# N Arul Murugan

List of Publications by Year
in descending order

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| 128 | 2,897 | 172457 | 243625 |
|---|---|---|---|
| papers | citations | 29 h-index | 44 g-index |

| 132 | 132 | 132 | 3817 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Exhibiting environment sensitive optical properties through multiscale modelling: A study of photoactivatable probes. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 425, 113672. | 3.9 | 2 |
| 2 | Molecular basis for stereoselective transport of fenoterol by the organic cation transporters 1 and 2. Biochemical Pharmacology, 2022, 197, 114871. | 4.4 | 7 |
| 3 | Data-driven approach towards identifying dyesensitizer molecules for higher power conversion efficiency in solar cells. New Journal of Chemistry, 2022, 46, 4395-4405. | 2.8 | 6 |
| 4 | A Review on Parallel Virtual Screening Softwares for High-Performance Computers. Pharmaceuticals, 2022, 15, 63. | 3.8 | 34 |
| 5 | Organosulfur/Seleniumâ€Based Highly Fluorogenic Molecular Probes for Liveâ€Cell Nucleolus Imaging. Chemistry - an Asian Journal, 2022, 17, . | 3.3 | 2 |
| 6 | Recent trends in computational tools and data-driven modeling for advanced materials. Materials Advances, 2022, 3, 4069-4087. | 5.4 | 17 |
| 7 | Structure-based drug repurposing: Traditional and advanced AI/ML-aided methods. Drug Discovery Today, 2022, 27, 1847-1861. | 6.4 | 46 |
| 8 | Improved Binding Affinity of Omicronâ€™s Spike Protein for the Human Angiotensin-Converting Enzyme 2 Receptor Is the Key behind Its Increased Virulence. International Journal of Molecular Sciences, 2022, 23, 3409. | 4.1 | 34 |
| 9 | Near-infrared emissive cyanine probes for selective visualization of the physiological and pathophysiological modulation of albumin levels. Journal of Materials Chemistry B, 2022, 10, 3657-3666. | 5.8 | 2 |
| 10 | Applying polypharmacology approach for drug repurposing for SARS-CoV2. Journal of Chemical Sciences, 2022, 134, 57. | 1.5 | 10 |
| 11 | Artificial intelligence in virtual screening: Models versus experiments. Drug Discovery Today, 2022, 27, 1913-1923. | 6.4 | 33 |
| 12 | Computational investigation on Andrographis paniculata phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4415-4426. | 3.5 | 73 |
| 13 | An unexpected role of an extra phenolic hydroxyl on the chemical reactivity and bioactivity of catechol or gallol modified hyaluronic acid hydrogels. Polymer Chemistry, 2021, 12, 2987-2991. | 3.9 | 12 |
| 14 | Peptide-Based Antiviral Drugs. Advances in Experimental Medicine and Biology, 2021, 1322, 261-284. | 1.6 | 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. International Journal of Molecular Sciences, 2021, 22, 3244. | 4.1 | 3 |
| 16 | DNA Minor Groove-Induced cisâ€“trans Isomerization of a Near-Infrared Fluorescent Probe. Biochemistry, 2021, 60, 2084-2097. | 2.5 | 5 |
| 17 | Cryptic Sites in Tau Fibrils Explain the Preferential Binding of the AV-1451 PET Tracer toward Alzheimerâ€™s Tauopathy. ACS Chemical Neuroscience, 2021, 12, 2437-2447. | 3.5 | 24 |
| 18 | Thiopheneâ€Based Dual Modulators of AÎ² and Tau Aggregation. ChemBioChem, 2021, 22, 3348-3357. | 2.6 | 8 |

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|---|---|---|---|
| 19 | Naphthalene Monoimide Derivative Ameliorates Amyloid Burden and Cognitive Decline in a Transgenic Mouse Model of Alzheimer's Disease. Advanced Therapeutics, 2021, 4, 2000225. | 3.2 | 18 |
| 20 | Identification of C5-NH<sub>2</sub> Modified Oseltamivir Derivatives as Novel Influenza Neuraminidase Inhibitors with Highly Improved Antiviral Activities and Favorable Druggability. Journal of Medicinal Chemistry, 2021, 64, 17992-18009. | 6.4 | 12 |
| 21 | Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Proteinâ€“Inhibitor Complexes in Relevance to Developing Parkinsonâ€™s Therapeutics. International Journal of Molecular Sciences, 2020, 21, 7648. | 4.1 | 9 |
