

N Arul Murugan

List of Publications by Year in descending order

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128
papers

2,897
citations

172207

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docs citations

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3817
citing authors

#	ARTICLE	IF	CITATIONS
1	Exhibiting environment sensitive optical properties through multiscale modelling: A study of photoactivatable probes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 425, 113672.	2.0	2
2	Molecular basis for stereoselective transport of fenoterol by the organic cation transporters 1 and 2. <i>Biochemical Pharmacology</i> , 2022, 197, 114871.	2.0	7
3	Data-driven approach towards identifying dyesensitizer molecules for higher power conversion efficiency in solar cells. <i>New Journal of Chemistry</i> , 2022, 46, 4395-4405.	1.4	6
4	A Review on Parallel Virtual Screening Softwares for High-Performance Computers. <i>Pharmaceuticals</i> , 2022, 15, 63.	1.7	34
5	Organosulfur/Selenium-Based Highly Fluorogenic Molecular Probes for Live-Cell Nucleolus Imaging. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	2
6	Recent trends in computational tools and data-driven modeling for advanced materials. <i>Materials Advances</i> , 2022, 3, 4069-4087.	2.6	17
7	Structure-based drug repurposing: Traditional and advanced AI/ML-aided methods. <i>Drug Discovery Today</i> , 2022, 27, 1847-1861.	3.2	46
8	Improved Binding Affinity of Omicron's Spike Protein for the Human Angiotensin-Converting Enzyme 2 Receptor Is the Key behind Its Increased Virulence. <i>International Journal of Molecular Sciences</i> , 2022, 23, 3409.	1.8	34
9	Near-infrared emissive cyanine probes for selective visualization of the physiological and pathophysiological modulation of albumin levels. <i>Journal of Materials Chemistry B</i> , 2022, 10, 3657-3666.	2.9	2
10	Applying polypharmacology approach for drug repurposing for SARS-CoV2. <i>Journal of Chemical Sciences</i> , 2022, 134, 57.	0.7	10
11	Artificial intelligence in virtual screening: Models versus experiments. <i>Drug Discovery Today</i> , 2022, 27, 1913-1923.	3.2	33
12	Computational investigation on <i>Andrographis paniculata</i> phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 4415-4426.	2.0	73
13	An unexpected role of an extra phenolic hydroxyl on the chemical reactivity and bioactivity of catechol or gallol modified hyaluronic acid hydrogels. <i>Polymer Chemistry</i> , 2021, 12, 2987-2991.	1.9	12
14	Peptide-Based Antiviral Drugs. <i>Advances in Experimental Medicine and Biology</i> , 2021, 1322, 261-284.	0.8	5
15	Assessment of Amyloid Forming Tendency of Peptide Sequences from Amyloid Beta and Tau Proteins Using Force-Field, Semi-Empirical, and Density Functional Theory Calculations. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3244.	1.8	3
16	DNA Minor Groove-Induced <i>cis</i> → <i>trans</i> Isomerization of a Near-Infrared Fluorescent Probe. <i>Biochemistry</i> , 2021, 60, 2084-2097.	1.2	5
17	Cryptic Sites in Tau Fibrils Explain the Preferential Binding of the AV-1451 PET Tracer toward Alzheimer's Tauopathy. <i>ACS Chemical Neuroscience</i> , 2021, 12, 2437-2447.	1.7	24
18	Thiophene-Based Dual Modulators of A β and Tau Aggregation. <i>ChemBioChem</i> , 2021, 22, 3348-3357.	1.3	8

