ArtÃ«m E Masunov

List of Publications by Year
in descending order

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149 papers	5,565 citations	57758 44 h-index	95266 68 g-index
152 all docs	152 docs citations	152 times ranked	6794 citing authors

#	Article	IF	Citations
1	Influence of Binary Diffusion Coefficients on Supercritical CO2Flame Characteristics of Methane/Natural Gas. , 2022, , .		0
2	Direct measurement of reaction rate for decomposition of diisopropyl methylphosphonate at high temperature using shock tube and laser absorption. International Journal of Chemical Kinetics, 2022, 54, 371-380.	1.6	5
3	Prediction of Crystal Structures and Mechanical Properties for Brittle, Plastic, and Elastic Polymorphs of 4-Bromophenyl 4-Bromobenzoate. Crystal Growth and Design, 2022, 22, 4546-4558.	3.0	3
4	How Many Isomers Do Metallic Clusters Have? Case of Magnesium Clusters of up to 55 Atoms. Journal of Physical Chemistry A, 2021, 125, 6543-6555.	2.5	3
5	Pseudocyclic Form of 4-Hydroxypyrrolidine-2-carboxanilide Podands with Trioxyethylene Chain: Modeling, Conformational Search, and NMR Analysis. Journal of Physical Chemistry A, 2021, 125, 6029-6041.	2.5	5
6	DMMP pyrolysis and oxidation studies at high temperature inside a shock tube using laser absorption measurements of CO. Combustion and Flame, 2020, 214, 14-24.	5.2	21
7	Virtual Tensile Test for Brittle, Plastic, and Elastic Polymorphs of 4-Bromophenyl 4-Bromobenzoate. Crystal Growth and Design, 2020, 20, 6093-6100.	3.0	9
8	High accuracy machine learning identification of fentanyl-relevant molecular compound classification via constituent functional group analysis. Scientific Reports, 2020, 10, 13569.	3.3	9
9	Three-Photon Spectroscopy of Porphyrins. Journal of Physical Chemistry A, 2020, 124, 11038-11050.	2.5	9
10	Global Structure Optimization of Pt Clusters Based on the Modified Empirical Potentials, Calibrated using Density Functional Theory. Journal of Physical Chemistry C, 2019, 123, 29024-29036.	3.1	16
11	Molecular dynamics of combustion reactions in supercritical carbon dioxide. Part 4: boxed MD study of formyl radical dissociation and recombination. Journal of Molecular Modeling, 2019, 25, 35.	1.8	6
12	Electronic Nature of Neutral and Charged Two-Photon Absorbing Squaraines for Fluorescence Bioimaging Application. ACS Omega, 2019, 4, 14669-14679.	3.5	19
13	Oxyphor 2P: A High-Performance Probe for Deep-Tissue Longitudinal Oxygen Imaging. Cell Metabolism, 2019, 29, 736-744.e7.	16.2	105
14	Molecular Dynamics of Combustion Reactions in Supercritical Carbon Dioxide. Part 5: Computational Study of Ethane Dissociation and Recombination Reactions C₂H₆ â‡Œ CH₃ + CH₃. Journal of Physical Chemistry A, 2019, 123, 4776-4784.	2.5	6
15	Theoretical Calculation of Reaction Rates and Combustion Kinetic Modeling Study of Triethyl Phosphate (TEP). Journal of Physical Chemistry A, 2019, 123, 4764-4775.	2.5	15
16	Molecular Dynamics of Combustion Reactions in Supercritical Carbon Dioxide. 6. Computational Kinetics of Reactions between Hydrogen Atom and Oxygen Molecule H + O₂ â‡Œ HO + O and H + O₂ â‡Œ HO₂. Journal of Physical Chemistry A, 2019, 123, 10772-10781.	2.5	7
17	Cover Image, Volume 51, Issue 1. International Journal of Chemical Kinetics, 2019, 51, i.	1.6	0
18	Quantum chemical and master equation study of OH + CH₂O â†’ H₂O + CHO reaction rates in supercritical CO₂ environment. International Journal of Chemical Kinetics, 2019, 51, 42-48.	1.6	12

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19	Theoretical study of chromophores for biological sensing: Understanding the mechanism of rhodol based multi-chromophoric systems. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 198, 123-135.	3.9	1