| 22 | Discovery of biphenyl pyrazole scaffold for neurodegenerative diseases: A novel class of acetylcholinesterase-centered multitargeted ligands. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127370. | 2.2 | 3 |
| 23 | Multiscale Modeling of Two-Photon Probes for Parkinsonâ€™s Diagnostics Based on Monoamine Oxidase B Biomarker. Journal of Chemical Information and Modeling, 2020, 60, 3854-3863. | 5.4 | 7 |
| 24 | Recognition of G-quadruplex topology through hybrid binding with implications in cancer theranostics. Theranostics, 2020, 10, 10394-10414. | 10.0 | 13 |
| 25 | Searching for target-specific and multi-targeting organics for Covid-19 in the Drugbank database with a double scoring approach. Scientific Reports, 2020, 10, 19125. | 3.3 | 47 |
| 26 | Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. Science Advances, 2020, 6, eabb8097. | 10.3 | 138 |
| 27 | Antioxidant Berberine-Derivative Inhibits Multifaceted Amyloid Toxicity. IScience, 2020, 23, 101005. | 4.1 | 63 |
| 28 | Structureâ€“Activity Relationship Exploration of NNIBP Tolerant Region I Leads to Potent HIV-1 NNRTIs. ACS Infectious Diseases, 2020, 6, 2225-2234. | 3.8 | 12 |
| 29 | Computational Insight into the Binding Profile of the Second-Generation PET Tracer PI2620 with Tau Fibrils. ACS Chemical Neuroscience, 2020, 11, 900-908. | 3.5 | 29 |
| 30 | Molecular Architectonics of Cyclic Dipeptide Amphiphiles and Their Application in Drug Delivery. ACS Applied Bio Materials, 2020, 3, 3413-3422. | 4.6 | 11 |
| 31 | Unraveling the Unbinding Pathways of Products Formed in Catalytic Reactions Involved in SIRT1â€“3: A Random Acceleration Molecular Dynamics Simulation Study. Journal of Chemical Information and Modeling, 2019, 59, 4100-4115. | 5.4 | 10 |
| 32 | Destabilization of amyloid fibrils on interaction with MoS<sub>2</sub>-based nanomaterials. RSC Advances, 2019, 9, 1613-1624. | 3.6 | 18 |
| 33 | The impact of the heteroatom in a five-membered ring on the photophysical properties of difluoroborates. Dyes and Pigments, 2019, 170, 107481. | 3.7 | 9 |
| 34 | Cross-interaction of tau PET tracers with monoamine oxidase B: evidence from in silico modelling and in vivo imaging. European Journal of Nuclear Medicine and Molecular Imaging, 2019, 46, 1369-1382. | 6.4 | 74 |
| 35 | Effect of Familial Mutations on the Interconversion of Î±-Helix to Î²-Sheet Structures in an Amyloid-Forming Peptide: Insight from Umbrella Sampling Simulations. ACS Chemical Neuroscience, 2019, 10, 1347-1354. | 3.5 | 16 |
| 36 | Identification of Dihydrofuro[3,4-d]pyrimidine Derivatives as Novel HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties. Journal of Medicinal Chemistry, 2019, 62, 1484-1501. | 6.4 | 70 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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 Î±-Synuclein Fibril Revealed by Multiscale Simulations. ACS Chemical Neuroscience, 2019, 10, 610-617. | 3.5 | 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. | 3.5 | 69 |
| 40 | Integrative approaches in HIV â€1 nonâ€nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328. | 14.6 | 10 |
| 41 | Cover Image, Volume 8, Issue 1. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1356. | 14.6 | 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. | 2.6 | 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. | 6.4 | 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. | 5.3 | 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. | 6.4 | 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. | 2.8 | 10 |
| 47 | Acetylene-sourced CVD-synthesised catalytically active graphene for electrochemical biosensing. Biosensors and Bioelectronics, 2017, 89, 496-504. | 10.1 | 27 |
| 48 | Development of an Efficient Gâ€Quadruplexâ€Stabilised Thrombinâ€Binding Aptamer Containing a Threeâ€Carbon Spacer Molecule. ChemBioChem, 2017, 18, 755-763. | 2.6 | 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. | 3.1 | 8 |
| 50 | AÎ² plaque-selective NIR fluorescence probe to differentiate Alzheimer's disease from tauopathies. Biosensors and Bioelectronics, 2017, 98, 54-61. | 10.1 | 83 |
