Ramakrishnan Parthasarathi

List of Publications by Year
in descending order

113 papers	6,874 citations	61945 43 h-index	62565 80 g-index
114 all docs	114 docs citations	114 times ranked	7271 citing authors

#	Article	IF	Citations
1	Electrophilicity-Based Charge Transfer Descriptor. Journal of Physical Chemistry A, 2007, 111, 1358-1361.	1.1	401
2	Design of low-cost ionic liquids for lignocellulosic biomass pretreatment. Green Chemistry, 2015, 17, 1728-1734.	4.6	384
3	Hydrogen Bonding without Borders:Â An Atoms-in-Molecules Perspective. Journal of Physical Chemistry A, 2006, 110, 3349-3351.	1.1	369
4	Electrophilicity index as a possible descriptor of biological activity. Bioorganic and Medicinal Chemistry, 2004, 12, 5533-5543.	1.4	363
5	Theoretical Study of the Remarkably Diverse Linkages in Lignin. Journal of Physical Chemistry Letters, 2011, 2, 2660-2666.	2.1	335
6	Efficient biomass pretreatment using ionic liquids derived from lignin and hemicellulose. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3587-95.	3.3	285
7	Recent innovations in analytical methods for the qualitative and quantitative assessment of lignin. Renewable and Sustainable Energy Reviews, 2015, 49, 871-906.	8.2	282
8	Intermolecular reactivity through the generalized philicity concept. Chemical Physics Letters, 2004, 394, 225-230.	1.2	225
9	Electrophilicity as a possible descriptor for toxicity prediction. Bioorganic and Medicinal Chemistry, 2005, 13, 3405-3412.	1.4	173
10	Hydrogen Bonding in Phenol, Water, and Phenolâ^'Water Clusters. Journal of Physical Chemistry A, 2005, 109, 843-850.	1.1	160
11	Chemical Reactivity Profiles of Two Selected Polychlorinated Biphenyls. Journal of Physical Chemistry A, 2003, 107, 10346-10352.	1.1	156
12	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
13	Understanding pretreatment efficacy of four cholinium and imidazolium ionic liquids by chemistry and computation. Green Chemistry, 2014, 16, 2546-2557.	4.6	138
14	Variation of electrophilicity during molecular vibrations and internal rotations. Theoretical Chemistry Accounts, 2005, 113, 257-266.	0.5	135
15	Understanding the role of water during ionic liquid pretreatment of lignocellulose: co-solvent or anti-solvent?. Green Chemistry, 2014, 16, 3830-3840.	4.6	129
16	Insights into Hydrogen Bonding and Stacking Interactions in Cellulose. Journal of Physical Chemistry A, 2011, 115, 14191-14202.	1.1	122
17	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	2.1	115
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	Group Philicity and Electrophilicity as Possible Descriptors for Modeling Ecotoxicity Applied to Chlorophenols. Chemical Research in Toxicology, 2006, 19, 356-364.	1.7	101
20	Ab Initio and DFT Studies on Methanolâ^'Water Clusters. Journal of Physical Chemistry A, 2010, 114, 2250-2258.	1.1	89
21	Nature and Kinetic Analysis of Carbonâ^'Carbon Bond Fragmentation Reactions of Cation Radicals Derived from SET-Oxidation of Lignin Model Compounds. Journal of Organic Chemistry, 2010, 75, 6549-6562.	1.7	88
22	Careful Scrutiny of the Philicity Concept. Journal of Physical Chemistry A, 2006, 110, 1084-1093.	1.1	87
23	Synthesis, characterization and DNA-binding properties of rac-[Ru(5,6-dmp)2(dppz)]2+ â€“ Enantiopreferential DNA binding and co-ligand promoted exciton coupling. Journal of Inorganic Biochemistry, 2006, 100, 3-17.	1.5	86
24	QSPR models for polychlorinated biphenyls: n-Octanol/water partition coefficient. Bioorganic and Medicinal Chemistry, 2006, 14, 1021-1028.	1.4	83
25	MOF-Based Catalysts for Selective Hydrogenolysis of Carbonâ€“Oxygen Ether Bonds. ACS Catalysis, 2016, 6, 55-59.	5.5	82
26	Effect of solvation on the condensed Fukui function and the generalized philicity index. Chemical Physics Letters, 2004, 383, 122-128.	1.2	80
27	Effect of electric field on the global and local reactivity indices. Chemical Physics Letters, 2003, 382, 48-56.	1.2	76
28	Bader's and Reactivity Descriptors' Analysis of DNA Base Pairs. Journal of Physical Chemistry A, 2004, 108, 3817-3828.	1.1	76
29	Synthesis and DNA-binding studies of two ruthenium(II) complexes of an intercalating ligand. European Journal of Medicinal Chemistry, 2009, 44, 2044-2051.	2.6	74
30	pKa Prediction Using Group Philicity. Journal of Physical Chemistry A, 2006, 110, 6540-6544.	1.1	64
31	Impact of engineered lignin composition on biomass recalcitrance and ionic liquid pretreatment efficiency. Green Chemistry, 2016, 18, 4884-4895.	4.6	64
32	CO2 enabled process integration for the production of cellulosic ethanol using bionic liquids. Energy and Environmental Science, 2016, 9, 2822-2834.	15.6	63
33	Interaction of chromium(III) complex of chiral binaphthyl tetradentate ligand with DNA. Bioorganic and Medicinal Chemistry, 2006, 14, 3300-3306.	1.4	60
34	Rapid room temperature solubilization and depolymerization of polymeric lignin at high loadings. Green Chemistry, 2016, 18, 6012-6020.	4.6	60
35	Molecular modeling and atomistic simulation strategies to determine surface properties of perfluorinated homopolymers and their random copolymers. Polymer, 2006, 47, 6914-6924.	1.8	55
36	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