20	Molecular Dynamics Study of Combustion Reactions in Supercritical Environment. Part 3: Boxed MD Study of CH₃ + HO₂ â†' CH₃O + OH Reaction Kinetics. Journal of Physical Chemistry A, 2018, 122, 3337-3345.	2.5	6
21	Molecular Dynamics Study of Combustion Reactions in a Supercritical Environment. Part 2: Boxed MD Study of CO + OH â†' CO₂ + H Reaction Kinetics. Journal of Physical Chemistry A, 2018, 122, 897-908.	2.5	12
22	Sarin simulants combustion at high temperature: Time-resolved laser absorption spectroscopy of intermediate products in a shock tube. , 2018, , .		0
23	Tuning structures and emissive properties in a series of Zn(<scp>ii</scp>) and Cd(<scp>ii</scp>) coordination polymers containing dicarboxylic acids and nicotinamide pillars. CrystEngComm, 2018, 20, 432-447.	2.6	22
24	Shock Tube/Laser Absorption and Kinetic Modeling Study of Triethyl Phosphate Combustion. Journal of Physical Chemistry A, 2018, 122, 3829-3836.	2.5	23
25	Nonlinear Optical Properties of Mixed Oxide Crystals CsNbMoO₆ and CsTaMoO₆: A Periodic CPHF/KS Study. Journal of Physical Chemistry C, 2018, 122, 24907-24916.	3.1	1
26	First-Principles Crystal Engineering of Nonlinear Optical Materials. II. Effect of Halogen Bonds on the Structure and Properties of Triiodobenzenes. Journal of Physical Chemistry C, 2018, 122, 22622-22631.	3.1	14
27	Catalytic Effect of Carbon Dioxide on Reaction OH + CO â†' H + CO₂ in Supercritical Environment: Master Equation Study. Journal of Physical Chemistry A, 2018, 122, 6355-6359.	2.5	11
28	Toward First-Principles Design of Organic Nonlinear Optical Materials: Crystal Structure Prediction and Halogen Bonding Impact on Hyperpolarizabilities of 2-Iodo-3-hydroxypyridine. Crystal Growth and Design, 2018, 18, 5069-5079.	3.0	22
29	Quantum Chemical Study of Supercritical Carbon Dioxide Effects on Combustion Kinetics. Journal of Physical Chemistry A, 2017, 121, 3728-3735.	2.5	19
30	Linear photophysics, two-photon absorption and femtosecond transient absorption spectroscopy of styryl dye bases. Journal of Luminescence, 2017, 183, 360-367.	3.1	10
31	Raman spectroscopy and theoretic study of hyperpolarizability effect in diiodobutenylâ€bisâ€thioquinolinium triiodide at low temperature. Journal of Raman Spectroscopy, 2017, 48, 1411-1413.	2.5	16
32	High temperature shock tube experiments and kinetic modeling study of diisopropyl ketone ignition and pyrolysis. Combustion and Flame, 2017, 177, 207-218.	5.2	33
33	Products and Pathways of Aldehydes Oxidation in the Negative Temperature Coefficient Region. Journal of Energy Resources Technology, Transactions of the ASME, 2017, 139, .	2.3	11
34	Quantum Chemical Study of CH₃ + O₂ Combustion Reaction System: Catalytic Effects of Additional CO₂ Molecule. Journal of Physical Chemistry A, 2017, 121, 5681-5689.	2.5	18
35	Stabilizing g-States in Centrosymmetric Tetrapyrroles: Two-Photon-Absorbing Porphyrins with Bright Phosphorescence. Journal of Physical Chemistry A, 2017, 121, 6243-6255.	2.5	22
36	First principles crystal engineering of nonlinear optical materials. I. Prototypical case of urea. Journal of Chemical Physics, 2017, 146, 244104.	3.0	16

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37	Chemical Reaction CO+OH^{â€¢} â†’ CO₂+H^{â€¢} Autocatalyzed by Carbon Dioxide: Quantum Chemical Study of the Potential Energy Surfaces. Journal of Physical Chemistry A, 2016, 120, 6023-6028.	2.5	26
38	Combustion of Aldehydes in the Negative Temperature Coefficient Region: Products and Pathways. , 2016, , .		0
39	Linear Photophysics and Femtosecond Nonlinear Spectroscopy of a Star-Shaped Squaraine Derivative with Efficient Two-Photon Absorption. Journal of Physical Chemistry C, 2016, 120, 11099-11110.	3.1	33
40	Molecular Dynamics Study of Combustion Reactions in a Supercritical Environment. Part 1: Carbon Dioxide and Water Force Field Parameters Refitting and Critical Isotherms of Binary Mixtures. Energy & Fuels, 2016, 30, 9622-9627.	5.1	17