| 51 | On/off-switchable LSPR nano-immunoassay for troponin-T. Scientific Reports, 2017, 7, 44027. | 3.3 | 36 |
| 52 | Progress in electronics and photonics with nanomaterials. Vacuum, 2017, 146, 304-307. | 3.5 | 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. | 3.5 | 8 |
| 54 | Cyclic Dipeptide-Based Ambidextrous Supergelators: Minimalistic Rational Design, Structure-Gelation Studies, and In Situ Hydrogelation. Biomacromolecules, 2017, 18, 3581-3590. | 5.4 | 36 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. Molecules, 2017, 22, 1643. | 3.8 | 15 |
| 56 | Elucidating the Mechanism of Zn<sup>2+</sup> Sensing by a Bipyridine Probe Based on Two-Photon Absorption. Journal of Physical Chemistry B, 2016, 120, 9067-9075. | 2.6 | 13 |
| 57 | The Culprit Is in the Cave: The Core Sites Explain the Binding Profiles of Amyloid-Specific Tracers. Journal of Physical Chemistry Letters, 2016, 7, 3313-3321. | 4.6 | 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. Journal of Physical Chemistry A, 2016, 120, 7175-7182. | 2.5 | 5 |
| 59 | Inflammation-sensitive in situ smart scaffolding for regenerative medicine. Nanoscale, 2016, 8, 17213-17222. | 5.6 | 17 |
| 60 | Multistep Modeling Strategy To Improve the Binding Affinity Prediction of PET Tracers to Aî²<sub>42</sub>: Case Study with Styrylbenzoxazole Derivatives. ACS Chemical Neuroscience, 2016, 7, 1698-1705. | 3.5 | 7 |
| 61 | Investigation into Biological Environments through (Non)linear Optics: A Multiscale Study of Laurdan Derivatives. Journal of Chemical Theory and Computation, 2016, 12, 6169-6181. | 5.3 | 25 |
| 62 | A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid Î² Aggregates. Scientific Reports, 2016, 6, 23668. | 3.3 | 90 |
| 63 | First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF<sub>2</sub>) Core Complex. Journal of Physical Chemistry B, 2016, 120, 2323-2332. | 2.6 | 28 |
| 64 | Studies on an on/off-switchable immunosensor for troponin T. Biosensors and Bioelectronics, 2015, 73, 100-107. | 10.1 | 22 |
| 65 | One- and Two-Photon Absorption of a Spiropyranâ€“Merocyanine System: Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2015, 119, 1515-1522. | 2.6 | 23 |
| 66 | Relation between Nonlinear Optical Properties of Pushâ€“Pull Molecules and Metric of Charge Transfer Excitations. Journal of Chemical Theory and Computation, 2015, 11, 4182-4188. | 5.3 | 39 |
| 67 | Synthesis, spectral characterization and DFT analysis for the validation of 2, 6 diaryl -piperidin-4-ones as potential sunscreens and UV filters. Journal of Molecular Structure, 2015, 1099, 560-566. | 3.6 | 7 |
| 68 | Investigation of the Binding Profiles of AZD2184 and Thioflavin T with Amyloid-Î²(1â€“42) Fibril by Molecular Docking and Molecular Dynamics Methods. Journal of Physical Chemistry B, 2015, 119, 11560-11567. | 2.6 | 48 |
| 69 | Advanced Glycation End Products Modulate Structure and Drug Binding Properties of Albumin. Molecular Pharmaceutics, 2015, 12, 3312-3322. | 4.6 | 39 |
| 70 | Toward Fully Nonempirical Simulations of Optical Band Shapes of Molecules in Solution: A Case Study of Heterocyclic Ketoimine Difluoroborates. Journal of Physical Chemistry A, 2015, 119, 5145-5152. | 2.5 | 39 |
| 71 | Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. Journal of Physical Chemistry C, 2015, 119, 653-664. | 3.1 | 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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1010-1017. | 3.9 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Studies of pH-Sensitive Optical Properties of the deGFP1 Green Fluorescent Protein Using a Unique Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 3492-3502. | 5.3 | 5 |
| 74 | Promising two-photon probes for in vivo detection of Î² amyloid deposits. Chemical Communications, 2014, 50, 11694-11697. | 4.1 | 25 |
| 75 | Simulations of Light Absorption of Carbon Particles in Nanoaerosol Clusters. Journal of Physical Chemistry A, 2014, 118, 1879-1886. | 2.5 | 8 |
