Elango Munusamy

List of Publications by Year
in descending order

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44 papers	1,866 citations	236612 25 h-index	253896 43 g-index
44 all docs	44 docs citations	44 times ranked	1987 citing authors

#	Article	IF	Citations
1	Intermolecular reactivity through the generalized philicity concept. Chemical Physics Letters, 2004, 394, 225-230.	1.2	225
2	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
3	Temperature dependence of chemical and biophysical rate processes: Phenomenological approach to deviations from Arrhenius law. Chemical Physics Letters, 2010, 498, 209-213.	1.2	138
4	Variation of electrophilicity during molecular vibrations and internal rotations. Theoretical Chemistry Accounts, 2005, 113, 257-266.	0.5	135
5	Stability and Reactivity of All-Metal Aromatic and Antiaromatic Systems in Light of the Principles of Maximum Hardness and Minimum Polarizability. Journal of Physical Chemistry A, 2005, 109, 9590-9597.	1.1	94
6	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
7	pKa Prediction Using Group Philicity. Journal of Physical Chemistry A, 2006, 110, 6540-6544.	1.1	64
8	Copper(II) Terpyridine Complexes: Effect of Substituent on DNA Binding and Nuclease Activity. European Journal of Inorganic Chemistry, 2007, 2007, 3484-3490.	1.0	56
9	Synthesis of Unsymmetrical Substituted 1,4-Dihydropyridines through Thermal and Microwave Assisted [4+2] Cycloadditions of 1-Azadienes and Allenic Esters. Journal of Organic Chemistry, 2008, 73, 2224-2233.	1.7	55
10	Initial Hardness Response and Hardness Profiles in the Study of Woodwardâ€“Hoffmann Rules for Electrocyclizations. Journal of Chemical Theory and Computation, 2008, 4, 595-602.	2.3	51
11	Time-Resolved Surface-Enhanced Coherent Sensing of Nanoscale Molecular Complexes. Scientific Reports, 2012, 2, 891.	1.6	50
12	Quantum Chemistry of C₃H₆O Molecules: Structure and Stability, Isomerization Pathways, and Chirality Changing Mechanisms. Journal of Physical Chemistry A, 2010, 114, 9864-9874.	1.1	49
13	Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. International Journal of Quantum Chemistry, 2011, 111, 318-332.	1.0	48
14	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
15	Chemical reactivity descriptor based aromaticity indices applied to and systems. Computational and Theoretical Chemistry, 2006, 759, 109-110.	1.5	39
16	On the Nature of the Stabilization of Benzeneâ‹…â‹…â‹…Dihalogen and Benzeneâ‹…â‹…â‹…Dinitrogen Complexes: CCSD(T)/CBS and DFTâ€“SAPT Calculations. ChemPhysChem, 2011, 12, 3253-3261.	1.0	38
17	Structure, Energetics, and Reactivity of Boric Acid Nanotubes: A Molecular Tailoring Approach. Journal of Physical Chemistry A, 2008, 112, 7699-7704.	1.1	36
18	Carbohydrate-Aromatic Interactions: The Role of Curvature on XHÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 2010, 114, 4313-4324.	1.1	35

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19	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
20	Structure and Stability of Water Chains (H2O)n, n = 5â˜’20. Journal of Physical Chemistry A, 2009, 113, 3744-3749.	1.1	32
21	Novel saccharideâ€“pyridine based gelators: selective gelation and diversity in superstructures. New Journal of Chemistry, 2009, 33, 1570.	1.4	30
22	Adsorption of hydrogen molecules on the alkali metal ion decorated boric acid clusters: A density functional theory investigation. International Journal of Hydrogen Energy, 2011, 36, 3922-3931.	3.8	30
23	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	0.7	29
24	Domino routes to substituted benzoindolizines: tandem reorganization of 1,3-dipolar cycloadducts of nitrones with allenic esters/ketones and alternative cycloadditionâ€“palladium catalyzed cyclization pathway. Tetrahedron, 2009, 65, 4593-4603.	1.0	28
25	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	1.5	27
26	Evolution of Aggregate Structure in Solutions of Anionic Monorhamnolipids: Experimental and Computational Results. Langmuir, 2017, 33, 7412-7424.	1.6	27
27	Design, synthesis and conformational analysis of turn inducer cyclopropane scaffolds: microwave assisted amidation of unactivated esters on catalytic solid support to obtain Î³-turn mimic scaffolds. Tetrahedron, 2009, 65, 240-246.	1.0	25
28	Investigations on synthesis of indole based constrained mimetic scaffolds through 1,3-dipolar cycloadditions of the C-(3-indolyl)-N-phenylnitrone with a variety of olefinic and allenic dipolarophiles under microwave irradiation. Tetrahedron, 2009, 65, 5928-5935.	1.0	24
29	Structural Properties of Nonionic Monorhamnolipid Aggregates in Water Studied by Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 5781-5793.	1.2	23
30	Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. Journal of Chemical Physics, 2013, 139, 094703.	1.2	22
31	Unraveling the Differential Aggregation of Anionic and Nonionic Monorhamnolipids at Airâ€“Water and Oilâ€“Water Interfaces: A Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 6403-6416.	1.2	21
32	A Classical Molecular Dynamics Simulation Study of Interfacial and Bulk Solution Aggregation Properties of Dirhamnolipids. Journal of Physical Chemistry B, 2020, 124, 814-827.	1.2	17
33	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
34	Quantum chemical and dynamical approaches to intra and intermolecular kinetics: The C_nH_{2n}O (n = 1, 2, 3) molecules. International Journal of Quantum Chemistry, 2011, 111, 1784-1791.	1.0	15
35	Molecular Dynamics Simulation of the Oil Sequestration Properties of a Nonionic Rhamnolipid. Journal of Physical Chemistry B, 2018, 122, 3944-3952.	1.2	13
36	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

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37	Alkylation of enolates: An electrophilicity perspective. International Journal of Quantum Chemistry, 2006, 106, 852-862.	1.0	11
38	Complex line shapes in surface-enhanced coherent Raman spectroscopy. Journal of Modern Optics, 2015, 62, 90-96.	0.6	11
39	Chemical reactivity patterns of [n]paracyclophanes. Computational and Theoretical Chemistry, 2007, 820, 1-6.	1.5	10
40	Density Functional Theoretical Investigation on Influence of Heterosubstitution and Benzannelation on the Thermal 6Ï€ Electrocyclization of cis-Cyclononatetraene. Journal of Physical Chemistry A, 2005, 109, 11870-11877.	1.1	9
41	Density Functional Theory Studies on Ice Nanotubes. Journal of Physical Chemistry A, 2011, 115, 12841-12851.	1.1	9
42	The Self-Assembly of Metaboric Acid Molecules into Bowls, Balls and Sheets. Journal of Physical Chemistry A, 2008, 112, 8107-8115.	1.1	7
43	Structure and stability of spiro-cyclic water clusters. Journal of Chemical Sciences, 2009, 121, 839-848.	0.7	6
44	A Molecular Dynamics Study of Small Molecules Bound to a Full Atomistic Model of Cardiac Thin Filament as a Method to Identify Possible Treatments for Genetic Cardiomyopathies. Biophysical Journal, 2020, 118, 326a.	0.2	0