Enrique R Batista

List of Publications by Year
in descending order

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92	3,751	117453	138251
papers	citations	34 h-index	58 g-index

96	96	96	3117
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spectroscopic and electrochemical characterization of a Pr⁴⁺ imidophosphorane complex and the redox chemistry of Nd³⁺ and Dy³⁺ complexes. Dalton Transactions, 2022, 51, 6696-6706.	1.6	11
2	Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. Journal of Chemical Theory and Computation, 2022, , .	2.3	3
3	An Allyl Uranium(IV) Sandwich Complex: Are Ï• Bonding Interactions Possible?. Chemistry - A European Journal, 2022, , e202200114.	1.7	7
4	A Comparative Review of Metalâ€Based Charge Carriers in Nonaqueous Flow Batteries. ChemSusChem, 2021, 14, 1214-1228.	3.6	11
5	Screening of metal complexes and organic solvents using the COSMOSAC-LANL model to enhance the energy density in a non-aqueous redox flow cell: an insight into the solubility. Physical Chemistry Chemical Physics, 2021, 23, 21106-21129.	1.3	1
6	RÃ¼cktitelbild: Structural and Spectroscopic Comparison of Softâ€Se vs. Hardâ€O Donor Bonding in Trivalent Americium/Neodymium Molecules (Angew. Chem. 17/2021). Angewandte Chemie, 2021, 133, 9812-9812.	1.6	0
7	Structural and Spectroscopic Comparison of Softâ€Se vs. Hardâ€O Donor Bonding in Trivalent Americium/Neodymium Molecules. Angewandte Chemie - International Edition, 2021, 60, 9459-9466.	7.2	23
8	Structural and Spectroscopic Comparison of Softâ€Se vs. Hardâ€O Donor Bonding in Trivalent Americium/Neodymium Molecules. Angewandte Chemie, 2021, 133, 9545-9552.	1.6	4
9	Complexation of Lanthanides and Heavy Actinides with Aqueous Sulfur-Donating Ligands. Inorganic Chemistry, 2021, 60, 6125-6134.	1.9	15
10	Two-Dimensional Nanomaterials as Anticorrosion Surface Coatings for Uranium Metal: Physical Insights from First-Principles Theory. ACS Applied Nano Materials, 2021, 4, 5038-5046.	2.4	4
11	Iron-iminopyridine complexes as charge carriers for non-aqueous redox flow battery applications. Energy Storage Materials, 2021, 37, 576-586.	9.5	18
12	Pairwise Difference Regression: A Machine Learning Meta-algorithm for Improved Prediction and Uncertainty Quantification in Chemical Search. Journal of Chemical Information and Modeling, 2021, 61, 3846-3857.	2.5	17
13	Complexation and redox chemistry of neptunium, plutonium and americium with a hydroxylaminato ligand. Chemical Science, 2021, 12, 13343-13359.	3.7	13
14	Computer-Assisted Design of Macrocyclic Chelators for Actinium-225 Radiotherapeutics. Inorganic Chemistry, 2021, 60, 623-632.	1.9	20
15	Using molten salts to probe outer-coordination sphere effects on lanthanide(<scp>iii</scp>)/(<scp>ii</scp>) electron-transfer reactions. Dalton Transactions, 2021, 50, 15696-15710.	1.6	10
16	First-principles modeling of conductivity at the (001), (110), and (111) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml heterointerfaces. Physical Review B, 2021, 104, .	1.1	0
17	Isolation and characterization of a californium metallocene. Nature, 2021, 599, 421-424.	13.7	25
18	â€œSweepingâ€•Ortho Substituents Drive Desolvation and Overwhelm Electronic Effects in Nd³⁺ Chelation: A Case of Three Aryldithiophosphinates. Inorganic Chemistry, 2020, 59, 161-171.	1.9	10