41	Potential Energy Surfaces for the Reactions of HO₂ Radical with CH₂O and HO₂ in CO₂ Environment. Journal of Physical Chemistry A, 2016, 120, 7681-7688.	2.5	17
42	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
43	Two-Photon Absorbing Phosphorescent Metalloporphyrins: Effects of Ï€-Extension and Peripheral Substitution. Journal of the American Chemical Society, 2016, 138, 15648-15662.	13.7	55
44	New Two-Photon Absorbing BODIPY-Based Fluorescent Probe: Linear Photophysics, Stimulated Emission, and Ultrafast Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 14317-14329.	3.1	30
45	From pink to blue and back to pink again: changing the Co(<scp>ii</scp>) ligation in a two-dimensional coordination network upon desolvation. CrystEngComm, 2016, 18, 384-389.	2.6	14
46	Aqueous medium induced optical transitions in cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2015, 17, 6217-6221.	2.8	13
47	Symmetry-Breaking in Cationic Polymethine Dyes: Part 2. Shape of Electronic Absorption Bands Explained by the Thermal Fluctuations of the Solvent Reaction Field. Journal of Physical Chemistry A, 2015, 119, 6807-6815.	2.5	39
48	Heisenberg coupling constant predicted for molecular magnets with pairwise spin-contamination correction. Journal of Magnetism and Magnetic Materials, 2015, 396, 222-227.	2.3	3
49	Atomistic mechanism of polyphenol amyloid aggregation inhibitors: molecular dynamics study of Curcumin, Exifone, and Myricetin interaction with the segment of tau peptide oligomer. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1399-1411.	3.5	53
50	Robust Packing Patterns and Luminescence Quenching in Mononuclear [Cu(II)(phen)₂] Sulfates. Journal of Physical Chemistry C, 2014, 118, 30087-30100.	3.1	31
51	Full length amylin oligomer aggregation: insights from molecular dynamics simulations and implications for design of aggregation inhibitors. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1651-1669.	3.5	18
52	Structure and properties of cerium oxides in bulk and nanoparticulate forms. Journal of Alloys and Compounds, 2014, 584, 199-208.	5.5	79
53	Adsorption of Glyoxal (CHOCHO) and Its UV Photolysis Products on the Surface of Atmospheric Ice Nanoparticles. DFT and Density Functional Tight-Binding Study. Journal of Physical Chemistry C, 2014, 118, 7398-7413.	3.1	21
54	The Atomic Level Interaction of Polyphenols with the AÎ² Oligomer Aggregate, A Molecular Dynamic Guidance for Rational Drug Design. , 2014, , 59-70.		1

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55	Mechanism of Nonlinear Optical Enhancement and Supramolecular Isomerism in 1D Polymeric Zn(II) and Cd(II) Sulfates with Pyridine-4-aldoxime Ligands. Journal of Physical Chemistry C, 2014, 118, 9217-9227.	3.1	25
56	Polymeric Luminescent Zn(II) and Cd(II) Dicarboxylates Decorated by Oxime Ligands: Tuning the Dimensionality and Adsorption Capacity. Crystal Growth and Design, 2014, 14, 3935-3948.	3.0	32
57	Predictions of the Spin Configuration in Mn₁₂ Molecular Magnets Made Accurate with the Help of Hubbard U on the Ligand Atoms. Journal of Physical Chemistry C, 2014, 118, 20605-20612.	3.1	5
58	Molecular Packing in Organic Solar Cell Materials: Insights from the Emission Line Shapes of P3HT/PCBM Polymer Blend Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 19975-19984.	3.1	21
59	Design and Electronic Structure of New Styryl Dye Bases: Steady-State and Time-Resolved Spectroscopic Studies. Journal of Physical Chemistry A, 2014, 118, 4502-4509.	2.5	15
60	Two-Photon Absorption Spectra Predicted by Semiempirical Methods. Journal of Computational and Theoretical Nanoscience, 2014, 11, 2208-2220.	0.4	5
61	Enhanced Intersystem Crossing Rate in Polymethine-Like Molecules: Sulfur-Containing Squaraines versus Oxygen-Containing Analogues. Journal of Physical Chemistry A, 2013, 117, 2333-2346.	2.5	44
