015, , .		0
61	NTChem: A highâ€performance software package for quantum molecular simulation. International Journal of Quantum Chemistry, 2015, 115, 349-359.	2.0	55
62	Theoretical investigation of enantioselectivity of cage-like supramolecular assembly: The insights into the shape complementarity and host-guest interaction. Journal of Computational Chemistry, 2015, 36, 459-466.	3.3	15
63	Gaussian-based cutoff scheme on Hartreeâ€“Fock exchange term of dielectric-dependent potential. Chemical Physics Letters, 2015, 634, 83-87.	2.6	5
64	Two-component relativistic time-dependent density functional theory study on spin-forbidden transitions for metal polypyridyl complexes. Chemical Physics Letters, 2015, 635, 152-156.	2.6	9
65	Computational Study of Catalytic Reaction of Quercetin 2,4-Dioxygenase. Journal of Physical Chemistry B, 2015, 119, 6952-6962.	2.6	16
66	Theoretical study of exciton dissociation through hot states at donorâ€“acceptor interface in organic photocell. Physical Chemistry Chemical Physics, 2015, 17, 12538-12544.	2.8	14
67	DFT calculations for Au adsorption onto a reduced TiO₂(110) surface with the coexistence of Cl. Molecular Physics, 2014, 112, 365-378.	1.7	15
68	DFT calculations for aerobic oxidation of alcohols over neutral Au6cluster. Molecular Physics, 2014, 112, 385-392.	1.7	13
69	Fine-Tuning of Magnetic Interactions in Organic Spin Ladders. Journal of the Physical Society of Japan, 2014, 83, 033707.	1.6	28
70	Theoretical investigation for the stability of the concaveâ€bound cyclopentadienyl iron complex of sumanene. International Journal of Quantum Chemistry, 2013, 113, 437-442.	2.0	7
71	Two-Dimensional Honeycomb Lattice Consisting of a New Organic Radical 2-Cl-6-F-V. Journal of the Physical Society of Japan, 2013, 82, 043713.	1.6	23
72	Theory of chemical bonds in metalloenzymes. XVII. Symmetry breaking in manganese cluster structures and chameleonic mechanisms for the Oï£¿O bond formation of water splitting reaction. International Journal of Quantum Chemistry, 2012, 112, 121-135.	2.0	21

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73	Theoretical studies on the structural and magnetic property of arginase active site. Supramolecular Chemistry, 2011, 23, 22-28.	1.2	3
74	Theoretical study of absorption spectrum of dirhodium tetracarboxylate complex [Rh2(CH3COO)4(H2O)2] in aqueous solution revisited. Supramolecular Chemistry, 2011, 23, 329-336.	1.2	7
75	Modification of MOF catalysts by manipulation of counter-ions: experimental and theoretical studies of photochemical hydrogen production from water over microporous diruthenium (II, III) coordination polymers. Supramolecular Chemistry, 2011, 23, 287-296.	1.2	32
76	Ab initio study of magnetic interactions of manganese-oxide clusters. Polyhedron, 2011, 30, 3256-3261.	2.2	18
77	Singletâ€“triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. Theoretical Chemistry Accounts, 2011, 130, 739-748.	1.4	30
78	Symmetry and broken symmetry in molecular orbital description of unstable molecules IV: comparison between single- and multi-reference computational results for antiaromtic molecules. Theoretical Chemistry Accounts, 2011, 130, 749-763.	1.4	40
79	Theoretical studies on the electronic structure of the synthetic complex of soluble methanemonooxygenase intermediate Q. Supramolecular Chemistry, 2011, 23, 83-87.	1.2	2
80	UNOâ€•and ULOâ€MRCC(Mk), APâ€UCC and APâ€UBD approaches to diradical systems. International Journal of Quantum Chemistry, 2010, 110, 3015-3026.	2.0	15
81	Theory of chemical bonds in metalloenzymes. XV. Local singlet and triplet diradical mechanisms for radical coupling reactions in the oxygen evolution complex. International Journal of Quantum Chemistry, 2010, 110, 3101-3128.	2.0	49
