Elango Munusamy

List of Publications by Year
in descending order

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Version: 2024-02-01

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	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
2	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
3	Molecular Dynamics Simulation of the Oil Sequestration Properties of a Nonionic Rhamnolipid. Journal of Physical Chemistry B, 2018, 122, 3944-3952.	1.2	13
4	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
5	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
6	Evolution of Aggregate Structure in Solutions of Anionic Monorhamnolipids: Experimental and Computational Results. Langmuir, 2017, 33, 7412-7424.	1.6	27
7	Complex line shapes in surface-enhanced coherent Raman spectroscopy. Journal of Modern Optics, 2015, 62, 90-96.	0.6	11
8	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
9	Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. Journal of Chemical Physics, 2013, 139, 094703.	1.2	22
10	Time-Resolved Surface-Enhanced Coherent Sensing of Nanoscale Molecular Complexes. Scientific Reports, 2012, 2, 891.	1.6	50
11	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
12	Density Functional Theory Studies on Ice Nanotubes. Journal of Physical Chemistry A, 2011, 115, 12841-12851.	1.1	9
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	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
15	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
16	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
17	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	1.5	27
18	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

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19	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
20	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
21	Structure and stability of spiro-cyclic water clusters. Journal of Chemical Sciences, 2009, 121, 839-848.	0.7	6
22	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
23	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
24	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
25	Novel saccharideâ€“pyridine based gelators: selective gelation and diversity in superstructures. New Journal of Chemistry, 2009, 33, 1570.	1.4	30
26	Structure and Stability of Water Chains (H2O)n, n = 5â^'20. Journal of Physical Chemistry A, 2009, 113, 3744-3749.	1.1	32
27	The Self-Assembly of Metaboric Acid Molecules into Bowls, Balls and Sheets. Journal of Physical Chemistry A, 2008, 112, 8107-8115.	1.1	7
28	Structure, Energetics, and Reactivity of Boric Acid Nanotubes: A Molecular Tailoring Approach. Journal of Physical Chemistry A, 2008, 112, 7699-7704.	1.1	36
29	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
30	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
31	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	1.1	141
32	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
33	Chemical reactivity patterns of [n]paracyclophanes. Computational and Theoretical Chemistry, 2007, 820, 1-6.	1.5	10
34	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
35	pKa Prediction Using Group Philicity. Journal of Physical Chemistry A, 2006, 110, 6540-6544.	1.1	64
36	Alkylation of enolates: An electrophilicity perspective. International Journal of Quantum Chemistry, 2006, 106, 852-862.	1.0	11

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37	Chemical reactivity descriptor based aromaticity indices applied to and systems. Computational and Theoretical Chemistry, 2006, 759, 109-110.	1.5	39
38	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
39	Variation of electrophilicity during molecular vibrations and internal rotations. Theoretical Chemistry Accounts, 2005, 113, 257-266.	0.5	135
40	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	0.7	29
41	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
42	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
43	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
44	Intermolecular reactivity through the generalized philicity concept. Chemical Physics Letters, 2004, 394, 225-230.	1.2	225