Krishnan Balasubramanian

List of Publications by Year
in descending order

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93	1,717	279798	345221
papers	citations	23 h-index	36 g-index

94	94	94	1061
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational and Artificial Intelligence Techniques for Drug Discovery and Administration. , 2022, , 553-616.		15
2	Structureâ€“activity relations for antiepileptic drugs through omega polynomials and topological indices. Molecular Physics, 2022, 120, .	1.7	15
3	Relativistic distance based and bond additive topological descriptors of zeolite RHO materials. Journal of Molecular Structure, 2022, 1250, 131798.	3.6	22
4	Graph entropies, enumeration of circuits, walks and topological properties of three classes of isoreticular metal organic frameworks. Journal of Mathematical Chemistry, 2022, 60, 695-732.	1.5	20
5	Induced representations of Dihedral groups ($$D_n$$) from its subgroups and to the Symmetric groups ($$S_n$$): Applications to Nanotubes, Gelâ€™fand states Tableaus and Spectroscopy. Journal of Mathematical Chemistry, 2022, 60, 733-751.	1.5	0
6	Degree-based entropies of graphene, graphyne and graphdiyne using Shannonâ€™s approach. Journal of Molecular Structure, 2022, 1260, 132797.	3.6	28
7	Symmetry and Combinatorial Concepts for Cyclopolyarenes, Nanotubes and 2D-Sheets: Enumerations, Isomers, Structures Spectra & Properties. Symmetry, 2022, 14, 34.	2.2	3
8	Two-dimensional coronene fractal structures: topological entropy measures, energetics, NMR and ESR spectroscopic patterns and existence of isentropic structures. Molecular Physics, 2022, 120, .	1.7	25
9	Three conjectures on extended twin primes and the existence of isoboolean and singular primes inspired by relativistic quantum computing. Journal of Mathematical Chemistry, 2022, 60, 1571-1583.	1.5	2
10	Face colorings and chiral face colorings of icosahedral giant fullerenes: C80 to C240. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 1-12.	2.1	6
11	Relativistic distance-based topological descriptors of Linde type A zeolites and their doped structures with very heavy elements. Molecular Physics, 2021, 119, e1798529.	1.7	31
12	Quantitative structural descriptors of sodalite materials. Journal of Molecular Structure, 2021, 1223, 128766.	3.6	26
13	Relativistic structural characterization of molybdenum and tungsten disulfide materials. International Journal of Quantum Chemistry, 2021, 121, e26492.	2.0	4
14	Tensor and Cartesian products for nanotori, nanotubes and zigâ€“zag polyhex nanotubes and their applications to¹³C NMR spectroscopy. Molecular Physics, 2021, 119, e1817594.	1.7	5
15	Combinatorial enumeration of relativistic states of actinide dimers. Journal of Mathematical Chemistry, 2021, 59, 315-363.	1.5	3
16	Biochemical and phylogenetic networks-II: X-trees and phylogenetic trees. Journal of Mathematical Chemistry, 2021, 59, 699-718.	1.5	2
17	Distance degree vector and scalar sequences of corona and lexicographic products of graphs with applications to dynamic NMR and dynamics of nonrigid molecules and proteins. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	4
18	Biochemical and phylogenetic networks-I: hypertrees and corona products. Journal of Mathematical Chemistry, 2021, 59, 676-698.	1.5	10