82	Theory of chemical bonds in metalloenzymes. XIV. Correspondence between magnetic coupling mode and radical coupling mechanism in hydroxylations with methane monooxygenase and related species. International Journal of Quantum Chemistry, 2010, 110, 2955-2981.	2.0	15
83	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. Molecular Physics, 2010, 108, 2533-2541.	1.7	10
84	MkMRCC, APUCC and APUBD approaches to 1,n-didehydropolyene diradicals: the nature of through-bond exchange interactions. Molecular Physics, 2010, 108, 2559-2578.	1.7	11
85	BS DFT and BS HDFT studies of Crï£¿Cr sextuple bond from the viewpoint of electron correlation effects. International Journal of Quantum Chemistry, 2009, 109, 3315-3324.	2.0	9
86	Estimation of effective exchange integral value of polyradical systems based on the band calculation. International Journal of Quantum Chemistry, 2009, 109, 3632-3640.	2.0	5
87	Approximately spinâ€projected Hessian for broken symmetry method and stretching frequencies of F₂ and singlet O₂. International Journal of Quantum Chemistry, 2009, 109, 3641-3648.	2.0	11
88	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. International Journal of Quantum Chemistry, 2009, 109, 3649-3658.	2.0	10
89	Theory of chemical bonds in metalloenzymes. VII. Hybridâ€density functional theory studies on the electronic structures of P450. International Journal of Quantum Chemistry, 2008, 108, 631-650.	2.0	20
90	DFT study for the heterojunction effect in the precious metal clusters. International Journal of Quantum Chemistry, 2008, 108, 2888-2895.	2.0	3

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91	Theory of chemical bonds in metalloenzymes XI: Full geometry optimization and vibration analysis of porphyrin ironâ€oxo species. International Journal of Quantum Chemistry, 2008, 108, 2950-2965.	2.0	6
92	Density functional study of manganese dimer. International Journal of Quantum Chemistry, 2007, 107, 3178-3190.	2.0	21
93	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. Molecular Crystals and Liquid Crystals, 2006, 455, 135-141.	0.9	1
94	Possibilities of molecule-based spintoronics of DNA wires, sheets, and related materials. International Journal of Quantum Chemistry, 2005, 105, 655-671.	2.0	9
95	Theoretical studies on magnetic interaction in one-dimensional spin chains of hydrogen atoms (Hn) and copper bromide (CunBrm). International Journal of Quantum Chemistry, 2004, 100, 907-917.	2.0	9
96	N-band Hubbard models II: Cooperative mechanisms of electron-phonon, electron correlation, and many-band effects toward high-Tc superconductors. International Journal of Quantum Chemistry, 2003, 92, 47-70.	2.0	11
97	Theoretical Studies on Magnetic Interactions of Aligned Tetrametal System by Using Hybrid Density Functional Method. Molecular Crystals and Liquid Crystals, 2002, 376, 347-352.	0.9	1
98	Theoretical Studies on Magnetic Interactions of Aligned Tetrametal Systems by Using Magnetic Effective Density Functional (MEDF) Method. Molecular Crystals and Liquid Crystals, 2002, 379, 525-530.	0.9	7
99	Field-induced Superconductivity. Molecular Crystals and Liquid Crystals, 2002, 379, 495-500.	0.9	0
100	Theoretical Studies with Ï€-Râ€¢ Cluster Models for Pure Organomagnetic Conductors. Molecular Crystals and Liquid Crystals, 2002, 379, 483-488.	0.9	3
101	Theoretical Studies on Magnetic Couplings of M-Ï€ Conjugated Systems via Pyrimidine Coupler. Molecular Crystals and Liquid Crystals, 2002, 379, 531-536.	0.9	1
102	Theoretical Studies on Ï€- d Magnetic Interactions Between BETS Donor and Transition Metal Halides in Î²-BETS 2 MX 4 Crystals. Molecular Crystals and Liquid Crystals, 2002, 379, 489-494.	0.9	1
103	Theoretical Studies on SDW and CDW States of Cu and Ag Oxides under the Periodic Boundary Condition. Molecular Crystals and Liquid Crystals, 2002, 379, 513-518.	0.9	0
104	Theoretical investigation of magnetic parameters in two-dimensional sheets of pure organic BEDT-TTF and BETS molecules by usingab initioMO and DFT methods. Molecular Physics, 2002, 100, 2641-2652.	1.7	14
