

Ramakrishnan Parthasarathi

List of Publications by Year in descending order

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113
papers

6,874
citations

61857

43
h-index

62479

80
g-index

114
all docs

114
docs citations

114
times ranked

7271
citing authors

#	ARTICLE	IF	CITATIONS
1	The dual role of phytochemicals on SARS-CoV-2 inhibition by targeting host and viral proteins. Journal of Traditional and Complementary Medicine, 2022, 12, 90-99.	1.5	15
2	Global, regional, and national sex differences in the global burden of tuberculosis by HIV status, 1990-2019: results from the Global Burden of Disease Study 2019. Lancet Infectious Diseases, The, 2022, 22, 222-241.	4.6	53
3	Developmental toxicity assessment of 4-MBC in Danio rerio embryo-larval stages. Science of the Total Environment, 2022, 804, 149920.	3.9	15
4	ToxDP2 Database: Toxicity prediction of dietary polyphenols. Food Chemistry, 2022, 370, 131350.	4.2	12
5	Computational risk assessment framework for the hazard analysis of bisphenols and quinone metabolites. Journal of Hazardous Materials, 2022, 426, 128031.	6.5	7
6	Artificial Intelligence in Clinical Toxicology. , 2022, , 1487-1501.		0
7	Integrated QSAR and Adverse Outcome Pathway Analysis of Chemicals Released on 3D Printing Using Acrylonitrile Butadiene Styrene. Chemical Research in Toxicology, 2021, 34, 355-364.	1.7	7
8	Analogue discovery of safer alternatives to HCQ and CQ drugs for SAR-CoV-2 by computational design. Computers in Biology and Medicine, 2021, 130, 104222.	3.9	12
9	Environmental survival of SARS-CoV-2 - A solid waste perspective. Environmental Research, 2021, 197, 111015.	3.7	46
10	In silico investigation and assessment of plausible novel tyrosinase inhibitory peptides from sesame seeds. LWT - Food Science and Technology, 2021, 147, 111619.	2.5	16
11	Chemical Reactivity and Skin Sensitization Studies on a Series of Chloro- and Fluoropyrroles - A Computational Approach. ACS Omega, 2021, 6, 21514-21524.	1.6	1
12	FOCUS-DB: An Online Comprehensive Database on Food Additive Safety. Journal of Chemical Information and Modeling, 2021, 61, 202-210.	2.5	3
13	Anti-hyperlipidaemic effects of synthetic analogues of nordihydroguaiaretic acid in dyslipidaemic rats. British Journal of Pharmacology, 2019, 176, 369-385.	2.7	4
14	IRMOF-74(<i>n</i>) - Mg: a novel catalyst series for hydrogen activation and hydrogenolysis of C=O bonds. Chemical Science, 2019, 10, 9880-9892.	3.7	23
15	In Silico Approaches in Predictive Genetic Toxicology. Methods in Molecular Biology, 2019, 2031, 351-373.	0.4	2
16	In Silico Approaches for Predictive Toxicology. , 2018, , 91-109.		19
17	Emerging Computational Methods for Predicting Chemically Induced Mutagenicity. , 2018, , 161-176.		1
18	One-pot integrated biofuel production using low-cost biocompatible protic ionic liquids. Green Chemistry, 2017, 19, 3152-3163.	4.6	115