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37	Global, regional, and national sex differences in the global burden of tuberculosis by HIV status, 1990â€“2019: results from the Global Burden of Disease Study 2019. Lancet Infectious Diseases, The, 2022, 22, 222-241.	4.6	53
38	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
39	Toxicity analysis of polychlorinated dibenzofurans through global and local electrophilicities. Computational and Theoretical Chemistry, 2006, 758, 119-125.	1.5	50
40	New Insights into the Vacuum UV Photodissociation of Peptides. Journal of the American Chemical Society, 2010, 132, 1606-1610.	6.6	49
41	Chemical Reactivity Indices for the Complete Series of Chlorinated Benzenes:Â Solvent Effect. Journal of Physical Chemistry A, 2006, 110, 2739-2745.	1.1	47
42	Molecular Structure, Reactivity, and Toxicity of the Complete Series of Chlorinated Benzenes. Journal of Physical Chemistry A, 2005, 109, 11043-11049.	1.1	46
43	Theoretical Insights into the Role of Water in the Dissolution of Cellulose Using IL/Water Mixed Solvent Systems. Journal of Physical Chemistry B, 2015, 119, 14339-14349.	1.2	46
44	Environmental survival of SARS-CoV-2 â€“ A solid waste perspective. Environmental Research, 2021, 197, 111015.	3.7	46
45	Activation of lignocellulosic biomass for higher sugar yields using aqueous ionic liquid at low severity process conditions. Biotechnology for Biofuels, 2016, 9, 160.	6.2	44
46	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
47	Hydrogen Bonding in Protonated Water Clusters:â€‰ An Atoms-in-Molecules Perspective. Journal of Physical Chemistry A, 2007, 111, 13287-13290.	1.1	40
48	Stacking Interactions in Benzene and Cytosine Dimers: From Molecular Electron Density Perspective. Structural Chemistry, 2005, 16, 243-255.	1.0	39
49	An atom counting strategy towards analyzing the biological activity of sex hormones. European Journal of Medicinal Chemistry, 2007, 42, 1365-1369.	2.6	39
50	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	0.7	36
51	DFT study of some aliphatic amines using generalized philicity concept. International Journal of Quantum Chemistry, 2005, 101, 690-702.	1.0	35
52	Hydrogen Peroxide Clusters:Â The Role of Open Book Motif in Cage and Helical Structures. Journal of Physical Chemistry A, 2006, 110, 6294-6300.	1.1	33
53	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
54	An Electrophilicity Based Analysis of Toxicity of Aromatic Compounds TowardsTetrahymena Pyriformis. QSAR and Combinatorial Science, 2006, 25, 114-122.	1.5	32