62	Comparison of TD-DFT Methods for the Calculation of Two-Photon Absorption Spectra of Oligophenylvinylenes. Journal of Physical Chemistry C, 2013, 117, 18170-18189.	3.1	68
63	Permanent dipole moments and energies of excited states from density functional theory compared with coupled cluster predictions: Case of para-nitroaniline. Computational and Theoretical Chemistry, 2013, 1019, 23-32.	2.5	10
64	Design of a New Optical Material with Broad Spectrum Linear and Two-Photon Absorption and Solvatochromism. Journal of Physical Chemistry C, 2013, 117, 23133-23147.	3.1	48
65	Preparation, Characterization, and Electronic Structure of Asymmetric Isonaphthalimide: Mechanism of Dual Fluorescence in Solid State. Journal of Physical Chemistry C, 2013, 117, 18154-18162.	3.1	13
66	New acentric materials constructed from aminopyridines and 4-nitrophenol. CrystEngComm, 2013, 15, 4700.	2.6	58
67	From discrete molecules to one-dimensional coordination polymers containing Mn(II), Zn(II) or Cd(II) pyridine-2-aldoxime building unit. Polyhedron, 2013, 60, 140-150.	2.2	26
68	Supramolecular step in design of nonlinear optical materials: Effect of Ï€â€¦Ï€ stacking aggregation on hyperpolarizability. Journal of Chemical Physics, 2013, 139, 094310.	3.0	77
69	Two-Photon Absorption Spectrum of a Single Crystal Cyanine-like Dye. Journal of Physical Chemistry Letters, 2012, 3, 1222-1228.	4.6	27
70	Quantum Chemical Study of the Initial Step of Ozone Addition to the Double Bond of Ethylene. Journal of Physical Chemistry A, 2012, 116, 10420-10434.	2.5	50
71	Solitonic waves in polyene dications and principles of charge carrier localization in Ï€â€conjugated organic materials. International Journal of Quantum Chemistry, 2012, 112, 2659-2667.	2.0	8
72	Alternative packing modes leading to amyloid polymorphism in five fragments studied with molecular dynamics. Biopolymers, 2012, 98, 131-144.	2.4	20

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74	Density functional theory study of small nickel clusters. Journal of Molecular Modeling, 2012, 18, 783-790.	1.8	36
75	Controlling the aggregation and rate of release in order to improve insulin formulation: molecular dynamics study of full-length insulin amyloid oligomer models. Journal of Molecular Modeling, 2012, 18, 1129-1142.	1.8	33
76	Theoretical Study of Photochromic Compounds: Part 3. Prediction of Thermal Stability. Journal of Physical Chemistry C, 2011, 115, 10292-10297.	3.1	55
77	Mechanism of Nitric Oxide Oxidation Reaction (2NO + O₂ â†' 2NO₂) Revisited. Journal of Chemical Theory and Computation, 2011, 7, 2021-2024.	5.3	45
78	Crystal Morphology as an Evidence of Supramolecular Organization in Adducts of 1,2-Bis(chloromercurio)tetrafluorobenzene with Organic Esters. Crystal Growth and Design, 2011, 11, 3964-3978.	3.0	17
79	Efficient Photochromic Transformation of a New Fluorenyl Diarylethene: One- and Two-Photon Absorption Spectroscopy. ACS Applied Materials & Interfaces, 2011, 3, 3559-3567.	8.0	23
80	Near-field enhancement of infrared intensities for f-f transitions in Er3+ ions close to the surface of silicon nanoparticles. Journal of Molecular Modeling, 2011, 17, 423-428.	1.8	6
81	Can molecular dynamics simulations assist in design of specific inhibitors and imaging agents of amyloid aggregation? Structure, stability and free energy predictions for amyloid oligomers of VQIVYK, MVGGVV and LYQLEN. Journal of Molecular Modeling, 2011, 17, 2423-2442.	1.8	19
82	Dissociation curves and binding energies of diatomic transition metal carbides from density functional theory. International Journal of Quantum Chemistry, 2011, 111, 4276-4287.	2.0	11
83	Molecular dynamic simulation of wild type and mutants of the polymorphic amyloid NNQNTF segments of elk prion: Structural stability and thermodynamic of association. Biopolymers, 2011, 95, 573-590.	2.4	33
