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	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
2	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
3	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
4	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
5	Phosphate ester hydrolysis of biologically relevant molecules by cerium oxide nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2010, 6, 738-744.	3.3	171
6	Applicability of hybrid density functional theory methods to calculation of molecular hyperpolarizability. Journal of Chemical Physics, 2008, 129, 044109.	3.0	150
7	Theoretical Study of Urea and Thiourea. 2. Chains and Ribbons. Journal of Physical Chemistry B, 2000, 104, 806-810.	2.6	145
8	Dopant-mediated oxygen vacancy tuning in ceria nanoparticles. Nanotechnology, 2009, 20, 085713.	2.6	133
9	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
10	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
11	Oxyphor 2P: A High-Performance Probe for Deep-Tissue Longitudinal Oxygen Imaging. Cell Metabolism, 2019, 29, 736-744.e7.	16.2	105
12	Theoretical Study of Urea. I. Monomers and Dimers. Journal of Physical Chemistry A, 1999, 103, 178-184.	2.5	95
13	Contributions to the binding free energy of ligands to avidin and streptavidin. Proteins: Structure, Function and Bioinformatics, 2002, 47, 194-208.	2.6	94
14	Protonated Nanoparticle Surface Governing Ligand Tethering and Cellular Targeting. ACS Nano, 2009, 3, 1203-1211.	14.6	82
15	Quantum chemistry of quantum dots: Effects of ligands and oxidation. Journal of Chemical Physics, 2009, 131, 044106.	3.0	80
16	Structure and properties of cerium oxides in bulk and nanoparticulate forms. Journal of Alloys and Compounds, 2014, 584, 199-208.	5.5	79
17	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
18	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

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19	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
20	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
21	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
22	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
23	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^— singlet states of linear polyenes: Time-dependent density-functional theory versus multiconfigurational methods. Physical Review A, 2008, 77, .	2.6	58
24	Quantum chemistry of the minimal CdSe clusters. Journal of Chemical Physics, 2008, 129, 074709.	3.0	58
25	Insight into how molecular structures of thiophene-based conjugated polymers affect crystallization behaviors. Polymer, 2011, 52, 2302-2309.	3.8	58
26	New acentric materials constructed from aminopyridines and 4-nitrophenol. CrystEngComm, 2013, 15, 4700.	2.6	58
27	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
28	Fluorescence Emission of Disperse Red 1 in Solution at Room Temperature. Journal of Physical Chemistry B, 2008, 112, 929-937.	2.6	55
29	Theoretical Study of Photochromic Compounds: Part 3. Prediction of Thermal Stability. Journal of Physical Chemistry C, 2011, 115, 10292-10297.	3.1	55
30	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
31	Untangling the Excited States of DR1 in Solution:â€‰ An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 3886-3890.	2.5	54
32	Distance and exposure dependent effective dielectric function. Journal of Computational Chemistry, 2002, 23, 1090-1099.	3.3	53
33	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
34	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
35	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
36	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

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37	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
38	DFT-Based Methods in the Design of Two-Photon Operated Molecular Switches. Journal of Physical Chemistry A, 2009, 113, 7080-7089.	2.5	49
39	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
40	Natural polyphenols as inhibitors of amyloid aggregation. Molecular dynamics study of GNNQQNY heptapeptide decamer. Biophysical Chemistry, 2010, 149, 12-21.	2.8	47
41	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
42	Two-Photon Absorption Properties of New Fluorene-Based Singlet Oxygen Photosensitizers. Journal of Physical Chemistry C, 2009, 113, 4706-4711.	3.1	45
43	Mechanism of Nitric Oxide Oxidation Reaction (2NO + O₂ â†' 2NO₂) Revisited. Journal of Chemical Theory and Computation, 2011, 7, 2021-2024.	5.3	45
44	Two-Photon Excitation of Substituted Enediynes. Journal of Physical Chemistry A, 2006, 110, 241-251.	2.5	44
45	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
46	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
47	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
48	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
49	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
50	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
51	Theoretical spectroscopy of carbocyanine dyes made accurate by frozen density correction to excitation energies obtained by TDâ€ÐFT. International Journal of Quantum Chemistry, 2010, 110, 3095-3100.	2.0	36
52	Density functional theory study of small nickel clusters. Journal of Molecular Modeling, 2012, 18, 783-790.	1.8	36
53	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
54	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

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55	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
56	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
57	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
58	Potential energy curves and electronic structure of 3d transition metal hydrides and their cations. Journal of Chemical Physics, 2008, 129, 214302.	3.0	32
59	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
60	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
61	Linear and nonlinear optical characterizations of a monomeric symmetric squaraine-based dye in solution. Journal of Chemical Physics, 2009, 130, 214504.	3.0	30
62	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
63	Molecular Orbital Study of Crystalline p-Benzoquinone. Journal of Physical Chemistry A, 1999, 103, 7042-7046.	2.5	29
64	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
65	Two-Photon Absorption Spectrum of a Single Crystal Cyanine-like Dye. Journal of Physical Chemistry Letters, 2012, 3, 1222-1228.	4.6	27
66	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
67	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
68	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
69	Understanding oxygen vacancy migration and clustering in barium strontiumcobalt iron oxide. Solid State Ionics, 2010, 181, 1067-1073.	2.7	25
70	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
71	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
72	Shock Tube/Laser Absorption and Kinetic Modeling Study of Triethyl Phosphate Combustion. Journal of Physical Chemistry A, 2018, 122, 3829-3836.	2.5	23