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55	Structure and Stability of Water Chains (H2O)n, n = 5â^'20. Journal of Physical Chemistry A, 2009, 113, 3744-3749.	1.1	32
56	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	0.7	29
57	Role of Aspartic Acid in Collagen Structure and Stability:Â A Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2006, 110, 20678-20685.	1.2	27
58	Structure and properties of polythiophene containing hetero aromatic side chains. Computational Materials Science, 2006, 37, 318-322.	1.4	27
59	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	1.5	27
60	Molecular Dynamics Investigations on the Effect of <scp>d</scp> Amino Acid Substitution in a Triple-Helix Structure and the Stability of Collagen. Journal of Physical Chemistry B, 2009, 113, 8983-8992.	1.2	27
61	Enantiopreferential DNA Binding: [{(5,6-dmp)2Ru}2(Î¼-bpm)]4+Induces a B-to-Z Conformational Change on DNA. Bulletin of the Chemical Society of Japan, 2005, 78, 835-844.	2.0	26
62	Hydrogen bonding of DNA base pairs and information entropy: From molecular electron density perspective. Chemical Physics Letters, 2006, 418, 530-534.	1.2	24
63	An atom counting and electrophilicity based QSTR approach. Journal of Chemical Sciences, 2007, 119, 475-488.	0.7	23
64	IRMOF-74(n)â€“Mg: a novel catalyst series for hydrogen activation and hydrogenolysis of Câ€“O bonds. Chemical Science, 2019, 10, 9880-9892.	3.7	23
65	Understanding the interaction of Lipoarabinomannan with membrane mimetic architectures. Tuberculosis, 2012, 92, 38-47.	0.8	22
66	Role of Length-Dependent Stability of Collagen-like Peptides. Journal of Physical Chemistry B, 2008, 112, 1533-1539.	1.2	21
67	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
68	Electron Density Topography, NMR, and NBO Analysis of Water Clusters. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2008, 38, 18-27.	0.6	19
69	In Silico Approaches for Predictive Toxicology. , 2018, , 91-109.		19
70	Embedded Single-Walled Carbon Nanotubes Locally Perturb DOPC Phospholipid Bilayers. Journal of Physical Chemistry B, 2012, 116, 12769-12782.	1.2	18
71	Structure and dynamics of a complex of cellulose with EDA: insights into the action of amines on cellulose. Cellulose, 2013, 20, 1563-1571.	2.4	18
72	Characterization of Hydrogen Bonding: From van der Waals Interactions to Covalency. , 2006, , 1-50.		16

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73	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
74	Chemical reactivity analysis on 33â€²44â€²55â€²-hexa chlorobiphenylâ€"A DFT approach. Computational and Theoretical Chemistry, 2005, 730, 221-226.	1.5	15
75	Bowls, Balls and Sheets of Boric Acid Clusters:Â The Role of Pentagon and Hexagon Motifs. Journal of Physical Chemistry A, 2005, 109, 8587-8593.	1.1	15
76	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
77	Developmental toxicity assessment of 4-MBC in Danio rerio embryo-larval stages. Science of the Total Environment, 2022, 804, 149920.	3.9	15
78	Solvation of H3O+by Phenol:Â Hydrogen Bonding vs Ï€ Complexation. Journal of Physical Chemistry A, 2007, 111, 2-5.	1.1	14
79	Theoretical Study on the Complete Series of Chloroanilines. Journal of Physical Chemistry A, 2006, 110, 9900-9907.	1.1	12
80	Photodissociation of Charge Tagged Peptides. Journal of the American Society for Mass Spectrometry, 2012, 23, 1182-1190.	1.2	12
81	The role of Câ€"H...Ï€ interaction in the stabilization of benzene and adamantane clusters#. Journal of Chemical Sciences, 2012, 124, 193-202.	0.7	12
82	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
83	ToxDP2 Database: Toxicity prediction of dietary polyphenols. Food Chemistry, 2022, 370, 131350.	4.2	12
84	Alkylation of enolates: An electrophilicity perspective. International Journal of Quantum Chemistry, 2006, 106, 852-862.	1.0	11
85	Do properties of bovine serum albumin at fluid/electrolyte interface follow the Hofmeister series?â€"An analysis using Langmuir and Langmuirâ€"Blodgett films. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1767-1774.	1.1	11
86	Philicity based site activation model towards understanding the Markovnikov regioselectivity rule. Computational and Theoretical Chemistry, 2007, 804, 17-20.	1.5	11
87	Synthesis, Spectral Characterization, and DNA Binding Studies oftrans-[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
88	Chemical information insights into the series of chloroanisoles â€" A theoretical approach. Computational and Theoretical Chemistry, 2006, 774, 49-57.	1.5	10
89	Chemical reactivity patterns of [n]paracyclophanes. Computational and Theoretical Chemistry, 2007, 820, 1-6.	1.5	10
90	A molecular dynamics analysis of ion pairs formed by lysine in collagen: Implication for collagen function and stability. Computational and Theoretical Chemistry, 2008, 851, 299-312.	1.5	9