84	Insight into how molecular structures of thiophene-based conjugated polymers affect crystallization behaviors. Polymer, 2011, 52, 2302-2309.	3.8	58
85	Fluorene-Based Metal-Ion Sensing Probe with High Sensitivity to Zn²⁺ and Efficient Two-Photon Absorption. Journal of Physical Chemistry B, 2010, 114, 9313-9321.	2.6	53
86	Are density functional theory predictions of the Raman spectra accurate enough to distinguish conformational transitions during amyloid formation?. Journal of Molecular Modeling, 2010, 16, 1093-1101.	1.8	8
87	Density functional study of oxygen vacancy formation and spin density distribution in octahedral ceria nanoparticles. Journal of Molecular Modeling, 2010, 16, 1617-1623.	1.8	22
88	Phosphate ester hydrolysis of biologically relevant molecules by cerium oxide nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2010, 6, 738-744.	3.3	171
89	Understanding oxygen vacancy migration and clustering in barium strontiumcobalt iron oxide. Solid State Ionics, 2010, 181, 1067-1073.	2.7	25
90	Natural polyphenols as inhibitors of amyloid aggregation. Molecular dynamics study of GNNQQNY heptapeptide decamer. Biophysical Chemistry, 2010, 149, 12-21.	2.8	47

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91	Theoretical spectroscopy of carbocyanine dyes made accurate by frozen density correction to excitation energies obtained by TDâ€DFT. International Journal of Quantum Chemistry, 2010, 110, 3095-3100.	2.0	36
92	Theory and computations of two-photon absorbing photochromic chromophores. European Journal of Chemistry, 2010, 1, 142-161.	0.6	16
93	Effective Generation of Triplet States and Singlet Oxygen by Sulfur-Containing Squaraines: Experimental and Theoretical Study. , 2010, , .		0
94	Two-photon Absorption in Single Crystals of Cyanine-like Dye. , 2010, , .		1
95	Near-Unity Quantum Yields for Intersystem Crossing and Singlet Oxygen Generation in Polymethine-like Molecules: Design and Experimental Realization. Journal of Physical Chemistry Letters, 2010, 1, 2354-2360.	4.6	62
96	Tuning Hydrated Nanoceria Surfaces: Experimental/Theoretical Investigations of Ion Exchange and Implications in Organic and Inorganic Interactions. Langmuir, 2010, 26, 7188-7198.	3.5	35
97	Weak antiferromagnetic coupling in molecular ring is predicted correctly by density functional theory plus Hubbard U. Journal of Chemical Physics, 2010, 132, 244104.	3.0	11
98	Thermally controlled preferential molecular aggregation state in a thiacarbocyanine dye. Journal of Chemical Physics, 2010, 133, 134508.	3.0	20
99	Predictions of Two Photon Absorption Profiles Using Time-Dependent Density Functional Theory Combined with SOS and CEO Formalisms. Lecture Notes in Computer Science, 2009, , 179-188.	1.3	1
100	Theoretical study of photochromic compounds, part 2: Thermal mechanism for byproduct formation and fatigue resistance of diarylethenes used as data storage materials. International Journal of Quantum Chemistry, 2009, 109, 3711-3722.	2.0	66
101	Symmetry breaking in cationic polymethine dyes, part 1: Ground state potential energy surfaces and solvent effects on electronic spectra of streptocyanines. International Journal of Quantum Chemistry, 2009, 109, 3592-3601.	2.0	29
102	Computational search for nonlinear optical materials: are polarization functions important in the hyperpolarizability predictions of molecules and aggregates?. Mendeleev Communications, 2009, 19, 311-313.	1.6	40
103	Electronic Properties of a New Two-Photon Absorbing Fluorene Derivative: The Role of Hartreeâ€“Fock Exchange in the Density Functional Theory Design of Improved Nonlinear Chromophores. Journal of Physical Chemistry C, 2009, 113, 20719-20724.	3.1	49
