# Anil Boda

List of Publications by Year
in descending order

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|---|---|---|---|
| 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 | 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 |
| 2 | 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 |
| 3 | Benzene-centered tripodal diglycolamides: synthesis, metal ion extraction, luminescence spectroscopy, and DFT studies. Dalton Transactions, 2017, 46, 1431-1438. | 3.3 | 53 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | Density Functional Theoretical Investigation of Remarkably High Selectivity of the Cs<sup>+</sup> Ion over the Na<sup>+</sup> Ion toward Macrocyclic Hybrid Calix-Bis-Crown Ether. Journal of Physical Chemistry A, 2012, 116, 8615-8623. | 2.5 | 40 |
| 8 | 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 |
| 9 | Dual mode of extraction for Cs<sup>+</sup> and Na<sup>+</sup> 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 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | Density Functional Theoretical Modeling of Selective Ligand for the Separation of Zr and Hf Metal Oxycations (ZrO<sup>2+</sup>and HfO<sup>2+</sup>). Separation Science and Technology, 2013, 48, 2397-2409. | 2.5 | 15 |
| 15 | Thorium decorporation efficacy of rationally-selected biocompatible compounds with relevance to human application. Journal of Hazardous Materials, 2019, 365, 952-961. | 12.4 | 15 |
| 16 | Adsorption of Gadolinium (Gd<sup>3+</sup>) 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 |
| 17 | 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 |
| 18 | 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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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. Chemosphere, 2022, 287, 132232. | 8.2 | 12 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory. Chemosphere, 2020, 249, 126116. | 8.2 | 9 |
| 28 | Mechanism unravelling for highly efficient and selective <sup>99</sup>TcO<sub>4</sub><sup>â^'</sup> sequestration utilising crown ether based solvent system from nuclear liquid waste: experimental and computational investigations. RSC Advances, 2022, 12, 3216-3226. | 3.6 | 9 |
| 29 | Scalar Relativistic Density Functional Theoretical Investigation of Higher Complexation Ability of Substituted 1,10â€Phenanthroline over Bipyridine Towards Am<sup>3+</sup>/Eu<sup>3+</sup> Ions. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 817-829. | 1.2 | 8 |
| 30 | Anion assisted extraction of U(VI) in alkylammonium ionic liquid: Experimental and DFT studies. Separation and Purification Technology, 2021, 261, 118275. | 7.9 | 8 |
| 31 | DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. Separation and Purification Technology, 2022, 289, 120709. | 7.9 | 8 |
| 32 | 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 |
| 33 | Ionic liquid as a novel partitioning media. Desalination and Water Treatment, 2012, 38, 323-331. | 1.0 | 5 |
| 34 | Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. Chemosphere, 2021, 271, 129547. | 8.2 | 5 |
| 35 | Elucidation of complexation of tetra and hexavalent actinides towards an amide ligand in polar and non-polar diluents: Combined experimental and theoretical approach. Polyhedron, 2017, 123, 234-242. | 2.2 | 4 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Conformational effect of dicyclo-hexano-18-crown-6 on isotopic fractionation of zinc: DFT approach. , 2014, , . | | 2 |
| 38 | 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 |
| 39 | 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 |