Sk Musharaf Ali

List of Publications by Year
in descending order

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122 papers	2,010 citations	279798 23 h-index	361022 35 g-index
124 all docs	124 docs citations	124 times ranked	1593 citing authors

#	Article	IF	Citations
1	Universal Scaling Laws of Diffusion in a Binary Fluid Mixture. Physical Review Letters, 2001, 87, 245901.	7.8	93
2	Novel amidoamine functionalized multi-walled carbon nanotubes for removal of mercury(II) ions from wastewater: Combined experimental and density functional theoretical approach. Chemical Engineering Journal, 2017, 313, 899-911.	12.7	79
3	Surface Engineering of PAMAM-SDB Chelating Resin with Diglycolamic Acid (DGA) Functional Group for Efficient Sorption of U(VI) and Th(IV) from Aqueous Medium. Journal of Hazardous Materials, 2017, 328, 1-11.	12.4	58
4	Complexation thermodynamics of diglycolamide with f-elements: solvent extraction and density functional theory analysis. Physical Chemistry Chemical Physics, 2016, 18, 9816-9828.	2.8	57
5	New Universal Scaling Laws of Diffusion and Kolmogorov-Sinai Entropy in Simple Liquids. Physical Review Letters, 2004, 92, 145901.	7.8	55
6	An amide functionalized task specific carbon nanotube for the sorption of tetra and hexa valent actinides: experimental and theoretical insight. RSC Advances, 2016, 6, 39553-39562.	3.6	54
7	Preferential interaction of charged alkali metal ions (guest) within a narrow cavity of cyclic crown ethers (neutral host): A quantum chemical investigation. Computational and Theoretical Chemistry, 2010, 941, 90-101.	1.5	53
8	DFT modeling on the suitable crown ether architecture for complexation with Cs+ and Sr2+ metal ions. Journal of Molecular Modeling, 2011, 17, 1091-1108.	1.8	52
9	Ab initio and density functional theoretical design and screening of model crown ether based ligand (host) for extraction of lithium metal ion (guest): effect of donor and electronic induction. Journal of Molecular Modeling, 2012, 18, 3507-3522.	1.8	49
10	Density functional theoretical analysis of structure, bonding, interaction and thermodynamic selectivity of hexavalent uranium (UO2 2+) and tetravalent plutonium (Pu4+) ion complexes of tetramethyl diglycolamide (TMDGA). Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	49
11	Mode coupling theory of self and cross diffusivity in a binary fluid mixture: Application to Lennard-Jones systems. Journal of Chemical Physics, 2001, 114, 10419-10429.	3.0	48
12	Oxidation state selective sorption behavior of plutonium using N,N-dialkylamide functionalized carbon nanotubes: experimental study and DFT calculation. RSC Advances, 2016, 6, 78692-78701.	3.6	37
13	Passage of TBPâ€“uranyl complexes from aqueousâ€“organic interface to the organic phase: insights from molecular dynamics simulation. Physical Chemistry Chemical Physics, 2016, 18, 23769-23784.	2.8	34
14	Dual mode of extraction for Cs⁺ and Na⁺ ions with dicyclohexano-18-crown-6 and bis(2-propyloxy)calix[4]crown-6 in ionic liquids: density functional theoretical investigation. RSC Advances, 2014, 4, 22911-22925.	3.6	31
15	Carbon nano tubes functionalized with novel functional group- amido-amine for sorption of actinides. Journal of Hazardous Materials, 2018, 345, 63-75.	12.4	31
16	Ligands for selective metal ion extraction: A molecular modeling approach. Desalination, 2008, 232, 181-190.	8.2	30
17	Microhydration of Cs+ ion: A density functional theory study on Cs+â€“(H2O)n clusters (n=1â€“10). Journal of Chemical Physics, 2007, 127, 044303.	3.0	28
18	Understanding the complexation of the Eu3+ ion with TODGA, CMPO, TOPO and DMDBTDMA: Extraction, luminescence and theoretical investigation. Polyhedron, 2016, 117, 612-622.	2.2	28

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19	Micro-solvation of the Zn2+ ionâ€"a case study. Physical Chemistry Chemical Physics, 2009, 11, 8285.	2.8	27
20	Diffusion, permeation and solubility of hydrogen, deuterium and tritium in crystalline tungsten: First principles DFT simulations. International Journal of Hydrogen Energy, 2020, 45, 29095-29109.	7.1	27