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19	An Overview of Ovarian Cancer: Molecular Processes Involved and Development of Target-based Chemotherapeutics. Current Topics in Medicinal Chemistry, 2021, 21, 329-346.	2.1	16
20	Topological characterization of hexagonal and rectangular tessellations of kekulenes as traps for toxic heavy metal ions. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	14
21	Combinatorial enumeration of stereo, chiral and position isomers of polysubstituted halocarbons: applications to machine learning of proton and 35Cl NMR spectroscopy of halocarbons. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
22	Combinatorics, Big Data, Neural Network & AI for Medicinal Chemistry & Drug Administration. Letters in Drug Design and Discovery, 2021, 18, 943-948.	0.7	21
23	Topological Characterization and Graph Entropies of Tessellations of Kekulene Structures: Existence of Isentropic Structures and Applications to Thermochemistry, Nuclear Magnetic Resonance, and Electron Spin Resonance. Journal of Physical Chemistry A, 2021, 125, 8140-8158.	2.5	46
24	Relativistic Quantum Chemical and Molecular Dynamics Techniques for Medicinal Chemistry of Bioinorganic Compounds. Topics in Medicinal Chemistry, 2021, , 133-193.	0.8	10
25	Symmetry, Combinatorics, Artificial Intelligence, Music and Spectroscopy. Symmetry, 2021, 13, 1850.	2.2	8
26	Topological Indices and Their Applications to Circumcised Donut Benzenoid Systems, Kekulenes and Drugs. Polycyclic Aromatic Compounds, 2020, 40, 280-303.	2.6	67
27	Topological Characterization of Coronoid Polycyclic Aromatic Hydrocarbons. Polycyclic Aromatic Compounds, 2020, 40, 784-802.	2.6	13
28	Enumeration of relativistic states for superheavy and transactinide dimers in the periodic table. Journal of Mathematical Chemistry, 2020, 58, 458-496.	1.5	2
29	Computations of Colorings 7Dâ€Hypercube's Hyperplanes for All Irreducible Representations. Journal of Computational Chemistry, 2020, 41, 653-686.	3.3	10
30	Computational combinatorics of hyperplane colorings of 6D-hypercube for all irreducible representations and applications. Journal of Mathematical Chemistry, 2020, 58, 204-272.	1.5	7
31	Combinatorics of Supergiant Fullerenes: Enumeration of Polysubstituted Isomers, Chirality, Nuclear Magnetic Resonance, Electron Spin Resonance Patterns, and Vibrational Modes from C70 to C150000. Journal of Physical Chemistry A, 2020, 124, 10359-10383.	2.5	7
32	Topological Peripheral Shapes and Distance-Based Characterization of Fullerenes C20-C720: Existence of Isoperipheral Fullerenes. Polycyclic Aromatic Compounds, 2020, , 1-19.	2.6	8
33	Combinatorics of Edge Symmetry: Chiral and Achiral Edge Colorings of Icosahedral Giant Fullerenes: C80, C180, and C240. Symmetry, 2020, 12, 1308.	2.2	3
34	Nonrigid water octamer: Computations with the 8â€cube. Journal of Computational Chemistry, 2020, 41, 2469-2484.	3.3	8
35	Topological and Thermodynamic Entropy Measures for COVID-19 Pandemic through Graph Theory. Symmetry, 2020, 12, 1992.	2.2	11
36	Enumeration of stereo, position and chiral isomers of polysubstituted giant fullerenes: applications to C₁₈₀ and C₂₄₀. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 687-696.	2.1	10