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19	CO2 enabled process integration for the production of cellulosic ethanol using bionic liquids. <i>Energy and Environmental Science</i> , 2016, 9, 2822-2834.	15.6	63
20	Activation of lignocellulosic biomass for higher sugar yields using aqueous ionic liquid at low severity process conditions. <i>Biotechnology for Biofuels</i> , 2016, 9, 160.	6.2	44
21	Rapid room temperature solubilization and depolymerization of polymeric lignin at high loadings. <i>Green Chemistry</i> , 2016, 18, 6012-6020.	4.6	60
22	Impact of engineered lignin composition on biomass recalcitrance and ionic liquid pretreatment efficiency. <i>Green Chemistry</i> , 2016, 18, 4884-4895.	4.6	64
23	MOF-Based Catalysts for Selective Hydrogenolysis of Carbon-Oxygen Ether Bonds. <i>ACS Catalysis</i> , 2016, 6, 55-59.	5.5	82
24	Recent innovations in analytical methods for the qualitative and quantitative assessment of lignin. <i>Renewable and Sustainable Energy Reviews</i> , 2015, 49, 871-906.	8.2	282
25	Concomitant Laparoscopic Intraperitoneal Onlay Mesh Repair with Other Clean Contaminated Procedures—Study of Feasibility and Safety. <i>Journal of Laparoendoscopic and Advanced Surgical Techniques - Part A</i> , 2015, 25, 33-36.	0.5	7
26	Theoretical Insights into the Role of Water in the Dissolution of Cellulose Using IL/Water Mixed Solvent Systems. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14339-14349.	1.2	46
27	Design of low-cost ionic liquids for lignocellulosic biomass pretreatment. <i>Green Chemistry</i> , 2015, 17, 1728-1734.	4.6	384
28	Efficient biomass pretreatment using ionic liquids derived from lignin and hemicellulose. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E3587-95.	3.3	285
29	Understanding the role of water during ionic liquid pretreatment of lignocellulose: co-solvent or anti-solvent?. <i>Green Chemistry</i> , 2014, 16, 3830-3840.	4.6	129
30	Understanding pretreatment efficacy of four cholinium and imidazolium ionic liquids by chemistry and computation. <i>Green Chemistry</i> , 2014, 16, 2546-2557.	4.6	138
31	Structure and dynamics of a complex of cellulose with EDA: insights into the action of amines on cellulose. <i>Cellulose</i> , 2013, 20, 1563-1571.	2.4	18
32	Embedded Single-Walled Carbon Nanotubes Locally Perturb DOPC Phospholipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12769-12782.	1.2	18
33	Photodissociation of Charge Tagged Peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1182-1190.	1.2	12
34	The role of H... interaction in the stabilization of benzene and adamantane clusters#. <i>Journal of Chemical Sciences</i> , 2012, 124, 193-202.	0.7	12
35	Understanding the interaction of Lipoarabinomannan with membrane mimetic architectures. <i>Tuberculosis</i> , 2012, 92, 38-47.	0.8	22
36	Density Functional Theory Studies on Ice Nanotubes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12841-12851.	1.1	9

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37	Elucidation of Carbohydrate-Phospholipid Interactions - a Quantum Chemical Study. <i>Biophysical Journal</i> , 2011, 100, 332a.	0.2	0
38	Theoretical Study of the Remarkably Diverse Linkages in Lignin. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2660-2666.	2.1	335
39	Role of Phospholipid Head Groups in Silver Nanoparticles Interaction with Membranes. <i>Biophysical Journal</i> , 2011, 100, 628a.	0.2	0
40	Insights into Hydrogen Bonding and Stacking Interactions in Cellulose. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14191-14202.	1.1	122
41	Quantum Chemical Study of Carbohydrate-Phospholipid Interactions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12826-12840.	1.1	7
42	Combustion synthesis of nanocrystalline nickel ferrite using hexamine as a fuel. <i>International Journal of Self-Propagating High-Temperature Synthesis</i> , 2011, 20, 236-240.	0.2	7
43	Bonding, aromaticity, and structure of trigonal dianion metal clusters. <i>Journal of Computational Chemistry</i> , 2010, 31, 1815-1821.	1.5	27
44	New Insights into the Vacuum UV Photodissociation of Peptides. <i>Journal of the American Chemical Society</i> , 2010, 132, 1606-1610.	6.6	49
45	Ab Initio and DFT Studies on Methanol-Water Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2250-2258.	1.1	89
46	Nature and Kinetic Analysis of Carbon-Carbon Bond Fragmentation Reactions of Cation Radicals Derived from SET-Oxidation of Lignin Model Compounds. <i>Journal of Organic Chemistry</i> , 2010, 75, 6549-6562.	1.7	88
47	Synthesis and DNA-binding studies of two ruthenium(II) complexes of an intercalating ligand. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 2044-2051.	2.6	74
48	Molecular mechanics and molecular dynamics study on azurin using extensible and systematic force field (ESFF). <i>Computational and Theoretical Chemistry</i> , 2009, 907, 1-8.	1.5	2
49	Molecular Dynamics Investigations on the Effect of Amino Acid Substitution in a Triple-Helix Structure and the Stability of Collagen. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8983-8992.	1.2	27
50	Structure and Stability of Water Chains (H ₂ O) _n , n = 5-20. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3744-3749.	1.1	32
51	A molecular dynamics analysis of ion pairs formed by lysine in collagen: Implication for collagen function and stability. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 299-312.	1.5	9
52	Role of Length-Dependent Stability of Collagen-like Peptides. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1533-1539.	1.2	21
53	Helix Forming Tendency of Valine Substituted Poly-Alanine: A Molecular Dynamics Investigation. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9100-9104.	1.2	7
54	Electron Density Topography, NMR, and NBO Analysis of Water Clusters. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2008, 38, 18-27.	0.6	19