104	Quantum Chemical Study of Trimolecular Reaction Mechanism between Nitric Oxide and Oxygen in the Gas Phase. Journal of Physical Chemistry A, 2009, 113, 9092-9101.	2.5	42
105	Theoretical Study of Photochromic Compounds. 1. Bond Length Alternation and Absorption Spectra for the Open and Closed Forms of 29 Diarylethene Derivatives. Journal of Physical Chemistry A, 2009, 113, 8409-8414.	2.5	61
106	Two-Photon Absorption Properties of New Fluorene-Based Singlet Oxygen Photosensitizers. Journal of Physical Chemistry C, 2009, 113, 4706-4711.	3.1	45
107	Electronic Hyperpolarizabilities for Donorâ"Acceptor Molecules with Long Conjugated Bridges: Calculations versus Experiment. Journal of Physical Chemistry A, 2009, 113, 10994-11001.	2.5	129
108	DFT-Based Methods in the Design of Two-Photon Operated Molecular Switches. Journal of Physical Chemistry A, 2009, 113, 7080-7089.	2.5	49

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109	Time-Dependent Density Functional Theory Study of Structure-Property Relationships in Diarylethene Photochromic Compounds. Lecture Notes in Computer Science, 2009, , 211-220.	1.3	4
110	Protonated Nanoparticle Surface Governing Ligand Tethering and Cellular Targeting. ACS Nano, 2009, 3, 1203-1211.	14.6	82
111	Prediction of Exchange Coupling Constant for Mn12 Molecular Magnet Using Dft+U. Lecture Notes in Computer Science, 2009, , 151-159.	1.3	3
112	Linear and nonlinear optical characterizations of a monomeric symmetric squaraine-based dye in solution. Journal of Chemical Physics, 2009, 130, 214504.	3.0	30
113	Quantum chemistry of quantum dots: Effects of ligands and oxidation. Journal of Chemical Physics, 2009, 131, 044106.	3.0	80
114	Water Deficient Environment Accelerates Proton Exchange: Acetoneâ^'Water Reaction Catalyzed by Calix[4]hydroquinone Nanotubes. Journal of Physical Chemistry C, 2009, 113, 10395-10401.	3.1	2
115	Dopant-mediated oxygen vacancy tuning in ceria nanoparticles. Nanotechnology, 2009, 20, 085713.	2.6	133
116	Modeling of Selective Carbon Nanotubes Growth for Non-classical Memory Applications. , 2009, , .		0
117	Structural Characterization Combined with the First Principles Simulations of Barium/Strontium Cobaltite/Ferrite as Promising Material for Solid Oxide Fuel Cells Cathodes and High-Temperature Oxygen Permeation Membranes. ACS Applied Materials & Interfaces, 2009, 1, 1512-1519.	8.0	50
118	Pairwise Spin-Contamination Correction Method and DFT Study of MnH and H2 Dissociation Curves. Lecture Notes in Computer Science, 2009, , 141-150.	1.3	5
119	Theoretical Photochemistry of the Photochromic Molecules Based on Density Functional Theory Methods. Lecture Notes in Computer Science, 2009, , 169-178.	1.3	2
120	Towards Multiscale Simulations of Carbon Nanotube Growth Process: A Density Functional Theory Study of Transition Metal Hydrides. Lecture Notes in Computer Science, 2009, , 765-774.	1.3	0
121	Conformational dependence of the first molecular hyperpolarizability in the computational design of nonlinear optical materials for optical switching. Mendeleev Communications, 2008, 18, 265-267.	1.6	40
122	Double excitations and state-to-state transition dipoles in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="none" display="inline"><mml:mrow><mml:mi>Ï€</mml:mi><mml:mtext>â^'</mml:mtext><mml:msup><mml:mi>Ï€</mml:mi><mml:mo>â^—</mml:mo></mml:msup></mml:mrow></mml:math> singlet states of linear polyenes: Time-dependent density-functional theory versus multiconfigurational methods. Physical Review A, 2008, 77, .	2.6	58
123	Fluorescence Emission of Disperse Red 1 in Solution at Room Temperature. Journal of Physical Chemistry B, 2008, 112, 929-937.	2.6	55
124	Applicability of hybrid density functional theory methods to calculation of molecular hyperpolarizability. Journal of Chemical Physics, 2008, 129, 044109.	3.0	150
