G Gopakumar

List of Publications by Year
in descending order

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48	1,549	331259	301761
papers	citations	21 h-index	39 g-index

58	58	58	1687
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Experimental and theoretical studies on solvent extraction of uranium(VI) with hexapropyl and hexabutyl phosphoramide extractants. Solvent Extraction and Ion Exchange, 2022, 40, 312-332.	0.8	4
2	Highly efficient functionalized MOF-LIC-1 for extraction of U(<scp>vi</scp>) and Th(<scp>iv</scp>) from aqueous solution: experimental and theoretical studies. Dalton Transactions, 2022, 51, 3557-3571.	1.6	12
3	Bright and Efficient Red Light-Emitting Electrochemical Cells with Nondoped Organic Small Molecules: A New Approach. ACS Photonics, 2022, 9, 203-210.	3.2	9
4	Insight into the Complexation of Heptavalent Technetium with Tri-n-Butyl Phosphate: A Computational Study. Chemical Physics Letters, 2022, , 139705.	1.2	0
5	Does the basicity of phosphoryl oxygen change with alkyl chain length in phosphate ligands?. Chemical Physics Letters, 2021, 775, 138641.	1.2	9
6	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
7	Exploring long-chain hexaalkyl phosphoramides for actinide extraction: A combined experimental and theoretical investigation. Inorganica Chimica Acta, 2021, 525, 120496.	1.2	8
8	Understanding water mediated proton migration in conversion of Ï€-bond in olefinic carbon atoms into Câ€“N bond to form Î²-amino adducts. Tetrahedron, 2021, 100, 132482.	1.0	1
9	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
10	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. Journal of Physical Chemistry A, 2021, 125, 9680-9690.	1.1	10
11	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
12	Introduction of heterocyclic ring to phenanthroimidazole moiety for efficient blue emitting ionic small molecule LECs. Organic Electronics, 2020, 87, 105939.	1.4	6
13	Experimental and theoretical studies on actinide extraction: dibutyl phenyl phosphonate versus tri-n-butyl phosphate. Journal of Coordination Chemistry, 2019, 72, 1480-1496.	0.8	12
14	Trihexyl phosphate to trihexyl phosphine oxide: Diverse effect on extraction behavior of actinides. Journal of Molecular Liquids, 2018, 256, 416-423.	2.3	17
15	Diphenylmorpholine CMPO: Synthesis, coordination behavior and extraction studies of actinides. Polyhedron, 2018, 141, 215-222.	1.0	9
16	Extraction of actinides by Tri-n-butyl phosphate derivatives: Effect of substituents. Inorganica Chimica Acta, 2018, 469, 123-132.	1.2	22
17	Luminescent versus non-luminescent uranylâ€“picolinate complexes. Journal of Radioanalytical and Nuclear Chemistry, 2018, 318, 2145-2156.	0.7	3
18	Experimental and theoretical studies on extraction of actinides and lanthanides by alicyclic H-phosphonates. Radiochimica Acta, 2017, 105, 329-339.	0.5	13