21	Insight into Speciation and Electrochemistry of Uranyl Ions in Deep Eutectic Solvents. Journal of Physical Chemistry B, 2020, 124, 181-189.	2.6	26
22	Interfacial insights on the dibenzo-based crown ether assisted cesium extraction in [BMIM][Tf2N]â€"water binary system. Journal of Radioanalytical and Nuclear Chemistry, 2017, 311, 427-438.	1.5	25
23	Unanticipated favoured adsorption affinity of Th(<scp>iv</scp>) ions towards bidentate carboxylate functionalized carbon nanotubes (CNTâ€"COOH) over tridentate diglycolamic acid functionalized CNT: density functional theoretical investigation. RSC Advances, 2015, 5, 80076-80088.	3.6	24
24	Sorption behaviour of Pu⁴⁺and PuO₂²⁺on amido amine-functionalized carbon nanotubes: experimental and computational study. RSC Advances, 2016, 6, 107011-107020.	3.6	23
25	Insight into the Complexation of Actinides and Lanthanides with Diglycolamide Derivatives: Experimental and Density Functional Theoretical Studies. Journal of Physical Chemistry B, 2017, 121, 2640-2649.	2.6	23
26	Diglycolamic acid-functionalized multiwalled carbon nanotubes as a highly efficient sorbent for f-block elements: experimental and theoretical investigations. New Journal of Chemistry, 2017, 41, 4531-4545.	2.8	22
27	Unusual extraction of trivalent f-cations using diglycolamide dendrimers in a room temperature ionic liquid: extraction, spectroscopic and DFT studies. Dalton Transactions, 2017, 46, 16541-16550.	3.3	22
28	Structural and dynamical properties of Li+-dibenzo-18-crown-6(DB18C6) complex in pure solvents and at the aqueous-organic interface. Journal of Molecular Modeling, 2014, 20, 2413.	1.8	21
29	From microhydration to bulk hydration of Sr2+ metal ion: DFT, MP2 and molecular dynamics study. Journal of Molecular Liquids, 2012, 172, 110-118.	4.9	20
30	Design and screening of suitable ligand/diluents systems for removal of Sr2+ ion from nuclear waste: Density functional theoretical modelling. Computational and Theoretical Chemistry, 2014, 1034, 38-52.	2.5	20
31	Tailoring of carbon nanotubes for the adsorption of heavy metal ions: molecular dynamics and experimental investigations. Molecular Systems Design and Engineering, 2018, 3, 917-929.	3.4	20
32	Reduction in Coordination Number of Eu(III) on Complexation with Pyrazine Mono- and Di-Carboxylates in Aqueous Medium. Inorganic Chemistry, 2019, 58, 11180-11194.	4.0	20
33	Highly Efficient N-Pivot Tripodal Diglycolamide Ligands for Trivalent f-Cations: Synthesis, Extraction, Spectroscopy, and Density Functional Theory Studies. Inorganic Chemistry, 2019, 58, 8633-8644.	4.0	20
34	Universal scaling laws of diffusion: Application to liquid metals. Journal of Chemical Physics, 2005, 123, 084505.	3.0	19
35	Molecular Dynamics Simulation for the Calibration of the OPLS Force Field Using DFT Derived Partial Charges for the Screening of Alkyl Phosphate Ligands by Studying Structure, Dynamics, and Thermodynamics. Journal of Chemical & Engineering Data, 2017, 62, 2280-2295.	1.9	19
36	Evaluation of 1st and 2nd generation of poly(amidoamine) dendrimer functionalized carbon nanotubes for the efficient removal of neptunium. Journal of Radioanalytical and Nuclear Chemistry, 2018, 315, 331-340.	1.5	19

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37	Thermodynamical Criteria of the Higher Selectivity of Zirconium Oxycations over Hafnium Oxycations towards Organophosphorus Ligands: Density Functional Theoretical Investigation. European Journal of Inorganic Chemistry, 2014, 2014, 1533-1545.	2.0	18
38	Thermodynamics of fluid conduction through hydrophobic channel of carbon nanotubes: The exciting force for filling of nanotubes with polar and nonpolar fluids. Journal of Chemical Physics, 2015, 142, 074501.	3.0	18
39	Understanding the sorption behavior of Pu⁴⁺ on poly(amidoamine) dendrimer functionalized carbon nanotube: sorption equilibrium, mechanism, kinetics, radiolytic stability, and back-extraction studies. Radiochimica Acta, 2017, 105, 677-688.	1.2	16