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37	Relativistic topological molecular descriptors of metal trihalides. Journal of Molecular Structure, 2020, 1217, 128368.	3.6	23
38	Edge Distanceâ€based Topological Indices of Strengthâ€weighted Graphs and their Application to Coronoid Systems, Carbon Nanocones and SiO₂ Nanostructures. Molecular Informatics, 2019, 38, e1900039.	2.5	29
39	Topological indices of the subdivision of a family of partial cubes and computation of $$hbox {SiO}_2$$ related structures. Journal of Mathematical Chemistry, 2019, 57, 1868-1883.	1.5	7
40	Computational multinomial combinatorics for colorings of 5D-hypercubes for all irreducible representations and applications. Journal of Mathematical Chemistry, 2019, 57, 655-689.	1.5	12
41	Distance-based topological indices of nanosheets, nanotubes and nanotori of $$hbox {SiO}_2$$ SiO 2. Journal of Mathematical Chemistry, 2019, 57, 343-369.	1.5	27
42	Mathematical and Computational Techniques for Drug Discovery: Promises and Developments. Current Topics in Medicinal Chemistry, 2019, 18, 2774-2799.	2.1	47
43	Quantum Molecular Dynamics, Topological, Group Theoretical and Graph Theoretical Studies of Protein-Protein Interactions. Current Topics in Medicinal Chemistry, 2019, 19, 426-443.	2.1	28
44	On certain topological indices of octahedral and icosahedral networks. IET Control Theory and Applications, 2018, 12, 215-220.	2.1	10
45	Quantum molecular modeling of hepatitis C virus inhibition through non-structural protein 5B polymerase receptor binding of C5-arylidene rhodanines. Computational Biology and Chemistry, 2018, 73, 147-158.	2.3	3
46	Hyper-Wiener and Wiener polarity indices of silicate and oxide frameworks. Journal of Mathematical Chemistry, 2018, 56, 1493-1510.	1.5	17
47	Relativity and the Jahnâ€“Teller, Berry pseudorotations of TBP clusters: group theory, spinâ€“orbit and combinatorial nuclear spin statistics of TBP Desarguesâ€“Levi isomerization graph. Journal of Mathematical Chemistry, 2018, 56, 2194-2225.	1.5	6
48	Combinatorial Enumeration of Isomers of Superaromatic Polysubstituted Cycloarenes and Coronoid Hydrocarbons with Applications to NMR. Journal of Physical Chemistry A, 2018, 122, 8243-8257.	2.5	14
49	Combinatorial multinomial generators for colorings of 4D-hypercubes and their applications. Journal of Mathematical Chemistry, 2018, 56, 2707-2723.	1.5	8
50	Computational Enumeration of Colorings of Hyperplanes of Hypercubes for all Irreducible Representations and Applications. Journal of Mathematical Sciences and Modelling, 2018, 1, 158-180.	0.3	7
51	Nested wreath groups and their applications to phylogeny in biology and Cayley trees in chemistry and physics. Journal of Mathematical Chemistry, 2017, 55, 195-222.	1.5	16
52	Quantum chemical insights into Alzheimer's disease: Curcumin's chelation with Cu(II), Zn(II), and Pd(II) as a mechanism for its prevention. International Journal of Quantum Chemistry, 2016, 116, 1107-1119.	2.0	23
53	Nuclear spin species, spin statistical weights and rovibronic tunnelling splittings of non-rigid water hexamer. Molecular Physics, 2016, 114, 1960-1973.	1.7	1
54	Quantum Chemical and Docking Insights into Bioavailability Enhancement of Curcumin by Piperine in Pepper. Journal of Physical Chemistry A, 2016, 120, 3643-3653.	2.5	53

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55	Analytical expressions for topological properties of polycyclic benzenoid networks. Journal of Chemometrics, 2016, 30, 682-697.	1.3	45
56	Combinatorics of Petersen graph and its compositions for all irreducible representations for Jahnâ€“Teller, non-rigid molecules and clusters. Journal of Mathematical Chemistry, 2016, 54, 1553-1574.	1.5	2
57	Vertex cut method for degree and distance-based topological indices and its applications to silicate networks. Journal of Mathematical Chemistry, 2016, 54, 1728-1747.	1.5	23
58	Analytical expressions for Wiener indices of n-circumscribed peri-condensed benzenoid graphs. Journal of Mathematical Chemistry, 2016, 54, 823-843.	1.5	11
59	Character tables of n-dimensional hyperoctahedral groups and their applications. Molecular Physics, 2016, 114, 1619-1633.	1.7	11
60	Metabolic Electron Attachment as a Primary Mechanism For Toxicity Potentials of Halocarbons. Current Computer-Aided Drug Design, 2016, 12, 62-72.	1.2	11
61	Generalization of the Hararyâ€“Palmer power group theorem to all irreducible representations of object and color groups- color combinatorial group theory. Journal of Mathematical Chemistry, 2014, 52, 703-728.	1.5	7
62	Photoelectron spectroscopy of the molecular anions, ZrOâ^', HfOâ^', HfHOâ^', and HfO2Hâ^'. Journal of Chemical Physics, 2012, 136, 154306.	3.0	8
63	Theoretical Study of the Interactions of In⁺ and In³⁺ with Stoneâ^'Wales Defect Single-Walled Carbon Nanotubes. Journal of Physical Chemistry Letters, 2010, 1, 457-462.	4.6	12
64	Closed-Cage Tungsten Oxide Clusters in the Gas Phase. Journal of Physical Chemistry A, 2010, 114, 5445-5452.	2.5	17
65	Group theoretical treatment of Jahnâ€“Teller versus spin-orbit effects on geometries, rovibronic levels and nuclear spin species of bismuth and antimony clusters. Molecular Physics, 2009, 107, 797-807.	1.7	16
66	Structural Insights into the Binding of Uranyl with Human Serum Protein Apotransferrin Structure and Spectra of Proteinâ^'Uranyl Interactions. Chemical Research in Toxicology, 2009, 22, 1613-1621.	3.3	28
67	New Insights into the Chemical and Electronic Properties of C69M [M = Inâ^', Tlâ^', Sb+, Bi+] Species. Journal of Physical Chemistry A, 2008, 112, 12179-12186.	2.5	2
68	Spectroscopic constants and potential energy curves of yttrium carbide (YC). Journal of Chemical Physics, 2007, 126, 224305.	3.0	6
69	Electronic states and stability of GeC2N radical. Chemical Physics Letters, 2007, 438, 162-168.	2.6	5
70	Unusual geometries and spectroscopic properties of electronic states of In2N2. Chemical Physics Letters, 2007, 439, 288-295.	2.6	8
71	Rovibronic symmetry and nuclear spin analysis of octanitrocubane. Chemical Physics Letters, 2007, 441, 29-38.	2.6	2
72	QSAR and SAR Studies on the Reduction of Some Aromatic Nitro Compounds by Xanthine Oxidase. Journal of Chemical Information and Modeling, 2006, 46, 103-110.	5.4	15