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19	Structural and Optical Properties of Phase-Pure UO₂, Î±-U₃O₈, and Î±-UO₃ Epitaxial Thin Films Grown by Pulsed Laser Deposition. ACS Applied Materials & Interfaces, 2020, 12, 35232-35241.	4.0	27
20	Mechanistic Study of the Production of NO_x Gases from the Reaction of Copper with Nitric Acid. Inorganic Chemistry, 2020, 59, 16833-16842.	1.9	1
21	SCC-DFTB Parameters for Feâ€“C Interactions. Journal of Physical Chemistry A, 2020, 124, 9674-9682.	1.1	3
22	Expanding the potential of redox carriers for flow battery applications. Journal of Materials Chemistry A, 2020, 8, 17808-17816.	5.2	5
23	Î´ and Ï† back-donation in AnIV metallacycles. Nature Communications, 2020, 11, 1558.	5.8	46
24	Water on Actinide Dioxide Surfaces: A Review of Recent Progress. Applied Sciences (Switzerland), 2020, 10, 4655.	1.3	13
25	The duality of electron localization and covalency in lanthanide and actinide metallocenes. Chemical Science, 2020, 11, 2796-2809.	3.7	48
26	Development of Density Functional Tight-Binding Parameters Using Relative Energy Fitting and Particle Swarm Optimization. Journal of Chemical Theory and Computation, 2020, 16, 1469-1481.	2.3	7
27	Tight-Binding Modeling of Uranium in an Aqueous Environment. Journal of Chemical Theory and Computation, 2020, 16, 3073-3083.	2.3	6
28	Comparison of tetravalent cerium and terbium ions in a conserved, homoleptic imidophosphorane ligand field. Chemical Science, 2020, 11, 6149-6159.	3.7	33
29	Computational screening of two-dimensional coatings for semiconducting photocathodes. Physical Review Materials, 2020, 4, .	0.9	8
30	Halide anion discrimination by a tripodal hydroxylamine ligand in gas and condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 19868-19878.	1.3	1
31	RÃ¼cktitelbild: [Am(C₅Me₄H)₃]: An Organometallic Americium Complex (Angew. Chem. 34/2019). Angewandte Chemie, 2019, 131, 12050-12050.	1.6	0
32	Design, Isolation, and Spectroscopic Analysis of a Tetravalent Terbium Complex. Journal of the American Chemical Society, 2019, 141, 13222-13233.	6.6	80
33	Solubility model of metal complex in ionic liquids from first principle calculations. RSC Advances, 2019, 9, 18506-18526.	1.7	19
34	Excess Electrons on Reduced AnO₂ (111) Surfaces (An = Th, U, Pu) and Their Impacts on Catalytic Water Splitting. Journal of Physical Chemistry C, 2019, 123, 30245-30251.	1.5	23
35	Soft-donor dipicolinamide derivatives for selective actinide(<scp>iii</scp>)/lanthanide(<scp>iii</scp>) separation: the role of S- vs. O-donor sites. Chemical Communications, 2019, 55, 2441-2444.	2.2	29
36	Linked Picolinamide Nickel Complexes as Redox Carriers for Nonaqueous Flow Batteries. ChemSusChem, 2019, 12, 1304-1309.	3.6	11

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37	[Am(C₅Me₄H)₃]: An Organometallic Americium Complex. Angewandte Chemie - International Edition, 2019, 58, 11695-11699.	7.2	29
38	[Am(C 5 Me 4 H) 3]: An Organometallic Americium Complex. Angewandte Chemie, 2019, 131, 11821-11825.	1.6	16
39	Homoleptic Imidophosphorane Stabilization of Tetravalent Cerium. Inorganic Chemistry, 2019, 58, 5289-5304.	1.9	40
40	Advancing Chelation Chemistry for Actinium and Other +3 f-Elements, Am, Cm, and La. Journal of the American Chemical Society, 2019, 141, 19404-19414.	6.6	46
41	Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. Frontiers in Physics, 2019, 6, .	1.0	9
42	Spectroscopic and Computational Characterization of Diethylenetriaminepentaacetic Acid/Transplutonium Chelates: Evidencing Heterogeneity in the Heavy Actinide(III) Series. Angewandte Chemie - International Edition, 2018, 57, 4521-4526.	7.2	33
43	Spectroscopic and Computational Characterization of Diethylenetriaminepentaacetic Acid/Transplutonium Chelates: Evidencing Heterogeneity in the Heavy Actinide(III) Series. Angewandte Chemie, 2018, 130, 4611-4616.	1.6	2
44	Bond Covalency and Oxidation State of Actinide Ions Complexed with Therapeutic Chelating Agent 3,4,3-LI(1,2-HOPO). Inorganic Chemistry, 2018, 57, 5352-5363.	1.9	88
45	Ligand induced shape transformation of thorium dioxide nanocrystals. Physical Chemistry Chemical Physics, 2018, 20, 17563-17573.	1.3	18
46	Coordination Chemistry of a Strongly-Donating Hydroxylamine with Early Actinides: An Investigation of Redox Properties and Electronic Structure. Inorganic Chemistry, 2018, 57, 4387-4394.	1.9	21
47	Plutonium coordination and redox chemistry with the CyMe₄-BTPhen polydentate N-donor extractant ligand. Chemical Communications, 2018, 54, 12582-12585.	2.2	10
48	Energy-Degeneracy-Driven Covalency in Actinide Bonding. Journal of the American Chemical Society, 2018, 140, 17977-17984.	6.6	108
49	Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. ACS Omega, 2018, 3, 14766-14778.	1.6	10
50	Perspectives on Designer Photocathodes for X-ray Free-Electron Lasers: Influencing Emission Properties with Heterostructures and Nanoengineered Electronic States. Physical Review Applied, 2018, 10, .	1.5	36
51	Revisiting complexation thermodynamics of transplutonium elements up to einsteinium. Chemical Communications, 2018, 54, 10578-10581.	2.2	20
52	A series of dithiocarbamates for americium, curium, and californium. Dalton Transactions, 2018, 47, 14452-14461.	1.6	49
53	Influence of Substituents on the Electronic Structure of Mono- and Bis(phosphido) Thorium(IV) Complexes. Inorganic Chemistry, 2018, 57, 7270-7278.	1.9	13
54	A Pseudotetrahedral Uranium(V) Complex. Inorganic Chemistry, 2018, 57, 8106-8115.	1.9	16