40	Partition coefficients of macrocyclic crown ethers in waterâ€“organic biphasic system: DFT/COSMO-RS approach. Fluid Phase Equilibria, 2010, 288, 111-120.	2.5	15
41	Density Functional Theoretical Modeling of Selective Ligand for the Separation of Zr and Hf Metal Oxycations (ZrO²⁺and HfO²⁺). Separation Science and Technology, 2013, 48, 2397-2409.	2.5	15
42	The entropic forces and dynamic integrity of single file water in hydrophobic nanotube confinements. Journal of Chemical Physics, 2015, 143, 184503.	3.0	15
43	Molecular dynamics simulation for the test of calibrated OPLS-AA force field for binary liquid mixture of tri-iso-amyl phosphate and n-dodecane. Journal of Chemical Physics, 2018, 148, 074502.	3.0	15
44	Breakdown of continuum model for water transport and desalination through ultrathin graphene nanopores: insights from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 21389-21406.	2.8	15
45	Nanoscopic insights of saline water in carbon nanotube appended filters using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 8529-8542.	2.8	15
46	Understanding of interfacial tension and interface thickness of liquid/liquid interface at a finite concentration of alkyl phosphate by molecular dynamics simulation. Journal of Molecular Liquids, 2019, 277, 217-232.	4.9	15
47	Thorium decorporation efficacy of rationally-selected biocompatible compounds with relevance to human application. Journal of Hazardous Materials, 2019, 365, 952-961.	12.4	15
48	Poly(amidoamine) Dendrimer Functionalized Carbon Nanotube for Efficient Sorption of Trivalent fâ€Elements: A Comparison Between 1st And 2nd Generation. ChemistrySelect, 2017, 2, 975-985.	1.5	14
49	Enhanced free energy of extraction of Eu³⁺ and Am³⁺ ions towards diglycolamide appended calix[4]arene: insights from DFT-D3 and COSMO-RS solvation models. Dalton Transactions, 2017, 46, 10886-10898.	3.3	14
50	Molecular Dynamics Simulation of Amorphous SiO₂, B₂O₃, Na₂Oâ€“SiO₂, Na₂Oâ€“B₂O₃, and Na₂Oâ€“B₂O₃â€“SiO₂ Glasses with Variable Compositions and with Cs₂O and SrO Dopants. Journal of Physical Chemistry B, 2019, 123, 6290-6302.	2.6	14
51	Adsorption of Gadolinium (Gd³⁺) Ions on the Dibenzo Crown Ether (DBCE) and Dicyclo Hexano Crown Ether (DCHCE) Grafted on the Polystyrene Surface: Insights from All Atom Molecular Dynamics Simulations and Experiments. Journal of Physical Chemistry C, 2019, 123, 12276-12285.	3.1	14
52	Amidoamine functionalized task specific carbon nanotube for efficient sorption of penta and hexavalent neptunium: Experimental and theoretical investigations. Journal of Environmental Chemical Engineering, 2017, 5, 3058-3064.	6.7	14
53	Density functional theoretical study on the preferential selectivity of macrocyclic dicyclohexano-18-crown-6 for Sr+2 ion over Th+4 ion during extraction from an aqueous phase to organic phases with different dielectric constants. Journal of Molecular Modeling, 2013, 19, 5277-5291.	1.8	13
54	Complexation of thorium with pyridine monocarboxylate-N-oxides: Thermodynamic and computational studies. Journal of Chemical Thermodynamics, 2018, 122, 13-22.	2.0	13

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55	Complexation thermodynamics of tetraalkyl diglycolamides with trivalent f-elements in ionic liquids: spectroscopic, microcalorimetric and computational studies. New Journal of Chemistry, 2018, 42, 708-716.	2.8	13
56	Ligand architectural effect on coordination, bonding, interaction, and selectivity of Am(<scp>iii</scp>) and Ln(<scp>iii</scp>) ions with bitopic ligands: synthesis, solvent extraction, and DFT studies. Physical Chemistry Chemical Physics, 2020, 22, 15448-15462.	2.8	13
57	Change in the Affinity of Ethylene Glycol Methacrylate Phosphate Monomer and Its Polymer Anchored on a Graphene Oxide Platform toward Uranium(VI) and Plutonium(IV) Ions. Journal of Physical Chemistry B, 2016, 120, 2942-2950.	2.6	12
58	Extraction of Gd³⁺ and UO₂²⁺ Ions Using Polystyrene Grafted Dibenzo Crown Ether (DB18C6) with Octanol and Nitrobenzene: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 1334-1344.	2.6	12