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55	Safety and Efficacy of Laparoscopic Surgery in Pregnancy: Experience of a Single Institution. Journal of Laparoendoscopic and Advanced Surgical Techniques - Part A, 2007, 17, 186-190.	0.5	52
56	Bader's Electron Density Analysis of Hydrogen Bonding in Secondary Structural Elements of Protein. Journal of Physical Chemistry A, 2007, 111, 7141-7148.	1.1	54
57	Hydrogen Bonding in Protonated Water Clusters: An Atoms-in-Molecules Perspective. Journal of Physical Chemistry A, 2007, 111, 13287-13290.	1.1	40
58	Solvation of H ₃ O ⁺ by Phenol: Hydrogen Bonding vs π Complexation. Journal of Physical Chemistry A, 2007, 111, 2-5.	1.1	14
59	Electrophilicity-Based Charge Transfer Descriptor. Journal of Physical Chemistry A, 2007, 111, 1358-1361.	1.1	401
60	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
61	Philicity based site activation model towards understanding the Markovnikov regioselectivity rule. Computational and Theoretical Chemistry, 2007, 804, 17-20.	1.5	11
62	Chemical reactivity patterns of [n]paracyclophanes. Computational and Theoretical Chemistry, 2007, 820, 1-6.	1.5	10
63	An atom counting strategy towards analyzing the biological activity of sex hormones. European Journal of Medicinal Chemistry, 2007, 42, 1365-1369.	2.6	39
64	Using QSPR Models to Predict the Enthalpy of Vaporization of 209 Polychlorinated Biphenyl Congeners. QSAR and Combinatorial Science, 2007, 26, 227-237.	1.5	20
65	Europium complex of a tridentate ligand: synthesis and spectroscopic properties. Transition Metal Chemistry, 2007, 32, 362-366.	0.7	8
66	An atom counting and electrophilicity based QSTR approach. Journal of Chemical Sciences, 2007, 119, 475-488.	0.7	23
67	Characterization of Hydrogen Bonding: From van der Waals Interactions to Covalency. , 2006, , 1-50.		16
68	Role of Aspartic Acid in Collagen Structure and Stability: A Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2006, 110, 20678-20685.	1.2	27
69	Group Philicity and Electrophilicity as Possible Descriptors for Modeling Ecotoxicity Applied to Chlorophenols. Chemical Research in Toxicology, 2006, 19, 356-364.	1.7	101
70	Hydrogen Bonding without Borders: An Atoms-in-Molecules Perspective. Journal of Physical Chemistry A, 2006, 110, 3349-3351.	1.1	369
71	Chemical Reactivity Indices for the Complete Series of Chlorinated Benzenes: Solvent Effect. Journal of Physical Chemistry A, 2006, 110, 2739-2745.	1.1	47
72	Hydrogen Peroxide Clusters: The Role of Open Book Motif in Cage and Helical Structures. Journal of Physical Chemistry A, 2006, 110, 6294-6300.	1.1	33

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73	Molecular Orbital Calculations on Polythiophenes Containing Heterocyclic Substituents: Effect of Structure on Electronic Transitions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14078-14086.	1.2	0
74	Theoretical Study on the Complete Series of Chloroanilines. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9900-9907.	1.1	12
75	Structure and properties of polythiophene containing hetero aromatic side chains. <i>Computational Materials Science</i> , 2006, 37, 318-322.	1.4	27
76	pKa Prediction Using Group Philicity. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6540-6544.	1.1	64
77	An Electrophilicity Based Analysis of Toxicity of Aromatic Compounds Towards <i>Tetrahymena Pyriformis</i> . <i>QSAR and Combinatorial Science</i> , 2006, 25, 114-122.	1.5	32
78	Alkylation of enolates: An electrophilicity perspective. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 852-862.	1.0	11
79	Hydrogen bonding of DNA base pairs and information entropy: From molecular electron density perspective. <i>Chemical Physics Letters</i> , 2006, 418, 530-534.	1.2	24
80	QSPR models for polychlorinated biphenyls: n-Octanol/water partition coefficient. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 1021-1028.	1.4	83
81	Interaction of chromium(III) complex of chiral binaphthyl tetradentate ligand with DNA. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 3300-3306.	1.4	60
82	Do properties of bovine serum albumin at fluid/electrolyte interface follow the Hofmeister series? An analysis using Langmuir and Langmuir-Blodgett films. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2006, 1764, 1767-1774.	1.1	11
83	Molecular modeling and atomistic simulation strategies to determine surface properties of perfluorinated homopolymers and their random copolymers. <i>Polymer</i> , 2006, 47, 6914-6924.	1.8	55
84	Synthesis, characterization and DNA-binding properties of rac-[Ru(5,6-dmp)2(dppz)]2+ Enantiopreferential DNA binding and co-ligand promoted exciton coupling. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 3-17.	1.5	86
85	Toxicity analysis of polychlorinated dibenzofurans through global and local electrophilicities. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 119-125.	1.5	50
86	Chemical information insights into the series of chloroanisoles A theoretical approach. <i>Computational and Theoretical Chemistry</i> , 2006, 774, 49-57.	1.5	10
87	Careful Scrutiny of the Philicity Concept. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1084-1093.	1.1	87
88	Analyzing Toxicity Through Electrophilicity. <i>Molecular Diversity</i> , 2006, 10, 119-131.	2.1	115
89	Computation of density of perfluoroalkyl methacrylates: a molecular modeling approach. <i>Theoretical Chemistry Accounts</i> , 2006, 117, 167-169.	0.5	6
90	Enantiopreferential DNA Binding: [(5,6-dmp)2Ru(1/4-bpm)]4+ Induces a B-to-Z Conformational Change on DNA. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 835-844.	2.0	26