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91	Density Functional Theory Studies on Ice Nanotubes. Journal of Physical Chemistry A, 2011, 115, 12841-12851.	1.1	9
92	Ab initio and density functional theory based studies on collagen triplets. Theoretical Chemistry Accounts, 2003, 110, 19-27.	0.5	8
93	Density functional theory calculations on dipeptideâ€“gallic acid interaction. Chemical Physics Letters, 2003, 369, 131-138.	1.2	8
94	Europium complex of a tridentate ligand: synthesis and spectroscopic properties. Transition Metal Chemistry, 2007, 32, 362-366.	0.7	8
95	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
96	Helix Forming Tendency of Valine Substituted Poly-Alanine: A Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2008, 112, 9100-9104.	1.2	7
97	Quantum Chemical Study of Carbohydrateâ€“Phospholipid Interactions. Journal of Physical Chemistry A, 2011, 115, 12826-12840.	1.1	7
98	Combustion synthesis of nanocrystalline nickel ferrite using hexamine as a fuel. International Journal of Self-Propagating High-Temperature Synthesis, 2011, 20, 236-240.	0.2	7
99	Concomitant Laparoscopic Intraperitoneal Onlay Mesh Repair with Other Clean Contaminated Proceduresâ€”Study of Feasibility and Safety. Journal of Laparoendoscopic and Advanced Surgical Techniques - Part A, 2015, 25, 33-36.	0.5	7
100	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
101	Computational risk assessment framework for the hazard analysis of bisphenols and quinone metabolites. Journal of Hazardous Materials, 2022, 426, 128031.	6.5	7
102	Computation of density of perfluoroalkyl methacrylates: a molecular modeling approach. Theoretical Chemistry Accounts, 2006, 117, 167-169.	0.5	6
103	Antiâ€hyperlipidaemic effects of synthetic analogues of nordihydroguaiaretic acid in dyslipidaemic rats. British Journal of Pharmacology, 2019, 176, 369-385.	2.7	4
104	FOCUS-DB: An Online Comprehensive Database on Food Additive Safety. Journal of Chemical Information and Modeling, 2021, 61, 202-210.	2.5	3
105	Molecular mechanics and molecular dynamics study on azurin using extensible and systematic force field (ESFF). Computational and Theoretical Chemistry, 2009, 907, 1-8.	1.5	2
106	Modeling Ecotoxicity as Applied to some Selected Aromatic Compounds. , 0, , 1-24.		2
107	In Silico Approaches in Predictive Genetic Toxicology. Methods in Molecular Biology, 2019, 2031, 351-373.	0.4	2
108	Emerging Computational Methods for Predicting Chemically Induced Mutagenicity. , 2018, , 161-176.		1

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109	Chemical Reactivity and Skin Sensitization Studies on a Series of Chloro- and Fluoropyrrolesâ€"A Computational Approach. ACS Omega, 2021, 6, 21514-21524.	1.6	1
110	Molecular Orbital Calculations on Polythiophenes Containing Heterocyclic Substituents:Â Effect of Structure on Electronic Transitions. Journal of Physical Chemistry B, 2006, 110, 14078-14086.	1.2	0
111	Elucidation of Carbohydrate-Phospholipid Interactions - a Quantum Chemical Study. Biophysical Journal, 2011, 100, 332a.	0.2	0
112	Role of Phospholipid Head Groups in Silver Nanoparticles Interaction with Membranes. Biophysical Journal, 2011, 100, 628a.	0.2	0
113	Artificial Intelligence in Clinical Toxicology. , 2022, , 1487-1501.		0