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19	Naphthalene Monoimide Derivative Ameliorates Amyloid Burden and Cognitive Decline in a Transgenic Mouse Model of Alzheimer's Disease. <i>Advanced Therapeutics</i> , 2021, 4, 2000225.	1.6	18
20	Identification of C5-NH ₂ Modified Oseltamivir Derivatives as Novel Influenza Neuraminidase Inhibitors with Highly Improved Antiviral Activities and Favorable Druggability. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 17992-18009.	2.9	12
21	Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Protein-Inhibitor Complexes in Relevance to Developing Parkinson's Therapeutics. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7648.	1.8	9
22	Discovery of biphenyl pyrazole scaffold for neurodegenerative diseases: A novel class of acetylcholinesterase-centered multitargeted ligands. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127370.	1.0	3
23	Multiscale Modeling of Two-Photon Probes for Parkinson's Diagnostics Based on Monoamine Oxidase B Biomarker. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3854-3863.	2.5	7
24	Recognition of G-quadruplex topology through hybrid binding with implications in cancer theranostics. <i>Theranostics</i> , 2020, 10, 10394-10414.	4.6	13
25	Searching for target-specific and multi-targeting organics for Covid-19 in the Drugbank database with a double scoring approach. <i>Scientific Reports</i> , 2020, 10, 19125.	1.6	47
26	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. <i>Science Advances</i> , 2020, 6, eabb8097.	4.7	138
27	Antioxidant Berberine-Derivative Inhibits Multifaceted Amyloid Toxicity. <i>IScience</i> , 2020, 23, 101005.	1.9	63
28	Structure-Activity Relationship Exploration of NNIBP Tolerant Region I Leads to Potent HIV-1 NNRTIs. <i>ACS Infectious Diseases</i> , 2020, 6, 2225-2234.	1.8	12
29	Computational Insight into the Binding Profile of the Second-Generation PET Tracer PI2620 with Tau Fibrils. <i>ACS Chemical Neuroscience</i> , 2020, 11, 900-908.	1.7	29
30	Molecular Architectonics of Cyclic Dipeptide Amphiphiles and Their Application in Drug Delivery. <i>ACS Applied Bio Materials</i> , 2020, 3, 3413-3422.	2.3	11
31	Unraveling the Unbinding Pathways of Products Formed in Catalytic Reactions Involved in SIRT1 ³ : A Random Acceleration Molecular Dynamics Simulation Study. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4100-4115.	2.5	10
32	Destabilization of amyloid fibrils on interaction with MoS ₂ -based nanomaterials. <i>RSC Advances</i> , 2019, 9, 1613-1624.	1.7	18
33	The impact of the heteroatom in a five-membered ring on the photophysical properties of difluoroborates. <i>Dyes and Pigments</i> , 2019, 170, 107481.	2.0	9
34	Cross-interaction of tau PET tracers with monoamine oxidase B: evidence from in silico modelling and in vivo imaging. <i>European Journal of Nuclear Medicine and Molecular Imaging</i> , 2019, 46, 1369-1382.	3.3	74
35	Effect of Familial Mutations on the Interconversion of β -Helix to β -Sheet Structures in an Amyloid-Forming Peptide: Insight from Umbrella Sampling Simulations. <i>ACS Chemical Neuroscience</i> , 2019, 10, 1347-1354.	1.7	16
36	Identification of Dihydrofuro[3,4- <i>d</i>]pyrimidine Derivatives as Novel HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1484-1501.	2.9	70