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91	Synthesis, Spectral Characterization, and DNA Binding Studies of trans-[Dichlorobis(2,3-dicyanodipyrido-N8,9-[3,2-f:2â€²,3â€²-h]quinoxaline)chromium(III)] Perchlorate Dihydrate. Bulletin of the Chemical Society of Japan, 2005, 78, 270-276.	2.0	10
92	Electrophilicity as a possible descriptor for toxicity prediction. Bioorganic and Medicinal Chemistry, 2005, 13, 3405-3412.	1.4	173
93	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
94	Chemical reactivity analysis on 3,3',4,4'-hexachlorobiphenyl: A DFT approach. Computational and Theoretical Chemistry, 2005, 730, 221-226.	1.5	15
95	Variation of electrophilicity during molecular vibrations and internal rotations. Theoretical Chemistry Accounts, 2005, 113, 257-266.	0.5	135
96	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	0.7	29
97	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	0.7	36
98	Stacking Interactions in Benzene and Cytosine Dimers: From Molecular Electron Density Perspective. Structural Chemistry, 2005, 16, 243-255.	1.0	39
99	DFT study of some aliphatic amines using generalized philicity concept. International Journal of Quantum Chemistry, 2005, 101, 690-702.	1.0	35
100	Molecular Structure, Reactivity, and Toxicity of the Complete Series of Chlorinated Benzenes. Journal of Physical Chemistry A, 2005, 109, 11043-11049.	1.1	46
101	Quantum chemical studies on polythiophenes containing heterocyclic substituents: Effect of structure on the band gap. Journal of Chemical Physics, 2005, 123, 164905.	1.2	32
102	Hydrogen Bonding in Phenol, Water, and Phenolâ€³Water Clusters. Journal of Physical Chemistry A, 2005, 109, 843-850.	1.1	160
103	Bowls, Balls and Sheets of Boric Acid Clusters: The Role of Pentagon and Hexagon Motifs. Journal of Physical Chemistry A, 2005, 109, 8587-8593.	1.1	15
104	Molecular dipoles at substrate/film interfaces influencing surface energy of Langmuirâ€“Blodgett films. Journal of Colloid and Interface Science, 2004, 271, 419-425.	5.0	7
105	Effect of solvation on the condensed Fukui function and the generalized philicity index. Chemical Physics Letters, 2004, 383, 122-128.	1.2	80
106	Intermolecular reactivity through the generalized philicity concept. Chemical Physics Letters, 2004, 394, 225-230.	1.2	225
107	Bader's and Reactivity Descriptors' Analysis of DNA Base Pairs. Journal of Physical Chemistry A, 2004, 108, 3817-3828.	1.1	76
108	Electrophilicity index as a possible descriptor of biological activity. Bioorganic and Medicinal Chemistry, 2004, 12, 5533-5543.	1.4	363

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109	Ab initio and density functional theory based studies on collagen triplets. Theoretical Chemistry Accounts, 2003, 110, 19-27.	0.5	8
110	Effect of electric field on the global and local reactivity indices. Chemical Physics Letters, 2003, 382, 48-56.	1.2	76
111	Density functional theory calculations on dipeptide-gallic acid interaction. Chemical Physics Letters, 2003, 369, 131-138.	1.2	8
112	Chemical Reactivity Profiles of Two Selected Polychlorinated Biphenyls. Journal of Physical Chemistry A, 2003, 107, 10346-10352.	1.1	156
113	Modeling Ecotoxicity as Applied to some Selected Aromatic Compounds. , 0, , 1-24.		2