105	Instability of a system and its estimation in terms of the hybrid density functional theory method: a magnetic effective density functional (MEDF) approach. Molecular Physics, 2002, 100, 1829-1838.	1.7	26
106	Antiferromagnetic coupling of transition metal spins across pyrimidine and pyrazine bridges in dinuclear manganese(ii), cobalt(ii), nickel(ii) and copper(ii) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate complexes. Dalton Transactions RSC, 2002, , 3177-3186.	2.3	91
107	Theoretical Studies on Magnetic Properties of TCNQ Organic Crystals with Ab initio and DFT Methods. Molecular Crystals and Liquid Crystals, 2002, 376, 411-416.	0.9	0
108	Analytical and ab initio studies of effective exchange interactions, polyradical character, unpaired electron density, and information entropy in radical clusters (R)N: Allyl radical cluster (N=2-10) and hydrogen radical cluster (N=50). International Journal of Quantum Chemistry, 2002, 90, 370-385.	2.0	122

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109	Theoretical studies on field-induced superconductivity in molecular crystals. International Journal of Quantum Chemistry, 2001, 85, 608-618.	2.0	9
110	Possibilities of molecular magnetic metals and highTc superconductors in field effect transistor configurations. International Journal of Quantum Chemistry, 2001, 85, 619-635.	2.0	10
111	Theoretical Studies of the Pressure Effects for Î²-Phase of p-NPNN. Molecular Crystals and Liquid Crystals, 1999, 335, 623-632.	0.3	3
112	Theoretical Studies of Magnetic Interactions in 3â€², 5â€²-Dihydroxyphenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1999, 335, 633-642.	0.3	1
113	Theoretical Studies of Intra- and Inter- Magnetic Interactions in TMAO(1,3,5,7 - Tetramethyl - 2, 6-) Tj ETQq1 1 0.784314 rgBT /Overlo	0.3	2
114	Path integral method by means of generalized coherent states and its numerical approach to molecular systems. I. Ensemble average of total energy. Journal of Chemical Physics, 1997, 107, 6283-6289.	3.0	9
115	Theoretical Studies of Magnetic Interactions in 2â€², 5â€²-Dihydroxyphenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1997, 306, 151-160.	0.3	9
116	Theoretical Studies of Magnetic Interactions in P-Cyanophenyl Nitronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1997, 306, 331-338.	0.3	4
117	Solid State ¹H-Mas-Nmr and Spin Densities on Protons of the Organic Ferromagnetic Tempo Derivatives. Molecular Crystals and Liquid Crystals, 1997, 306, 307-314.	0.3	7
118	Magnetic Interaction Via Î²-Hydrogen Atoms in Tempo Derivatives. Molecular Crystals and Liquid Crystals, 1997, 306, 141-150.	0.3	16
119	Calculation of Magnetization by Path Integral Method II. Molecular Crystals and Liquid Crystals, 1996, 286, 177-184.	0.3	4
120	Calculation of Magnetization by Path Integral Method I. Molecular Crystals and Liquid Crystals, 1996, 286, 171-176.	0.3	4
121	Theoretical Calculation of Effective Exchange Integrals for One-and Two-Dimensional Poly(Phenylenemethylene) Systems. Possibilities of Organic Ferro-and Ferri-Magnetic Solids. Molecular Crystals and Liquid Crystals, 1996, 279, 9-18.	0.3	9
122	Theoretical Studies of the Ferromagnetic Inter-Molecular Interaction of P-Carboxylate Phenyl Nitronyl Nitroxide. Molecular Crystals and Liquid Crystals, 1996, 279, 29-38.	0.3	11
123	Theoretical Studies of Spin Populations on Nitronyl Nitroxide, Phenyl Nitronyl Nitroxide and P-NPNN. Molecular Crystals and Liquid Crystals, 1995, 271, 19-28.	0.3	2
124	Theoretical Approaches to Molecular Magnetism II: No-Overlap and Orientation Principles for Ferromagnetic Interactions. Molecular Crystals and Liquid Crystals, 1995, 272, 117-129.	0.3	8
125	QM/MM study of hydrolysis of arginine catalysed by arginase. Molecular Physics, 0, , 1-9.	1.7	4