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37	Recent Advancements in Computing Reliable Binding Free Energies in Drug Discovery Projects. Challenges and Advances in Computational Chemistry and Physics, 2019, , 221-246.	0.6	1
38	Mechanistic Insight into the Binding Profile of DCVJ and β -Synuclein Fibril Revealed by Multiscale Simulations. ACS Chemical Neuroscience, 2019, 10, 610-617.	1.7	18
39	Different Positron Emission Tomography Tau Tracers Bind to Multiple Binding Sites on the Tau Fibril: Insight from Computational Modeling. ACS Chemical Neuroscience, 2018, 9, 1757-1767.	1.7	69
40	Integrative approaches in HIV α 1 non-nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328.	6.2	10
41	Cover Image, Volume 8, Issue 1. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1356.	6.2	0
42	Free Energy Landscape for Alpha-Helix to Beta-Sheet Interconversion in Small Amyloid Forming Peptide under Nanoconfinement. Journal of Physical Chemistry B, 2018, 122, 9654-9664.	1.2	16
43	Structure-Based Optimization of N-Substituted Oseltamivir Derivatives as Potent Anti-Influenza A Virus Agents with Significantly Improved Potency against Oseltamivir-Resistant N1-H274Y Variant. Journal of Medicinal Chemistry, 2018, 61, 9976-9999.	2.9	35
44	Combining (Non)linear Optical and Fluorescence Analysis of DiD To Enhance Lipid Phase Recognition. Journal of Chemical Theory and Computation, 2018, 14, 5350-5359.	2.3	11
45	Optimization of N-Substituted Oseltamivir Derivatives as Potent Inhibitors of Group-1 and -2 Influenza A Neuraminidases, Including a Drug-Resistant Variant. Journal of Medicinal Chemistry, 2018, 61, 6379-6397.	2.9	46
46	Unusual binding-site-specific photophysical properties of a benzothiazole-based optical probe in amyloid beta fibrils. Physical Chemistry Chemical Physics, 2018, 20, 20334-20339.	1.3	10
47	Acetylene-sourced CVD-synthesised catalytically active graphene for electrochemical biosensing. Biosensors and Bioelectronics, 2017, 89, 496-504.	5.3	27
48	Development of an Efficient Ca^{2+} -Quadruplex-Stabilised Thrombin-Binding Aptamer Containing a Three-Carbon Spacer Molecule. ChemBioChem, 2017, 18, 755-763.	1.3	26
49	Atomic level simulations of the interaction of asphaltene with quartz surfaces: role of chemical modifications and aqueous environment. Materials and Structures/Materiaux Et Constructions, 2017, 50, 1.	1.3	8
50	Al^{3+} plaque-selective NIR fluorescence probe to differentiate Alzheimer's disease from tauopathies. Biosensors and Bioelectronics, 2017, 98, 54-61.	5.3	83
51	On/off-switchable LSPR nano-immunoassay for troponin-T. Scientific Reports, 2017, 7, 44027.	1.6	36
52	Progress in electronics and photonics with nanomaterials. Vacuum, 2017, 146, 304-307.	1.6	27
53	Effect of Alzheimer Familial Chromosomal Mutations on the Amyloid Fibril Interaction with Different PET Tracers: Insight from Molecular Modeling Studies. ACS Chemical Neuroscience, 2017, 8, 2655-2666.	1.7	8
54	Cyclic Dipeptide-Based Ambidextrous Supergelators: Minimalistic Rational Design, Structure-Gelation Studies, and In Situ Hydrogelation. Biomacromolecules, 2017, 18, 3581-3590.	2.6	36

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55	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. <i>Molecules</i> , 2017, 22, 1643.	1.7	15
56	Elucidating the Mechanism of Zn ²⁺ Sensing by a Bipyridine Probe Based on Two-Photon Absorption. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9067-9075.	1.2	13
57	The Culprit Is in the Cave: The Core Sites Explain the Binding Profiles of Amyloid-Specific Tracers. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3313-3321.	2.1	35
58	Origin of the Absorption Band of Bromophenol Blue in Acidic and Basic pH: Insight from a Combined Molecular Dynamics and TD-DFT/MM Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7175-7182.	1.1	5
59	Inflammation-sensitive in situ smart scaffolding for regenerative medicine. <i>Nanoscale</i> , 2016, 8, 17213-17222.	2.8	17
60	Multistep Modeling Strategy To Improve the Binding Affinity Prediction of PET Tracers to A β ₄₂ : Case Study with Styrylbenzoxazole Derivatives. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1698-1705.	1.7	7
61	Investigation into Biological Environments through (Non)linear Optics: A Multiscale Study of Laurdan Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6169-6181.	2.3	25
62	A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid β Aggregates. <i>Scientific Reports</i> , 2016, 6, 23668.	1.6	90
63	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF ₂) Core Complex. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2323-2332.	1.2	28
64	Studies on an on/off-switchable immunosensor for troponin T. <i>Biosensors and Bioelectronics</i> , 2015, 73, 100-107.	5.3	22
65	One- and Two-Photon Absorption of a Spiropyran-Merocyanine System: Experimental and Theoretical Studies. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1515-1522.	1.2	23
66	Relation between Nonlinear Optical Properties of Push-Pull Molecules and Metric of Charge Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4182-4188.	2.3	39
67	Synthesis, spectral characterization and DFT analysis for the validation of 2, 6 diaryl -piperidin-4-ones as potential sunscreens and UV filters. <i>Journal of Molecular Structure</i> , 2015, 1099, 560-566.	1.8	7
68	Investigation of the Binding Profiles of AZD2184 and Thioflavin T with Amyloid- β (1-42) Fibril by Molecular Docking and Molecular Dynamics Methods. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11560-11567.	1.2	48
69	Advanced Glycation End Products Modulate Structure and Drug Binding Properties of Albumin. <i>Molecular Pharmaceutics</i> , 2015, 12, 3312-3322.	2.3	39
70	Toward Fully Nonempirical Simulations of Optical Band Shapes of Molecules in Solution: A Case Study of Heterocyclic Ketoimine Difluoroborates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5145-5152.	1.1	39
71	Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. <i>Journal of Physical Chemistry C</i> , 2015, 119, 653-664.	1.5	15
72	Synthesis, characterization of (3E)-1-(6-chloro-2-methyl-4-phenyl quinolin-3-yl)-3-aryl prop-2-en-1-ones through IR, NMR, single crystal X-ray diffraction and insights into their electronic structure using DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1010-1017.	2.0	4