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55	Identification of the Formal +2 Oxidation State of Neptunium: Synthesis and Structural Characterization of {Np^{II}[C₅H₃(SiMe₃)₂]₃}^{1â€“}. Journal of the American Chemical Society, 2018, 140, 7425-7428.	6.6	81
56	Overcoming the quantum efficiency-lifetime tradeoff of photocathodes by coating with atomically thin two-dimensional nanomaterials. Npj 2D Materials and Applications, 2018, 2, .	3.9	21
57	Synthesis and Characterization of the Actinium Aquo Ion. ACS Central Science, 2017, 3, 176-185.	5.3	53
58	Bonding in Uranium(V) Hexafluoride Based on the Experimental Electron Density Distribution Measured at 20 K. Inorganic Chemistry, 2017, 56, 1775-1778.	1.9	23
59	Covalency in Americium(III) Hexachloride. Journal of the American Chemical Society, 2017, 139, 8667-8677.	6.6	89
60	Degradation of Alkali-Based Photocathodes from Exposure to Residual Gases: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 8399-8408.	1.5	26
61	Evaluating the electronic structure of formal Ln^{II}ions in Ln^{II}(C₅H₄SiMe₃)₃^{1â^’}using XANES spectroscopy and DFT calculations. Chemical Science, 2017, 8, 6076-6091.	3.7	42
62	Assessment of Tuned Range Separated Exchange Functionals for Spectroscopies and Properties of Uranium Complexes. Journal of Chemical Theory and Computation, 2017, 13, 3614-3625.	2.3	17
63	Quantitative Evidence for Lanthanide-Oxygen Orbital Mixing in CeO₂, PrO₂, and TbO₂. Journal of the American Chemical Society, 2017, 139, 18052-18064.	6.6	75
64	On the Origin of Covalent Bonding in Heavy Actinides. Journal of the American Chemical Society, 2017, 139, 9901-9908.	6.6	95
65	Kinetics of alkali-based photocathode degradation. AIP Advances, 2016, 6, .	0.6	15
66	Spectroscopic and computational investigation of actinium coordination chemistry. Nature Communications, 2016, 7, 12312.	5.8	73
67	A Linear trans-Bis(imido) Neptunium(V) Actinyl Analog: Np^V(NDipp)₂(^tBu₂bipy)₂Cl (Dipp = 2,6-ⁱPr₂C₆H₃). Journal of the American Chemical Society, 2015, 137, 9583-9586.	6.6	33
68	Covalency in Lanthanides. An X-ray Absorption Spectroscopy and Density Functional Theory Study of LnCl₆^{xâ€“}(x= 3, 2). Journal of the American Chemical Society, 2015, 137, 2506-2523.	6.6	182
69	Using solution- and solid-state S K-edge X-ray absorption spectroscopy with density functional theory to evaluate Mâ€“S bonding for MS₄^{2â^’}(M = Cr, Mo, W) dianions. Dalton Transactions, 2014, 43, 17283-17295.	1.6	15
70	New evidence for 5f covalency in actinocenes determined from carbon K-edge XAS and electronic structure theory. Chemical Science, 2014, 5, 351-359.	3.7	131
71	Electronic structure and O K-edge XAS spectroscopy of U3O8. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 81-87.	0.8	26
72	Covalency in Metalâ€“Oxygen Multiple Bonds Evaluated Using Oxygen K-edge Spectroscopy and Electronic Structure Theory. Journal of the American Chemical Society, 2013, 135, 1864-1871.	6.6	57