| 76 | Solvatochromism in a Pyridinium Cyclopentadienylide: Insights from a Sequential Carâ€“Parrinello QM/MM and TD-DFT/Semicontinuum Approach. Journal of Physical Chemistry B, 2014, 118, 7358-7366. | 2.6 | 2 |
| 77 | Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. Journal of Physical Chemistry B, 2014, 118, 1715-1725. | 2.6 | 19 |
| 78 | Role of Protonation State and Solvation on the pH Dependent Optical Properties of Bromocresol Green. Journal of Chemical Theory and Computation, 2014, 10, 3958-3968. | 5.3 | 3 |
| 79 | Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. Journal of Chemical Theory and Computation, 2014, 10, 778-788. | 5.3 | 12 |
| 80 | In silicomodeling and experimental evidence of coagulant protein interaction with precursors for nanoparticle functionalization. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1182-1190. | 3.5 | 6 |
| 81 | pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. Journal of Chemical Theory and Computation, 2013, 9, 3660-3669. | 5.3 | 12 |
| 82 | Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867. | 2.0 | 41 |
| 83 | EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. Physical Chemistry Chemical Physics, 2013, 15, 2427. | 2.8 | 4 |
| 84 | Twoâ€Photon Solvatochromism II: Experimental and Theoretical Study of Solvent Effects on the Twoâ€Photon Absorption Spectrum of Reichardtâ€™s Dye. ChemPhysChem, 2013, 14, 3731-3739. | 2.1 | 32 |
| 85 | Spatial spin-charge separation in neutral endohedral metallofullerene: A combined restricted open-shell MP2 and Carâ€“Parrinello molecular dynamics study. Chemical Physics Letters, 2013, 557, 71-75. | 2.6 | 0 |
| 86 | Hybrid density functionalâ€“molecular mechanics calculations for core-electron binding energies of glycine in water solution. Physical Chemistry Chemical Physics, 2013, 15, 244-254. | 2.8 | 15 |
| 87 | Solvent-Dependent Conformational States of a [2]Rotaxane-Based Molecular Machine: A Molecular Dynamics Perspective. Journal of Physical Chemistry C, 2013, 117, 25059-25068. | 3.1 | 12 |
| 88 | Association Dynamics and Linear and Nonlinear Optical Properties of an N-Acetylaladanamide Probe in a POPC Membrane. Journal of the American Chemical Society, 2013, 135, 13590-13597. | 13.7 | 27 |
| 89 | Revealing Spectral Features in Two-Photon Absorption Spectrum of Hoechst 33342: A Combined Experimental and Quantum-Chemical Study. Journal of Physical Chemistry B, 2013, 117, 12013-12019. | 2.6 | 22 |
| 90 | Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77. | 4.6 | 29 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Differences in first neighbor orientation behind the anomalies in the low and high density trans-1,2-dichloroethene liquid. Journal of Chemical Physics, 2012, 136, 124514. | 3.0 | 10 |
| 92 | Solvent Polarity-Induced Conformational Unlocking of Asparagine. Journal of Physical Chemistry A, 2012, 116, 11702-11708. | 2.5 | 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. Journal of Chemical Theory and Computation, 2012, 8, 4766-4774. | 5.3 | 8 |
| 94 | How Crucial Are Finite Temperature and Solvent Effects on Structure and Absorption Spectra of Si<sub>10</sub>?. Journal of Physical Chemistry C, 2012, 116, 26618-26624. | 3.1 | 4 |
| 95 | Al3+ induced planarization, conformational arrest and metallochromic shift in a pyrimidine dione dye: insight from integrated hybrid quantumâ€“classical calculations. Physical Chemistry Chemical Physics, 2012, 14, 2339. | 2.8 | 1 |
| 96 | Color modeling of protein optical probes. Physical Chemistry Chemical Physics, 2012, 14, 1107-1112. | 2.8 | 40 |
| 97 | Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263. | 5.3 | 19 |
| 98 | NMR Spinâ€“Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. Chemistry - A European Journal, 2012, 18, 11677-11684. | 3.3 | 14 |
| 99 | The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181. | 2.6 | 40 |
| 100 | Solvent Dependence of Structure, Charge Distribution, and Absorption Spectrum in the Photochromic Merocyanineâ^'Spiropyran Pair. Journal of Physical Chemistry B, 2011, 115, 4025-4032. | 2.6 | 43 |