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73	Studies of pH-Sensitive Optical Properties of the deGFP1 Green Fluorescent Protein Using a Unique Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3492-3502.	2.3	5
74	Promising two-photon probes for in vivo detection of β^2 amyloid deposits. <i>Chemical Communications</i> , 2014, 50, 11694-11697.	2.2	25
75	Simulations of Light Absorption of Carbon Particles in Nanoaerosol Clusters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1879-1886.	1.1	8
76	Solvatochromism in a Pyridinium Cyclopentadienylide: Insights from a Sequential Carâ€Parrinello QM/MM and TD-DFT/Semicontinuum Approach. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7358-7366.	1.2	2
77	Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1715-1725.	1.2	19
78	Role of Protonation State and Solvation on the pH Dependent Optical Properties of Bromocresol Green. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3958-3968.	2.3	3
79	Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 778-788.	2.3	12
80	<i>In silico</i> modeling and experimental evidence of coagulant protein interaction with precursors for nanoparticle functionalization. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1182-1190.	2.0	6
81	pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3660-3669.	2.3	12
82	Dioxygen spectra and bioactivation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1847-1867.	1.0	41
83	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2427.	1.3	4
84	Two-Photon Solvatochromism II: Experimental and Theoretical Study of Solvent Effects on the Two-Photon Absorption Spectrum of Reichardtâ€™s Dye. <i>ChemPhysChem</i> , 2013, 14, 3731-3739.	1.0	32
85	Spatial spin-charge separation in neutral endohedral metallofullerene: A combined restricted open-shell MP2 and Carâ€Parrinello molecular dynamics study. <i>Chemical Physics Letters</i> , 2013, 557, 71-75.	1.2	0
86	Hybrid density functionalâ€molecular mechanics calculations for core-electron binding energies of glycine in water solution. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 244-254.	1.3	15
87	Solvent-Dependent Conformational States of a [2]Rotaxane-Based Molecular Machine: A Molecular Dynamics Perspective. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25059-25068.	1.5	12
88	Association Dynamics and Linear and Nonlinear Optical Properties of an <i>N</i> -Acetylaladanamide Probe in a POPC Membrane. <i>Journal of the American Chemical Society</i> , 2013, 135, 13590-13597.	6.6	27
89	Revealing Spectral Features in Two-Photon Absorption Spectrum of Hoechst 33342: A Combined Experimental and Quantum-Chemical Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12013-12019.	1.2	22
90	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 70-77.	2.1	29

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91	Differences in first neighbor orientation behind the anomalies in the low and high density trans-1,2-dichloroethene liquid. <i>Journal of Chemical Physics</i> , 2012, 136, 124514.	1.2	10
92	Solvent Polarity-Induced Conformational Unlocking of Asparagine. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11702-11708.	1.1	7
93	Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4766-4774.	2.3	8
94	How Crucial Are Finite Temperature and Solvent Effects on Structure and Absorption Spectra of Si₁₀?. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26618-26624.	1.5	4
95	Al ³⁺ induced planarization, conformational arrest and metallochromic shift in a pyrimidine dione dye: insight from integrated hybrid quantum-classical calculations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2339.	1.3	1
96	Color modeling of protein optical probes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1107-1112.	1.3	40
97	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 257-263.	2.3	19
98	NMR Spin-Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. <i>Chemistry - A European Journal</i> , 2012, 18, 11677-11684.	1.7	14
99	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8169-8181.	1.2	40
100	Solvent Dependence of Structure, Charge Distribution, and Absorption Spectrum in the Photochromic Merocyanine-Spiropyran Pair. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4025-4032.	1.2	43
101	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12506.	1.3	64
102	Density Functional Theory/Molecular Mechanics Approach for Electronic $\langle i g i \rangle$ -Tensors of Solvated Molecules. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4350-4358.	1.2	20
103	Modeling Solvatochromism of a Quinolinium Betaine Dye in Water Solvent Using Sequential Hybrid QM/MM and Semicontinuum Approach. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1056-1061.	1.2	18
104	Density Functional Restricted-Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3261-3271.	2.3	18
105	Demystifying the solvatochromic reversal in Brooker's merocyanine dye. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1290-1292.	1.3	55
106	Modeling solvatochromism of Nile red in water. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1521-1530.	1.0	21
107	Solvatochromic shift of phenol blue in water from a combined Car-Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and $\langle \text{sc} \rangle \text{ZINDO} \langle \text{sc} \rangle$ approach. <i>Journal of Chemical Physics</i> , 2010, 132, 234508.	1.2	25
108	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13349-13357.	1.2	52