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19	Extraction and coordination behavior of diphenyl hydrogen phosphine oxide towards actinides. Journal of Coordination Chemistry, 2017, 70, 3338-3352.	0.8	9
20	Investigations on synthesis, coordination behavior and actinide recovery of unexplored dicyclohexylphosphinic acid. Polyhedron, 2016, 117, 741-748.	1.0	10
21	Complexation Behavior of the Tri-n-butyl Phosphate Ligand with Pu(IV) and Zr(IV): A Computational Study. Journal of Physical Chemistry A, 2016, 120, 4201-4210.	1.1	39
22	Experimental and theoretical studies on extraction behavior of di-n-alkyl phosphine oxides towards actinides. RSC Advances, 2015, 5, 107421-107429.	1.7	23
23	Jahnâ€“Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. Journal of Physical Chemistry A, 2015, 119, 4237-4243.	1.1	5
24	Bisâ€•and Tris(pyrazolyl)borate/Methaneâ€Stabilized P^{III}â€Centered Cations. Chemistry - A European Journal, 2014, 20, 8575-8578.	1.7	8
25	Jahnâ€“Teller instability in cationic boron and carbon buckyballs B80+ and C60+: a comparative study. Physical Chemistry Chemical Physics, 2013, 15, 2829.	1.3	19
26	Synthesis and Structure of Carbeneâ€Stabilized Nâ€Centered Cations [L₂N]⁺, [L₂NR]²⁺, [LNR₃]²⁺, and [L₃N]³⁺. Chemistry - A European Journal, 2013, 19, 3542-3546.	1.7	39
27	Stabilization of a Twoâ€Coordinate [GeCl]⁺ Cation by Simultaneous Ïƒ and Ï€â€…Donation from a Monodentate Carbodiphosphorane. Angewandte Chemie - International Edition, 2013, 52, 5644-5647.	7.2	92
28	The Cinchona Primary Amine-Catalyzed Asymmetric Epoxidation and Hydroperoxidation of Î±,Î²-Unsaturated Carbonyl Compounds with Hydrogen Peroxide. Journal of the American Chemical Society, 2013, 135, 6677-6693.	6.6	141
29	Palladiumâ€Catalyzed Allylic Substitution at Fourâ€Memberedâ€Ring Systems: Formation of Î·¹â€Allyl Complexes and Electrocyclic Ring Opening. Angewandte Chemie - International Edition, 2013, 52, 6313-6316.	7.2	30
30	Polycationic Ligands in Gold Catalysis: Synthesis and Applications of Extremely Ï€-Acidic Catalysts. Journal of the American Chemical Society, 2013, 135, 18815-18823.	6.6	123
31	Hydroxylation Catalysis by Mononuclear and Dinuclear Iron Oxo Catalysts: a Methane Monooxygenase Model System versus the Fenton Reagent Fe^{IV}O(H₂O)₅²⁺. Inorganic Chemistry, 2012, 51, 63-75.	1.9	24
32	One-Point Binding Ligands for Asymmetric Gold Catalysis: Phosphoramidites with a TADDOL-Related but Acyclic Backbone. Journal of the American Chemical Society, 2012, 134, 15331-15342.	6.6	202
33	The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B112. Physical Chemistry Chemical Physics, 2011, 13, 7524.	1.3	44
34	Investigations of the Boron Buckyball B80: Bonding Analysis and Chemical Reactivity. Progress in Theoretical Chemistry and Physics, 2011, , 265-278.	0.2	1
35	Origin of the Unusual Stability of B₁₂and B₁₃⁺Clusters. Inorganic Chemistry, 2009, 48, 9965-9967.	1.9	52
36	Lithium-Doped Germanium Nanowire? Experimental and Theoretical Indication. Journal of Physical Chemistry C, 2009, 113, 10858-10867.	1.5	22

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37	Experimental Detection and Theoretical Characterization of Germanium-Doped Lithium Clusters Li_nGe (n = 1â˜7). Journal of Physical Chemistry A, 2009, 113, 9080-9091.	1.1	25
38	The boron buckyball has an unexpected Th symmetry. Chemical Physics Letters, 2008, 450, 175-177.	1.2	75
39	Chemical bonding in the boron buckyball. Chemical Physics Letters, 2008, 461, 226-228.	1.2	53
40	Electronic Structure of Germanium Monohydrides GenH, n = 1â˜3. Journal of Physical Chemistry A, 2008, 112, 12187-12195.	1.1	15
41	Molecular Mechanism for H2Release from BH3NH3, Including the Catalytic Role of the Lewis Acid BH3. Journal of Physical Chemistry A, 2007, 111, 679-690.	1.1	161
42	Chromium-Doped Germanium Clusters CrGe_n (n = 1â˜5):â€‰ Geometry, Electronic Structure, and Topology of Chemical Bonding. Journal of Physical Chemistry A, 2007, 111, 13544-13553.	1.1	70
43	Interaction of Triatomic Germanium with Lithium Atoms:â€‰ Electronic Structure and Stability of Ge3Lin Clusters. Journal of Physical Chemistry A, 2007, 111, 4353-4361.	1.1	28
44	Molecular mechanism of hydrogen release reactions: Topological analysis using the electron localization function. Computational and Theoretical Chemistry, 2007, 811, 77-89.	1.5	9
45	The triplet state of indigo: Electronic structure calculations. Chemical Physics Letters, 2007, 449, 11-17.	1.2	10
46	Interaction of diatomic germanium with lithium atoms: Electronic structure and stability. Journal of Chemical Physics, 2006, 124, 214312.	1.2	25
47	Energetics and chemical bonding of the 1,3,5-tridehydrobenzene triradical and its protonated form. Chemical Physics, 2005, 316, 125-140.	0.9	27
48	The 5-Dehydro-m-xylylene Triradical and Its Nitrogen and Phosphorus Derivatives:Â Open-Shell Doublet versus Quartet Ground State. Journal of Physical Chemistry A, 2004, 108, 8411-8418.	1.1	11