59	Structural, luminescence, thermodynamic and theoretical studies on mononuclear complexes of Eu(III) with pyridine monocarboxylate-N-oxides in aqueous solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 150-163.	3.9	12
60	Molecular Dynamics Simulation Studies on Structure, Dynamics, and Thermodynamics of Uranyl Nitrate Solution at Various Acid Concentrations. Journal of Physical Chemistry B, 2019, 123, 4571-4586.	2.6	12
61	Experimental and theoretical insight into the extraction mechanism, kinetics, thermodynamics, complexation and radiolytic stability of novel calix crown ether in ionic liquid with Sr2+. Journal of Molecular Liquids, 2020, 316, 113864.	4.9	12
62	Exploring functionalized titania for task specific application of efficient separation of trivalent f-block elements. New Journal of Chemistry, 2020, 44, 6151-6162.	2.8	12
63	Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. Chemosphere, 2022, 287, 132232.	8.2	12
64	Adsorption, Absorption, Diffusion, and Permeation of Hydrogen and Its Isotopes in bcc Bulk Fe and Fe(100) Surface: Plane Wave-Based Density Functional Theoretical Investigations. Journal of Physical Chemistry C, 2019, 123, 23951-23966.	3.1	11
65	DFT and MD simulation supplemented experiments for isotopic fractionation of zinc compounds using a macrocyclic crown ether appended polymeric resin. Physical Chemistry Chemical Physics, 2020, 22, 14682-14693.	2.8	11
66	Chemisorption, diffusion and permeation of hydrogen isotopes in bcc bulk cr and cr(100) surface: First-principles dft simulations. Journal of Nuclear Materials, 2021, 543, 152538.	2.7	11
67	A new bisglycolamide substituted calix[4]arene-benzo-crown-6 for the selective removal of cesium ion: combined experimental and density functional theoretical investigation. RSC Advances, 2016, 6, 47120-47129.	3.6	10
68	Conformational effect on the preferential binding of alkali metal cation with crown ether: A molecular level investigation. Desalination and Water Treatment, 2009, 12, 93-99.	1.0	9
69	From microhydration to bulk hydration of Rb+ metal ion: DFT, MP2 and AIMD simulation study. Journal of Molecular Liquids, 2013, 179, 34-45.	4.9	9
70	Insights into the Interaction Energy for Cs+â€“Crown Ether Complex by Molecular Dynamics Simulations. Energy Procedia, 2016, 90, 395-400.	1.8	9
71	Curious Characteristics of Polar and Nonpolar Molecules Confined within Carbon Nanotubes (CNT) of Varied Diameter: Insights from Molecular Dynamics Simulation. Journal of Chemical & Engineering Data, 2017, 62, 2307-2315.	1.9	9
72	Extractive insights in the cesium ion partitioning with bis(2-propyloxy)-calix [4]crown-6 and dicyclohexano-18-crown-6 in ionic liquid-water biphasic systems. Journal of Molecular Liquids, 2017, 241, 279-291.	4.9	9

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73	Molecular engineering of functionalized crown ether resins for the isotopic enrichment of gadolinium: from computer to column chromatography. Molecular Systems Design and Engineering, 2017, 2, 640-652.	3.4	9
74	Partitioning of Cs⁺ and Na⁺ ions by dibenzo-18-crown-6 ionophore in biphasic aqueous systems of octanol and ionic liquid. Radiochimica Acta, 2018, 106, 477-495.	1.2	9
75	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory. Chemosphere, 2020, 249, 126116.	8.2	9
76	New Greener and Sustainable Methodology for Direct Sequestering and Analysis of Uranium Using a Maline Supramolecular Scaffold and Mechanistic Understanding through Speciation and Interaction Studies. ACS Sustainable Chemistry and Engineering, 2021, 9, 7846-7862.	6.7	9
77	In Situ Preconcentration during the Di-(2-ethylhexyl) Phosphoric Acid-Assisted Dissolution of Uranium Trioxide in an Ionic Liquid: Spectroscopic, Electrochemical, and Theoretical Studies. Inorganic Chemistry, 2021, 60, 10147-10157.	4.0	9
78	Mechanism unravelling for highly efficient and selective ⁹⁹TcO₄^{â¯} sequestration utilising crown ether based solvent system from nuclear liquid waste: experimental and computational investigations. RSC Advances, 2022, 12, 3216-3226.	3.6	9