| 101 | Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. Physical Chemistry Chemical Physics, 2011, 13, 12506. | 2.8 | 64 |
| 102 | Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358. | 2.6 | 20 |
| 103 | Modeling Solvatochromism of a Quinolinium Betaine Dye in Water Solvent Using Sequential Hybrid QM/MM and Semicontinuum Approach. Journal of Physical Chemistry B, 2011, 115, 1056-1061. | 2.6 | 18 |
| 104 | Density Functional Restrictedâ€“Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271. | 5.3 | 18 |
| 105 | Demystifying the solvatochromic reversal in Brookerâ€™s merocyanine dye. Physical Chemistry Chemical Physics, 2011, 13, 1290-1292. | 2.8 | 55 |
| 106 | Modeling solvatochromism of Nile red in water. International Journal of Quantum Chemistry, 2011, 111, 1521-1530. | 2.0 | 21 |
| 107 | Solvatochromic shift of phenol blue in water from a combined Carâ€“Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and <scp>ZINDO</scp> approach. Journal of Chemical Physics, 2010, 132, 234508. | 3.0 | 25 |
| 108 | Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357. | 2.6 | 52 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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. | 7.1 | 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. | 2.6 | 8 |
| 111 | Role of Dynamic Flexibility in Computing Solvatochromic Properties of Dyeâ^'Solvent Systems: o-Betaine in Water. Journal of Physical Chemistry A, 2009, 113, 2572-2577. | 2.5 | 27 |
| 112 | Thermal behavior of disordered phase of caffeine molecular crystal: Insights from Monte Carlo simulation studies. Journal of Chemical Physics, 2009, 130, 204514. | 3.0 | 14 |
| 113 | Conformations, structural transitions and visible near-infrared absorption spectra of four-, five- and six-coordinated Cu(<scp>ii</scp>) aqua complexes. Physical Chemistry Chemical Physics, 2009, 11, 508-519. | 2.8 | 51 |
| 114 | Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Carâ^'Parrinello Molecular Dynamics Investigation. Journal of Physical Chemistry A, 2009, 113, 4833-4839. | 2.5 | 23 |
| 115 | Solvent Dependence of Conformational Distribution, Molecular Geometry, and Electronic Structure in Adenosine. Journal of Physical Chemistry B, 2009, 113, 1012-1021. | 2.6 | 14 |
| 116 | Pressure dependence of crystal structure and molecular packing in anthracene. Molecular Physics, 2009, 107, 1689-1695. | 1.7 | 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. | 2.8 | 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. | 2.8 | 6 |
| 119 | Solvent Dependence on Conformational Transition, Dipole Moment, and Molecular Geometry of 1,2-Dichloroethane: Insight from Carâ^'Parrinello Molecular Dynamics Calculations. Journal of Physical Chemistry B, 2008, 112, 14673-14677. | 2.6 | 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. | 3.0 | 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. | 3.0 | 6 |
| 122 | Orientational Melting and Reorientational Motion in a Cubane Molecular Crystal: A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 23955-23962. | 2.6 | 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. | 2.6 | 3 |
| 124 | High-Pressure Study of Adamantane:Â Variable Shape Simulations up to 26 GPa. Journal of Physical Chemistry B, 2005, 109, 17296-17303. | 2.6 | 8 |
| 125 | Pressure Induced Orientational Ordering inp-Terphenyl. Journal of Physical Chemistry B, 2005, 109, 1433-1440. | 2.6 | 19 |
| 126 | Pressure-Induced Ordering in Adamantane: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2005, 109, 2014-2020. | 2.6 | 12 |

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|---|---|---|---|
| 127 | Structure, Energetics, and Dynamics of Pedal-Like Motion in Stilbene from Molecular Simulation and ab Initio Calculations. Journal of Physical Chemistry B, 2004, 108, 17403-17411. | 2.6 | 14 |
| 128 | High Pressure Phase of Biphenyl at Room Temperature:â€‰ A Monte Carlo Study. Journal of Physical Chemistry B, 2004, 108, 4178-4184. | 2.6 | 18 |