

G Gopakumar

List of Publications by Year in descending order

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48
papers

1,549
citations

331538

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h-index

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39
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58
all docs

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docs citations

58
times ranked

1687
citing authors

#	ARTICLE	IF	CITATIONS
1	One-Point Binding Ligands for Asymmetric Gold Catalysis: Phosphoramidites with a TADDOL-Related but Acyclic Backbone. <i>Journal of the American Chemical Society</i> , 2012, 134, 15331-15342.	6.6	202
2	Molecular Mechanism for H ₂ Release from BH ₃ NH ₃ , Including the Catalytic Role of the Lewis Acid BH ₃ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 679-690.	1.1	161
3	The Cinchona Primary Amine-Catalyzed Asymmetric Epoxidation and Hydroperoxidation of $\hat{1}\pm, \hat{1}^2$ -Unsaturated Carbonyl Compounds with Hydrogen Peroxide. <i>Journal of the American Chemical Society</i> , 2013, 135, 6677-6693.	6.6	141
4	Polycationic Ligands in Gold Catalysis: Synthesis and Applications of Extremely $\hat{1}$ -Acidic Catalysts. <i>Journal of the American Chemical Society</i> , 2013, 135, 18815-18823.	6.6	123
5	Stabilization of a Two-coordinate [GeCl] ⁺ Cation by Simultaneous $\hat{1}$ and $\hat{1}$...Donation from a Monodentate Carbodiphosphorane. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 5644-5647.	7.2	92
6	The boron buckyball has an unexpected Th symmetry. <i>Chemical Physics Letters</i> , 2008, 450, 175-177.	1.2	75
7	Chromium-Doped Germanium Clusters CrGe _n (<i>n</i> = 1-5): Geometry, Electronic Structure, and Topology of Chemical Bonding. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13544-13553.	1.1	70
8	Chemical bonding in the boron buckyball. <i>Chemical Physics Letters</i> , 2008, 461, 226-228.	1.2	53
9	Origin of the Unusual Stability of B ₁₂ and B ₁₃ ⁺ Clusters. <i>Inorganic Chemistry</i> , 2009, 48, 9965-9967.	1.9	52
10	The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B ₁₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7524.	1.3	44
11	Synthesis and Structure of Carbene-Stabilized N-Centered Cations [L ₂ N] ⁺ , [L ₂ NR] ²⁺ , [LNR ₃] ²⁺ , and [L ₃ N] ³⁺ . <i>Chemistry - A European Journal</i> , 2013, 19, 3542-3546.	1.7	39
12	Complexation Behavior of the Tri- <i>n</i> -butyl Phosphate Ligand with Pu(IV) and Zr(IV): A Computational Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4201-4210.	1.1	39
13	Palladium-Catalyzed Allylic Substitution at Four-Membered Ring Systems: Formation of $\hat{1}^1$ Allyl Complexes and Electrocyclic Ring Opening. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6313-6316.	7.2	30
14	Interaction of Triatomic Germanium with Lithium Atoms: Electronic Structure and Stability of Ge ₃ Li _n Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4353-4361.	1.1	28
15	Energetics and chemical bonding of the 1,3,5-tridehydrobenzene triradical and its protonated form. <i>Chemical Physics</i> , 2005, 316, 125-140.	0.9	27
16	Interaction of diatomic germanium with lithium atoms: Electronic structure and stability. <i>Journal of Chemical Physics</i> , 2006, 124, 214312.	1.2	25
17	Experimental Detection and Theoretical Characterization of Germanium-Doped Lithium Clusters Li _n Ge (<i>n</i> = 1-7). <i>Journal of Physical Chemistry A</i> , 2009, 113, 9080-9091.	1.1	25
18	Hydroxylation Catalysis by Mononuclear and Dinuclear Iron Oxo Catalysts: a Methane Monooxygenase Model System versus the Fenton Reagent Fe ^{IV} O(H ₂ O) ₅ ²⁺ . <i>Inorganic Chemistry</i> , 2012, 51, 63-75.	1.9	24