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73	Carbon K-Edge X-ray Absorption Spectroscopy and Time-Dependent Density Functional Theory Examination of Metalâ€“Carbon Bonding in Metallocene Dichlorides. Journal of the American Chemical Society, 2013, 135, 14731-14740.	6.6	43
74	Tetrahalide Complexes of the [U(NR)₂]²⁺ Ion: Synthesis, Theory, and Chlorine K-Edge X-ray Absorption Spectroscopy. Journal of the American Chemical Society, 2013, 135, 2279-2290.	6.6	87
75	A Screened Hybrid DFT Study of Actinide Oxides, Nitrides, and Carbides. Journal of Physical Chemistry C, 2013, 117, 13122-13128.	1.5	52
76	Role of Geometric Distortion and Polarization in Localizing Electronic Excitations in Conjugated Polymers. Journal of Chemical Theory and Computation, 2013, 9, 1144-1154.	2.3	50
77	Screened hybrid and DFT +Ustudies of the structural, electronic, and optical properties of U₃O₈. Journal of Physics Condensed Matter, 2013, 25, 025501.	0.7	26
78	Effect of spin-orbit coupling on the actinide dioxides AnO2 (An=Th, Pa, U, Np, Pu, and Am): A screened hybrid density functional study. Journal of Chemical Physics, 2012, 137, 154707.	1.2	108
79	Determining Relative f and d Orbital Contributions to Mâ€“Cl Covalency in MCl₆^{2â€“} (M = Ti, Zr, Hf, U) and UOCl₅^{â€“} Using Cl K-Edge X-ray Absorption Spectroscopy and Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2012, 134, 5586-5597.	6.6	175
80	Theoretical Examination of the Thermodynamic Factors in the Selective Extraction of Am3+ from Eu3+ by Dithiophosphinic Acids. Inorganic Chemistry, 2012, 51, 13-15.	1.9	49
81	Sulfur K-edge X-ray Absorption Spectroscopy and Time-Dependent Density Functional Theory of Dithiophosphinate Extractants: Minor Actinide Selectivity and Electronic Structure Correlations. Journal of the American Chemical Society, 2012, 134, 14408-14422.	6.6	65
82	Probing Ni[S₂PR₂]₂ Electronic Structure to Generate Insight Relevant to Minor Actinide Extraction Chemistry. Inorganic Chemistry, 2012, 51, 7551-7560.	1.9	16
83	Experimental and Theoretical Comparison of the O K-Edge Nonresonant Inelastic X-ray Scattering and X-ray Absorption Spectra of NaReO4. Journal of the American Chemical Society, 2010, 132, 13914-13921.	6.6	37
84	Calculation of One-Electron Redox Potentials Revisited. Is It Possible to Calculate Accurate Potentials with Density Functional Methods?. Journal of Physical Chemistry A, 2009, 113, 6745-6750.	1.1	270
85	Trends in Covalency for d- and f-Element Metallocene Dichlorides Identified Using Chlorine K-Edge X-ray Absorption Spectroscopy and Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2009, 131, 12125-12136.	6.6	169
86	Uranium(VI) Bis(imido) Chalcogenate Complexes: Synthesis and Density Functional Theory Analysis. Inorganic Chemistry, 2009, 48, 2693-2700.	1.9	71
87	Theoretical Studies on the Redox Potentials of Fe Dinuclear Complexes as Models for Hydrogenase. Inorganic Chemistry, 2008, 47, 9228-9237.	1.9	72
88	Covalency Trends in Group IV Metallocene Dichlorides. Chlorine K-Edge X-Ray Absorption Spectroscopy and Time Dependent-Density Functional Theory. Inorganic Chemistry, 2008, 47, 5365-5371.	1.9	47
89	Electron Localization in the Ground State of the Ruthenium Blue Dimer. Journal of the American Chemical Society, 2007, 129, 7224-7225.	6.6	31
90	Synthesis of Imido Analogs of the Uranyl Ion. Science, 2005, 310, 1941-1943.	6.0	211

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91	Electronic Structure and Spectroscopy of f-Element Tris(cyclopentadienyl) Complexes. ACS Symposium Series, 0, , 285-327.	0.5	1
92	Synthesis, solid-state, solution, and theoretical characterization of an â€œin-cageâ€•scandium-NOTA complex. Dalton Transactions, 0, , .	1.6	0