125	Potential energy curves and electronic structure of 3d transition metal hydrides and their cations. Journal of Chemical Physics, 2008, 129, 214302.	3.0	32
126	Catalytic Role of Calix[4]hydroquinone in Acetoneâ^'Water Proton Exchange: A Quantum Chemical Study of Proton Transfer via Ketoâ^'Enol Tautomerism. Journal of Physical Chemistry A, 2008, 112, 10405-10412.	2.5	8

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128	Quantum chemistry of the minimal CdSe clusters. Journal of Chemical Physics, 2008, 129, 074709.	3.0	58
129	Two-Photon Excitation of Substituted Enediynes. Journal of Physical Chemistry A, 2006, 110, 241-251.	2.5	44
130	Role of Donorâ^'Acceptor Strengths and Separation on the Two-Photon Absorption Response of Cytotoxic Dyes:â€‰ A TD-DFT Study. Journal of Physical Chemistry A, 2005, 109, 7276-7284.	2.5	55
131	Theoretical study of the effects of solvent environment on photophysical properties and electronic structure of paracyclophane chromophores. Journal of Chemical Physics, 2005, 122, 224505.	3.0	59
132	Calculations of the third-order nonlinear optical responses in pushâ€“pull chromophores with a time-dependent density functional theory. Chemical Physics Letters, 2004, 392, 444-451.	2.6	38
133	Prediction of Two-Photon Absorption Properties for Organic Chromophores Using Time-Dependent Density-Functional Theory. Journal of Physical Chemistry B, 2004, 108, 899-907.	2.6	178
134	Potentials of Mean Force between Ionizable Amino Acid Side Chains in Water. Journal of the American Chemical Society, 2003, 125, 1722-1730.	13.7	190
135	A Disilapentalene and a Stable Diradical from the Reaction of a Dilithiosilole with a Dichlorocyclopropene. Journal of the American Chemical Society, 2003, 125, 5767-5773.	13.7	25
136	Distance and exposure dependent effective dielectric function. Journal of Computational Chemistry, 2002, 23, 1090-1099.	3.3	53
137	Contributions to the binding free energy of ligands to avidin and streptavidin. Proteins: Structure, Function and Bioinformatics, 2002, 47, 194-208.	2.6	94
138	Câ^'H Bond-Shortening upon Hydrogen Bond Formation:Â Influence of an Electric Field. Journal of Physical Chemistry A, 2001, 105, 4737-4740.	2.5	203
139	ACD/I-Lab 4.5:â€‰ An Internet Service Review. Journal of Chemical Information and Computer Sciences, 2001, 41, 1093-1095.	2.8	13
140	Theoretical Study of Urea and Thiourea. 2. Chains and Ribbons. Journal of Physical Chemistry B, 2000, 104, 806-810.	2.6	145
141	Theoretical Study of Urea. I. Monomers and Dimers. Journal of Physical Chemistry A, 1999, 103, 178-184.	2.5	95
142	Are Hydrogen Bonds Covalent or Electrostatic? A Molecular Orbital Comparison of Molecules in Electric Fields and H-Bonding Environments. Journal of Physical Chemistry A, 1999, 103, 7083-7086.	2.5	105
143	Molecular Orbital Study of Crystalline p-Benzoquinone. Journal of Physical Chemistry A, 1999, 103, 7042-7046.	2.5	29
144	Proximity effects on nuclear spinâ€“spin coupling constants. Part 2.â€”The electric field effect on1J(CH) couplings. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3029-3033.	1.7	46

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146	Topological properties of electron density in the Hâ^'+ H2CO reaction system. Journal of Molecular Structure, 1994, 311, 161-167.	3.6	1
147	Topological properties of electron density in the Hâ^'+H2CO reaction system. Computational and Theoretical Chemistry, 1994, 311, 161-167.	1.5	1
148	Donor-acceptor nature of specific nonbonded interactions of sulfur and halogen atoms. Influence on the geometry and packing of molecules. Journal of Structural Chemistry, 1992, 33, 423-435.	1.0	14
149	Structure and Properties of 1237 Low-Lying Isomers of Magnesium Clusters Mgn (nâ€‰=â€‰2â€“32) Predicted with the DFT Global Optimization. Journal of Cluster Science, 0, , .	3.3	1