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19	Experimental and theoretical studies on extraction behavior of di-n-alkyl phosphine oxides towards actinides. <i>RSC Advances</i> , 2015, 5, 107421-107429.	1.7	23
20	Lithium-Doped Germanium Nanowire? Experimental and Theoretical Indication. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10858-10867.	1.5	22
21	Extraction of actinides by Tri-n-butyl phosphate derivatives: Effect of substituents. <i>Inorganica Chimica Acta</i> , 2018, 469, 123-132.	1.2	22
22	Jahnâ€Teller instability in cationic boron and carbon buckyballs B80+ and C60+: a comparative study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2829.	1.3	19
23	Trihexyl phosphate to trihexyl phosphine oxide: Diverse effect on extraction behavior of actinides. <i>Journal of Molecular Liquids</i> , 2018, 256, 416-423.	2.3	17
24	Electronic Structure of Germanium Monohydrides GenH, n = 1âˆ³. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12187-12195.	1.1	15
25	Experimental and theoretical studies on extraction of actinides and lanthanides by alicyclic H-phosphonates. <i>Radiochimica Acta</i> , 2017, 105, 329-339.	0.5	13
26	Experimental and theoretical studies on actinide extraction: dibutyl phenyl phosphonate <i>versus</i> tri-<i>n</i>-butyl phosphate. <i>Journal of Coordination Chemistry</i> , 2019, 72, 1480-1496.	0.8	12
27	Highly efficient functionalized MOF-LIC-1 for extraction of U(<sc>vi</sc>) and Th(<sc>iv</sc>) from aqueous solution: experimental and theoretical studies. <i>Dalton Transactions</i> , 2022, 51, 3557-3571.	1.6	12
28	The 5-Dehydro-m-xyllylene Triradical and Its Nitrogen and Phosphorus Derivatives:Â Open-Shell Doublet versus Quartet Ground State. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8411-8418.	1.1	11
29	The triplet state of indigo: Electronic structure calculations. <i>Chemical Physics Letters</i> , 2007, 449, 11-17.	1.2	10
30	Investigations on synthesis, coordination behavior and actinide recovery of unexplored dicyclohexylphosphinic acid. <i>Polyhedron</i> , 2016, 117, 741-748.	1.0	10
31	Molecular and Spectroscopic Insights into a Metal Salt-Based Deep Eutectic Solvent: A Combined Quantum Theory of Atoms in Molecules, Noncovalent Interaction, and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9680-9690.	1.1	10
32	Molecular mechanism of hydrogen release reactions: Topological analysis using the electron localization function. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 77-89.	1.5	9
33	Extraction and coordination behavior of diphenyl hydrogen phosphine oxide towards actinides. <i>Journal of Coordination Chemistry</i> , 2017, 70, 3338-3352.	0.8	9
34	Diphenylmorpholine CMPO: Synthesis, coordination behavior and extraction studies of actinides. <i>Polyhedron</i> , 2018, 141, 215-222.	1.0	9
35	Does the basicity of phosphoryl oxygen change with alkyl chain length in phosphate ligands?. <i>Chemical Physics Letters</i> , 2021, 775, 138641.	1.2	9
36	Bright and Efficient Red Light-Emitting Electrochemical Cells with Nondoped Organic Small Molecules: A New Approach. <i>ACS Photonics</i> , 2022, 9, 203-210.	3.2	9

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37	Bis- and Tris(pyrazolyl)borate/Methane-stabilized P ^{III} -Centered Cations. Chemistry - A European Journal, 2014, 20, 8575-8578.	1.7	8
38	On the Nature of the Carbonyl versus Phosphoryl Binding in Uranyl Nitrate Complexes. Journal of Physical Chemistry A, 2020, 124, 7805-7815.	1.1	8
39	Exploring long-chain hexaalkyl phosphoramides for actinide extraction: A combined experimental and theoretical investigation. Inorganica Chimica Acta, 2021, 525, 120496.	1.2	8
40	Introduction of heterocyclic ring to phenanthroimidazole moiety for efficient blue emitting ionic small molecule LECs. Organic Electronics, 2020, 87, 105939.	1.4	6
41	Novel Thenil-Based Ionic Small Molecules for Nondoped Light-Emitting Electrochemical Cells for Ultrapure Green Emission. Journal of Physical Chemistry C, 2021, 125, 17993-18001.	1.5	6
42	Jahn-Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. Journal of Physical Chemistry A, 2015, 119, 4237-4243.	1.1	5
43	Experimental and theoretical studies on solvent extraction of uranium(VI) with hexapropyl and hexabutyl phosphoramidate extractants. Solvent Extraction and Ion Exchange, 2022, 40, 312-332.	0.8	4
44	Furil-based ionic small molecules for green-emitting non-doped LECs with improved color purity. New Journal of Chemistry, 2021, 45, 12576-12584.	1.4	4
45	Luminescent versus non-luminescent uranyl-picolate complexes. Journal of Radioanalytical and Nuclear Chemistry, 2018, 318, 2145-2156.	0.7	3
46	Understanding water mediated proton migration in conversion of C=C bond in olefinic carbon atoms into C=N bond to form β -amino adducts. Tetrahedron, 2021, 100, 132482.	1.0	1
47	Investigations of the Boron Buckyball B80: Bonding Analysis and Chemical Reactivity. Progress in Theoretical Chemistry and Physics, 2011, , 265-278.	0.2	1
48	Insight into the Complexation of Heptavalent Technetium with Tri-n-Butyl Phosphate: A Computational Study. Chemical Physics Letters, 2022, , 139705.	1.2	0