

Anil Boda

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3824454/publications.pdf>

Version: 2024-02-01

39
papers

728
citations

623734

14
h-index

552781

26
g-index

40
all docs

40
docs citations

40
times ranked

552
citing authors

#	ARTICLE	IF	CITATIONS
1	Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. <i>Chemosphere</i> , 2022, 287, 132232.	8.2	12
2	Mechanism unravelling for highly efficient and selective $^{99}\text{TcO}_4^-$ sequestration utilising crown ether based solvent system from nuclear liquid waste: experimental and computational investigations. <i>RSC Advances</i> , 2022, 12, 3216-3226.	3.6	9
3	DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. <i>Separation and Purification Technology</i> , 2022, 289, 120709.	7.9	8
4	Density functional theoretical analysis of micro-adsorption of isotopes of hydrogen molecule and atom by uranium. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 18441-18467.	7.1	2
5	Chemisorption, diffusion and permeation of hydrogen isotopes in bcc bulk cr and cr(100) surface: First-principles dft simulations. <i>Journal of Nuclear Materials</i> , 2021, 543, 152538.	2.7	11
6	Density functional theoretical tailoring of electronic effect through various substituents on calix[4]arene-crown for efficient Cs ⁺ ion encapsulation and extraction. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26436.	2.0	1
7	Anion assisted extraction of U(VI) in alkylammonium ionic liquid: Experimental and DFT studies. <i>Separation and Purification Technology</i> , 2021, 261, 118275.	7.9	8
8	Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. <i>Chemosphere</i> , 2021, 271, 129547.	8.2	5
9	The aqueous interaction of neodymium with two omnipresent biomolecules – a mechanistic understanding by experimental and theoretical studies. <i>Dalton Transactions</i> , 2021, 50, 16191-16204.	3.3	3
10	Diffusion, permeation and solubility of hydrogen, deuterium and tritium in crystalline tungsten: First principles DFT simulations. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 29095-29109.	7.1	27
11	Experimental and theoretical insight into the extraction mechanism, kinetics, thermodynamics, complexation and radiolytic stability of novel calix crown ether in ionic liquid with Sr ²⁺ . <i>Journal of Molecular Liquids</i> , 2020, 316, 113864.	4.9	12
12	DFT and MD simulation supplemented experiments for isotopic fractionation of zinc compounds using a macrocyclic crown ether appended polymeric resin. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14682-14693.	2.8	11
13	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory. <i>Chemosphere</i> , 2020, 249, 126116.	8.2	9
14	Reduction in Coordination Number of Eu(III) on Complexation with Pyrazine Mono- and Di-Carboxylates in Aqueous Medium. <i>Inorganic Chemistry</i> , 2019, 58, 11180-11194.	4.0	20
15	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. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23951-23966.	3.1	11
16	Scalar Relativistic Density Functional Theoretical Investigation of Higher Complexation Ability of Substituted 1,10-Phenanthroline over Bipyridine Towards Am ³⁺ /Eu ³⁺ Ions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2019, 645, 817-829.	1.2	8
17	Adsorption of Gadolinium (Gd ³⁺) Ions on the Dibenzo Crown Ether (DBCE) and Dicyclohexano Crown Ether (DCHCE) Grafted on the Polystyrene Surface: Insights from All Atom Molecular Dynamics Simulations and Experiments. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12276-12285.	3.1	14
18	Thorium decorporation efficacy of rationally-selected biocompatible compounds with relevance to human application. <i>Journal of Hazardous Materials</i> , 2019, 365, 952-961.	12.4	15

#	ARTICLE	IF	CITATIONS
19	Complexation of thorium with pyridine monocarboxylate-N-oxides: Thermodynamic and computational studies. <i>Journal of Chemical Thermodynamics</i> , 2018, 122, 13-22.	2.0	13
20	Structural, luminescence, thermodynamic and theoretical studies on mononuclear complexes of Eu(III) with pyridine monocarboxylate-N-oxides in aqueous solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 150-163.	3.9	12
21	Elucidation of complexation of tetra and hexavalent actinides towards an amide ligand in polar and non-polar diluents: Combined experimental and theoretical approach. <i>Polyhedron</i> , 2017, 123, 234-242.	2.2	4
22	Benzene-centered tripodal diglycolamides: synthesis, metal ion extraction, luminescence spectroscopy, and DFT studies. <i>Dalton Transactions</i> , 2017, 46, 1431-1438.	3.3	53
23	Molecular modeling guided isotope separation of gadolinium with strong cation exchange resin using displacement chromatography. <i>Separation Science and Technology</i> , 2017, 52, 2300-2307.	2.5	7
24	Molecular engineering of functionalized crown ether resins for the isotopic enrichment of gadolinium: from computer to column chromatography. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 640-652.	3.4	9
25	An amide functionalized task specific carbon nanotube for the sorption of tetra and hexa valent actinides: experimental and theoretical insight. <i>RSC Advances</i> , 2016, 6, 39553-39562.	3.6	54
26	Oxidation state selective sorption behavior of plutonium using N,N-dialkylamide functionalized carbon nanotubes: experimental study and DFT calculation. <i>RSC Advances</i> , 2016, 6, 78692-78701.	3.6	37
27	Density functional theoretical analysis of structure, bonding, interaction and thermodynamic selectivity of hexavalent uranium (UO ₂ ²⁺) and tetravalent plutonium (Pu ⁴⁺) ion complexes of tetramethyl diglycolamide (TMDGA). <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	49
28	Conformational effect of dicyclo-hexano-18-crown-6 on isotopic fractionation of zinc: DFT approach. , 2014, , .		2
29	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. <i>RSC Advances</i> , 2014, 4, 22911-22925.	3.6	31
30	Density Functional Theoretical Modeling of Selective Ligand for the Separation of Zr and Hf Metal Oxycations (ZrO ²⁺ and HfO ²⁺). <i>Separation Science and Technology</i> , 2013, 48, 2397-2409.	2.5	15
31	From microhydration to bulk hydration of Rb ⁺ metal ion: DFT, MP2 and AIMD simulation study. <i>Journal of Molecular Liquids</i> , 2013, 179, 34-45.	4.9	9
32	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. <i>Journal of Molecular Modeling</i> , 2013, 19, 5277-5291.	1.8	13
33	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. <i>Journal of Molecular Modeling</i> , 2012, 18, 3507-3522.	1.8	49
34	Ionic liquid as a novel partitioning media. <i>Desalination and Water Treatment</i> , 2012, 38, 323-331.	1.0	5
35	From microhydration to bulk hydration of Sr ²⁺ metal ion: DFT, MP2 and molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2012, 172, 110-118.	4.9	20
36	Density Functional Theoretical Investigation of Remarkably High Selectivity of the Cs ⁺ Ion over the Na ⁺ Ion toward Macrocyclic Hybrid Calix-Bis-Crown Ether. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8615-8623.	2.5	40

#	ARTICLE	IF	CITATIONS
37	DFT modeling on the suitable crown ether architecture for complexation with Cs ⁺ and Sr ²⁺ metal ions. <i>Journal of Molecular Modeling</i> , 2011, 17, 1091-1108.	1.8	52
38	Preferential interaction of charged alkali metal ions (guest) within a narrow cavity of cyclic crown ethers (neutral host): A quantum chemical investigation. <i>Computational and Theoretical Chemistry</i> , 2010, 941, 90-101.	1.5	53
39	Partition coefficients of macrocyclic crown ethers in water-organic biphasic system: DFT/COSMO-RS approach. <i>Fluid Phase Equilibria</i> , 2010, 288, 111-120.	2.5	15