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73	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
74	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
75	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
76	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
77	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
78	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
79	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
80	Thermally controlled preferential molecular aggregation state in a thiacarbocyanine dye. Journal of Chemical Physics, 2010, 133, 134508.	3.0	20
81	Alternative packing modes leading to amyloid polymorphism in five fragments studied with molecular dynamics. Biopolymers, 2012, 98, 131-144.	2.4	20
82	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
83	Quantum Chemical Study of Supercritical Carbon Dioxide Effects on Combustion Kinetics. Journal of Physical Chemistry A, 2017, 121, 3728-3735.	2.5	19
84	Electronic Nature of Neutral and Charged Two-Photon Absorbing Squaraines for Fluorescence Bioimaging Application. ACS Omega, 2019, 4, 14669-14679.	3.5	19
85	Unique example of amyloid aggregates stabilized by main chain H-bond instead of the steric zipper: molecular dynamics study of the amyloidogenic segment of amylin wild-type and mutants. Journal of Molecular Modeling, 2012, 18, 891-903.	1.8	18
86	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
87	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
88	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
89	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
90	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

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91	Theory and computations of two-photon absorbing photochromic chromophores. European Journal of Chemistry, 2010, 1, 142-161.	0.6	16
92	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
93	First principles crystal engineering of nonlinear optical materials. I. Prototypical case of urea. Journal of Chemical Physics, 2017, 146, 244104.	3.0	16
94	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
95	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
96	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
97	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
98	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
99	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
100	ACD/I-Lab 4.5:â€‰ An Internet Service Review. Journal of Chemical Information and Computer Sciences, 2001, 41, 1093-1095.	2.8	13
101	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
102	Aqueous medium induced optical transitions in cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2015, 17, 6217-6221.	2.8	13
103	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
104	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
105	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
106	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
107	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
108	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

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109	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
110	Linear photophysics, two-photon absorption and femtosecond transient absorption spectroscopy of styryl dye bases. Journal of Luminescence, 2017, 183, 360-367.	3.1	10
111	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
112	High accuracy machine learning identification of fentanyl-relevant molecular compound classification via constituent functional group analysis. Scientific Reports, 2020, 10, 13569.	3.3	9
113	Three-Photon Spectroscopy of Porphyrins. Journal of Physical Chemistry A, 2020, 124, 11038-11050.	2.5	9
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	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
122	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
123	Two-Photon Absorption Spectra Predicted by Semiempirical Methods. Journal of Computational and Theoretical Nanoscience, 2014, 11, 2208-2220.	0.4	5
124	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
125	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
126	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

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127	A theoretical investigation of the Cî—¸H Â·Â·Â· O interaction between substituted phenylacetylenes and water. Computational and Theoretical Chemistry, 1996, 371, 17-19.	1.5	4
128	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
129	Prediction of Exchange Coupling Constant for Mn12 Molecular Magnet Using Dft+U. Lecture Notes in Computer Science, 2009, , 151-159.	1.3	3
130	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
131	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
132	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
133	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
134	Theoretical Photochemistry of the Photochromic Molecules Based on Density Functional Theory Methods. Lecture Notes in Computer Science, 2009, , 169-178.	1.3	2
135	Topological properties of electron density in the Hâ^'+ H2CO reaction system. Journal of Molecular Structure, 1994, 311, 161-167.	3.6	1
136	Topological properties of electron density in the Hâ^'+H2CO reaction system. Computational and Theoretical Chemistry, 1994, 311, 161-167.	1.5	1
137	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
138	Two-photon Absorption in Single Crystals of Cyanine-like Dye. , 2010, , .		1
139	The Atomic Level Interaction of Polyphenols with the AÎ² Oligomer Aggregate, A Molecular Dynamic Guidance for Rational Drug Design. , 2014, , 59-70.		1
140	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
141	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
142	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
143	Modeling of Selective Carbon Nanotubes Growth for Non-classical Memory Applications. , 2009, , .		0
144	Effective Generation of Triplet States and Singlet Oxygen by Sulfur-Containing Squaraines: Experimental and Theoretical Study. , 2010, , .		0

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145	Combustion of Aldehydes in the Negative Temperature Coefficient Region: Products and Pathways. , 2016, , .		0
146	Sarin simulants combustion at high temperature: Time-resolved laser absorption spectroscopy of intermediate products in a shock tube. , 2018, , .		0
147	Cover Image, Volume 51, Issue 1. International Journal of Chemical Kinetics, 2019, 51, i.	1.6	0
148	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
149	Influence of Binary Diffusion Coefficients on Supercritical CO2Flame Characteristics of Methane/Natural Gas. , 2022, , .		0