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73	Molecular Orbital Basis for Yellow Curry Spice Curcumin's Prevention of Alzheimer's Disease. Journal of Agricultural and Food Chemistry, 2006, 54, 3512-3520.	5.2	165
74	Complex Graph Matrix Representations and Characterizations of Proteomic Maps and Chemically Induced Changes to Proteomes. Journal of Proteome Research, 2006, 5, 1133-1142.	3.7	17
75	A Simple Algorithm for Unique Representation of Chemical StructuresCyclic/Acyclic Functionalized Achiral Molecules. Journal of Chemical Information and Modeling, 2006, 46, 52-56.	5.4	8
76	Electron affinity and inversion distortion of dibenzo-p-dioxin. Chemical Physics Letters, 2005, 410, 142-146.	2.6	3
77	New theoretical insight into the interactions and properties of formic acid: Development of a quantum-based pair potential for formic acid. Journal of Chemical Physics, 2005, 123, 144702.	3.0	33
78	Ab initio based force field and molecular dynamics simulations of crystalline TATB. Journal of Chemical Physics, 2004, 120, 7059-7066.	3.0	90
79	Group theoretical analysis of vibrational modes and rovibronic levels of extended aromatic C48N12 azafullerene. Chemical Physics Letters, 2004, 391, 64-68.	2.6	41
80	Group theory, nuclear spin statistics and tunneling splittings of 1,3,5-triamino-2,4,6-trinitrobenzene. Chemical Physics Letters, 2004, 398, 15-21.	2.6	17
81	Group theoretical analysis of vibrational modes and rovibronic levels of extended aromatic C48N12 azafullerene. Chemical Physics Letters, 2004, 391, 64-64.	2.6	1
82	Theoretical Study on the Reaction of OH Radicals with Polychlorinated Dibenzo-p-dioxins. Journal of Physical Chemistry A, 2004, 108, 607-614.	2.5	43
83	Molecular interactions of TATB clusters. Chemical Physics Letters, 2003, 374, 286-296.	2.6	33
84	Prediction of Cellular Toxicity of Halocarbons from Computed Chemodescriptors:â€‰ A Hierarchical QSAR Approach. Journal of Chemical Information and Computer Sciences, 2003, 43, 1103-1109.	2.8	43
85	The treacherous potential energy hypersurface of AgSiO. Journal of Chemical Physics, 2003, 118, 10623-10630.	3.0	4
86	Title is missing!. Journal of Mathematical Chemistry, 2000, 28, 213-239.	1.5	5
87	Use of Statistical and Neural Net Approaches in Predicting Toxicity of Chemicals. Journal of Chemical Information and Computer Sciences, 2000, 40, 885-890.	2.8	85
88	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
89	Characterization of Isospectral Graphs Using Graph Invariants and Derived Orthogonal Parameters. Journal of Chemical Information and Computer Sciences, 1998, 38, 367-373.	2.8	29
90	Correlation between energetics and toxicities of single-carbon halides. Chemical Physics, 1996, 204, 233-237.	1.9	22

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91	Exact dimer statistics and characteristic polynomials of cacti lattices. Theoretica Chimica Acta, 1989, 76, 315-329.	0.8	24
92	Graph edge colorings and their chemical applications. Theoretica Chimica Acta, 1988, 74, 111-122.	0.8	5
93	Combinatorics of chiral and stereo isomers of substituted nanotubes: applications of Eulerian character indices and comparison with bondonic formalism. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-19.	2.1	3