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	Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. Chemosphere, 2022, 287, 132232.	8.2	12
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. Chemosphere, 2021, 271, 129547.	8.2	5
14	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
15	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
16	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
17	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
18	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

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19	Insight into Speciation and Electrochemistry of Uranyl Ions in Deep Eutectic Solvents. Journal of Physical Chemistry B, 2020, 124, 181-189.	2.6	26
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	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
22	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
23	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
24	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
25	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
26	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory. Chemosphere, 2020, 249, 126116.	8.2	9
27	Unusual behavior of Stokesâ€“Einstein relation in liquid mixtures. AIP Advances, 2020, 10, .	1.3	4
28	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
29	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, 6299-6312.	2.6	14
30	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
31	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
32	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
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	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
35	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
36	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

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37	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
38	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
39	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
40	Thorium decorporation efficacy of rationally-selected biocompatible compounds with relevance to human application. Journal of Hazardous Materials, 2019, 365, 952-961.	12.4	15
41	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
42	Complexation of thorium with pyridine monocarboxylate-N-oxides: Thermodynamic and computational studies. Journal of Chemical Thermodynamics, 2018, 122, 13-22.	2.0	13
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	TBP Assisted Uranyl Extraction in Water-Dodecane Biphasic System: Insights from Molecular Dynamics Simulation. Chemical Product and Process Modeling, 2017, 12, .	0.9	5
67	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
68	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
69	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
70	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
71	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
72	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

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73	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
74	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
75	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
76	Self diffusion and wetting transition of fluids in carbon nanotubes. AIP Conference Proceedings, 2016, , .	0.4	3
77	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
78	Insights into the Interaction Energy for Cs+â€“Crown Ether Complex by Molecular Dynamics Simulations. Energy Procedia, 2016, 90, 395-400.	1.8	9
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	The entropic forces and dynamic integrity of single file water in hydrophobic nanotube confinements. Journal of Chemical Physics, 2015, 143, 184503.	3.0	15
87	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
88	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
89	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
90	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

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91	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
92	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
93	Conformational effect of dicyclo-hexano-18-crown-6 on isotopic fractionation of zinc: DFT approach. , 2014, , .		2
94	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
95	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
96	Nano Cavity Induced Isotope Separation of Zinc: Density Functional Theoretical Modeling. Journal of Chemical & Engineering Data, 2014, 59, 2472-2484.	1.9	8
97	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
98	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
99	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
100	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
101	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
102	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
103	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
104	Designing of ligands for solvent extraction of Cs⁺using molecular modeling approach. Desalination and Water Treatment, 2012, 38, 1-7.	1.0	8
105	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
106	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
107	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
108	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

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109	Micro-solvation of the Zn2+ ionâ€"a case study. Physical Chemistry Chemical Physics, 2009, 11, 8285.	2.8	27
110	Ligands for selective metal ion extraction: A molecular modeling approach. Desalination, 2008, 232, 181-190.	8.2	30
111	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
112	Simple theoretical model of shear viscosity in isotopic fluid mixtures. Molecular Physics, 2007, 105, 387-393.	1.7	5
113	Mass dependence of shear viscosity in a binary fluid mixture: Mode-coupling theory. Physical Review E, 2006, 74, 051201.	2.1	8
114	A stretched exponential model of collective dynamic structure factor in simple dense fluids. Chemical Physics Letters, 2006, 429, 299-303.	2.6	1
115	Scaling law of shear viscosity in atomic liquid and liquid mixtures. Journal of Chemical Physics, 2006, 124, 144504.	3.0	8
116	Time-dependent friction and solvation time correlation function. New Journal of Physics, 2005, 7, 27-27.	2.9	2
117	Universal scaling laws of diffusion: Application to liquid metals. Journal of Chemical Physics, 2005, 123, 084505.	3.0	19
118	New Universal Scaling Laws of Diffusion and Kolmogorov-Sinai Entropy in Simple Liquids. Physical Review Letters, 2004, 92, 145901.	7.8	55
119	Theory of cross-diffusivity in a binary fluid mixture. Chemical Physics, 2002, 276, 301-308.	1.9	8
120	A microscopic theory of tracer diffusivity: crossover to the hydrodynamic limit. Chemical Physics Letters, 2002, 357, 217-222.	2.6	6
121	Universal Scaling Laws of Diffusion in a Binary Fluid Mixture. Physical Review Letters, 2001, 87, 245901.	7.8	93
122	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