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109	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16453-16458.	3.3	84
110	1,2-Dichloroethane in Haloalkane Dehalogenase Protein and in Water Solvent: A Case Study of the Confinement Effect on Structural and Dynamical Properties. Journal of Physical Chemistry B, 2009, 113, 3257-3263.	1.2	8
111	Role of Dynamic Flexibility in Computing Solvatochromic Properties of Dye~Solvent Systems: <i>o</i> -Betaine in Water. Journal of Physical Chemistry A, 2009, 113, 2572-2577.	1.1	27
112	Thermal behavior of disordered phase of caffeine molecular crystal: Insights from Monte Carlo simulation studies. Journal of Chemical Physics, 2009, 130, 204514.	1.2	14
113	Conformations, structural transitions and visible near-infrared absorption spectra of four-, five- and six-coordinated Cu(II) aqua complexes. Physical Chemistry Chemical Physics, 2009, 11, 508-519.	1.3	51
114	Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Car~Parrinello Molecular Dynamics Investigation. Journal of Physical Chemistry A, 2009, 113, 4833-4839.	1.1	23
115	Solvent Dependence of Conformational Distribution, Molecular Geometry, and Electronic Structure in Adenosine. Journal of Physical Chemistry B, 2009, 113, 1012-1021.	1.2	14
116	Pressure dependence of crystal structure and molecular packing in anthracene. Molecular Physics, 2009, 107, 1689-1695.	0.8	6
117	Solvation shell structure of cyclooctylpyranone in water solvent and its comparative structure, dynamics and dipole moment in HIV protease. Physical Chemistry Chemical Physics, 2009, 11, 6482.	1.3	2
118	Investigations into conformational transitions and solvation structure of a 7-piperidino-5,9-methanobenzo[8] annulene in water. Physical Chemistry Chemical Physics, 2008, 10, 6135.	1.3	6
119	Solvent Dependence on Conformational Transition, Dipole Moment, and Molecular Geometry of 1,2-Dichloroethane: Insight from Car~Parrinello Molecular Dynamics Calculations. Journal of Physical Chemistry B, 2008, 112, 14673-14677.	1.2	13
120	What does pressure decide to cook with orientationally disordered plastic phase of cubane: An orientational glass or crystal?. Journal of Chemical Physics, 2005, 123, 244514.	1.2	1
121	Temperature-induced dynamical conformational disorder in 4-vinyl benzoic acid molecular crystals: A molecular simulation study. Journal of Chemical Physics, 2005, 123, 094508.	1.2	6
122	Orientalional Melting and Reorientational Motion in a Cubane Molecular Crystal: A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 23955-23962.	1.2	9
123	Effect of Pressure on Pedal Motion in Stilbene Molecular Crystals and Its Dependence on the Crystallographic Site. Journal of Physical Chemistry B, 2005, 109, 12107-12114.	1.2	3
124	High-Pressure Study of Adamantane:~Variable Shape Simulations up to 26 GPa. Journal of Physical Chemistry B, 2005, 109, 17296-17303.	1.2	8
125	Pressure Induced Orientalional Ordering in p-Terphenyl. Journal of Physical Chemistry B, 2005, 109, 1433-1440.	1.2	19
126	Pressure-Induced Ordering in Adamantane: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2005, 109, 2014-2020.	1.2	12

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127	Structure, Energetics, and Dynamics of Pedal-Like Motion in Stilbene from Molecular Simulation and ab Initio Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17403-17411.	1.2	14
128	High Pressure Phase of Biphenyl at Room Temperature: A Monte Carlo Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4178-4184.	1.2	18