79	Theory of cross-diffusivity in a binary fluid mixture. Chemical Physics, 2002, 276, 301-308.	1.9	8
80	Mass dependence of shear viscosity in a binary fluid mixture: Mode-coupling theory. Physical Review E, 2006, 74, 051201.	2.1	8
81	Scaling law of shear viscosity in atomic liquid and liquid mixtures. Journal of Chemical Physics, 2006, 124, 144504.	3.0	8
82	Designing of ligands for solvent extraction of Cs⁺using molecular modeling approach. Desalination and Water Treatment, 2012, 38, 1-7.	1.0	8
83	Nano Cavity Induced Isotope Separation of Zinc: Density Functional Theoretical Modeling. Journal of Chemical & Engineering Data, 2014, 59, 2472-2484.	1.9	8
84	Experimental and DFT studies for selective separation of Sb(<scp>iii</scp>) and Sb(<scp>v</scp>) from mixtures with Zr(<scp>iv</scp>)/Co(<scp>ii</scp>) using thiourea grafted polystyrene adsorbent. RSC Advances, 2015, 5, 71393-71401.	3.6	8
85	Interfacial Behavior of Cs⁺, K⁺, Na⁺, and Rb⁺ Extraction in the Presence of Dibenzo-18-Crown-6 from the Nitrobenzeneâ€“Water Biphasic System: Experimental, Quantum Chemical, and Molecular Dynamic Studies. ACS Omega, 2018, 3, 1663-1674.	3.5	8
86	Alkali Metal Ion Partitioning with Calix[4]arene-benzo-crown-6 Ionophore in Acidic Medium: Insights from Experiments, Statistical Mechanical Framework, and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 2102-2112.	2.6	8
87	Structure, Dynamics, and Adsorption of Charged Guest within the Nanocavity of Polymer-Functionalized Neutral Macrocyclic Host. ACS Applied Materials & Interfaces, 2018, 10, 20968-20982.	8.0	8
88	Sorption of different metal ions on magnetic nanoparticles and their effect on nanoparticles settlement. Environmental Nanotechnology, Monitoring and Management, 2019, 11, 100202.	2.9	8
89	Scalar Relativistic Density Functional Theoretical Investigation of Higher Complexation Ability of Substituted 1,10â€Phenanthroline over Bipyridine Towards Am³⁺/Eu³⁺ Ions. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 817-829.	1.2	8
90	Molecular dynamics simulations of simplified sodium borosilicate glasses: the effect of composition on structure and dynamics. Physical Chemistry Chemical Physics, 2021, 23, 14898-14912.	2.8	8

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91	Molecular modeling guided isotope separation of gadolinium with strong cation exchange resin using displacement chromatography. Separation Science and Technology, 2017, 52, 2300-2307.	2.5	7
92	Sequestration of Am3+ and Eu3+ into ionic liquid containing Aza-macrocycle based multiple-diglycolamide ligands: Extraction, complexation, luminescence and DFT studies. Journal of Molecular Liquids, 2022, 347, 118291.	4.9	7
93	Efficient separation of strontium ions from aqueous solution by dibenzo-18-crown-6 functionalized resin: Static and dynamic adsorption studies with computational DFT insights. Chemical Engineering Journal Advances, 2022, 11, 100308.	5.2	7
94	A microscopic theory of tracer diffusivity: crossover to the hydrodynamic limit. Chemical Physics Letters, 2002, 357, 217-222.	2.6	6
95	Theoretical prediction of distribution coefficients of Sr2+ in nuclear waste/ionic liquid phases using COSMO-RS model. Separation and Purification Technology, 2014, 133, 138-148.	7.9	6
96	Diglycolamic Acid Functionalized CNTs for Preferential Selection of Eu(III) over Am(III) Ion: Density Functional Theoretical Modelling Validated by Experiments. Separation Science and Technology, 2015, 50, 395-403.	2.5	6
97	High Complexation Selectivity of U(VI) over Rare Earths by N,Nâ€Dihexylâ€2â€ethylhexanamide (DH2EHA): Experimental and Theoretical Evidence. ChemistrySelect, 2017, 2, 2348-2354.	1.5	6
98	Extraction of uranium(VI) by tri iso-amyl phosphate (TiAP) in ionic liquids. Journal of Radioanalytical and Nuclear Chemistry, 2017, 312, 255-262.	1.5	6
99	Role of Ligand Straining in Complexation of Eu³⁺â€“Am³⁺ Ions by TPEN and PPDEN, Scalar Relativistic DFT Exploration in Conjunction with COSMO-RS. ACS Omega, 2018, 3, 13104-13116.	3.5	6
100	The effect of alkyl chain length attached to the diglycolamide and n-paraffin on the aggregation behaviour of diglycolamide and MD simulation of aggregates. Journal of Molecular Structure, 2020, 1221, 128795.	3.6	6
101	Highly efficient diglycolamide-functionalized dendrimers for the sequestration of tetravalent actinides: solvent extraction and theoretical studies. New Journal of Chemistry, 2021, 45, 9462-9471.	2.8	6
102	New deep eutectic solvents based on imidazolium cation: Probing redox speciation of uranium oxides by electrochemical and theoretical simulations. Journal of Electroanalytical Chemistry, 2021, 901, 115752.	3.8	6
103	Simple theoretical model of shear viscosity in isotopic fluid mixtures. Molecular Physics, 2007, 105, 387-393.	1.7	5
104	Test of Universal Scaling Law for Molecular Diffusion of Liquids in Bulk and Nanotube Confinement. Journal of Physical Chemistry C, 2017, 121, 11968-11974.	3.1	5
105	TBP Assisted Uranyl Extraction in Water-Dodecane Biphasic System: Insights from Molecular Dynamics Simulation. Chemical Product and Process Modeling, 2017, 12, .	0.9	5
106	Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. Chemosphere, 2021, 271, 129547.	8.2	5
107	Dispersion corrected interaction of polar and nonpolar fluids confined within carbon nanotubes: Density functional theoretical analysis using <scp>G</scp>rimme's D3 scheme. International Journal of Quantum Chemistry, 2018, 118, e25578.	2.0	4
108	Unusual behavior of Stokesâ€“Einstein relation in liquid mixtures. AIP Advances, 2020, 10, .	1.3	4

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109	Self diffusion and wetting transition of fluids in carbon nanotubes. AIP Conference Proceedings, 2016, , .	0.4	3
110	A molecular dynamics study for the extraction of Cs+ and Na+ ions using dicyclohexano-18-crown-6 with octanol. Separation Science and Technology, 2017, 52, 2291-2299.	2.5	3
111	Does uranyl-TBP complex formation happen at the aqueous-organic interface? Revelation by molecular dynamics simulations. Journal of Molecular Liquids, 2021, 330, 115621.	4.9	3
112	The aqueous interaction of neodymium with two omni existent biomoieties â€“ a mechanistic understanding by experimental and theoretical studies. Dalton Transactions, 2021, 50, 16191-16204.	3.3	3
113	Tuning Network Connectivity of Silicate and Sodium Borosilicate Glasses by TiO₂ for Enhanced Chemical Durability: Molecular Dynamics Simulation Investigations. Langmuir, 2022, 38, 7639-7663.	3.5	3
114	Time-dependent friction and solvation time correlation function. New Journal of Physics, 2005, 7, 27-27.	2.9	2
115	Conformational effect of dicyclo-hexano-18-crown-6 on isotopic fractionation of zinc: DFT approach. , 2014, , .		2
116	Macrocyclic host appended carbon nanotubes for selective adsorption of metal ions: combined experimental, DFT and MD studies. Molecular Systems Design and Engineering, 2019, 4, 616-625.	3.4	2
117	Deciphering the curved profile of uranyl ions at the aqueous-organic interface by atomistic simulations. Journal of Molecular Liquids, 2021, 343, 117599.	4.9	2
118	Density functional theoretical analysis of micro-adsorption of isotopes of hydrogen molecule and atom by uranium. International Journal of Hydrogen Energy, 2022, 47, 18441-18467.	7.1	2
119	A stretched exponential model of collective dynamic structure factor in simple dense fluids. Chemical Physics Letters, 2006, 429, 299-303.	2.6	1
120	Density functional theoretical tailoring of electronic effect through various substituents on calix[4]areneâ€crownâ€6 for efficient Cs + ion encapsulation and extraction. International Journal of Quantum Chemistry, 2021, 121, e26436.	2.0	1
121	Exploring the reaction pathway involved in the dibenzoâ€18â€crownâ€6 synthesis from catechol and bis(2â€chloroethyl) ether in presence of base. Journal of Physical Organic Chemistry, 2022, 35, .	1.9	1
122	Molecular Facts on the Structure and Dynamics of Electrolyte Species in Cuâ€“Cl Cycle for Hydrogen Generation: An Insight from Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2018, 122, 4115-4130.	2.6	0