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	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
2	Synthesis of Imido Analogs of the Uranyl Ion. Science, 2005, 310, 1941-1943.	6.0	211
3	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
4	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
5	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
6	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
7	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
8	Energy-Degeneracy-Driven Covalency in Actinide Bonding. Journal of the American Chemical Society, 2018, 140, 17977-17984.	6.6	108
9	On the Origin of Covalent Bonding in Heavy Actinides. Journal of the American Chemical Society, 2017, 139, 9901-9908.	6.6	95
10	Covalency in Americium(III) Hexachloride. Journal of the American Chemical Society, 2017, 139, 8667-8677.	6.6	89
11	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
12	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
13	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
14	Design, Isolation, and Spectroscopic Analysis of a Tetravalent Terbium Complex. Journal of the American Chemical Society, 2019, 141, 13222-13233.	6.6	80
15	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
16	Spectroscopic and computational investigation of actinium coordination chemistry. Nature Communications, 2016, 7, 12312.	5.8	73
17	Theoretical Studies on the Redox Potentials of Fe Dinuclear Complexes as Models for Hydrogenase. Inorganic Chemistry, 2008, 47, 9228-9237.	1.9	72
18	Uranium(VI) Bis(imido) Chalcogenate Complexes: Synthesis and Density Functional Theory Analysis. Inorganic Chemistry, 2009, 48, 2693-2700.	1.9	71

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19	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
20	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
21	Synthesis and Characterization of the Actinium Aquo Ion. ACS Central Science, 2017, 3, 176-185.	5.3	53
22	A Screened Hybrid DFT Study of Actinide Oxides, Nitrides, and Carbides. Journal of Physical Chemistry C, 2013, 117, 13122-13128.	1.5	52
23	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
24	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
25	A series of dithiocarbamates for americium, curium, and californium. Dalton Transactions, 2018, 47, 14452-14461.	1.6	49
26	The duality of electron localization and covalency in lanthanide and actinide metallocenes. Chemical Science, 2020, 11, 2796-2809.	3.7	48
27	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
28	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
29	Î´ and Ï† back-donation in AnIV metallacycles. Nature Communications, 2020, 11, 1558.	5.8	46
30	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
31	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
32	Homoleptic Imidophosphorane Stabilization of Tetravalent Cerium. Inorganic Chemistry, 2019, 58, 5289-5304.	1.9	40
33	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
34	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
35	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
36	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

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37	Comparison of tetravalent cerium and terbium ions in a conserved, homoleptic imidophosphorane ligand field. Chemical Science, 2020, 11, 6149-6159.	3.7	33
38	Electron Localization in the Ground State of the Ruthenium Blue Dimer. Journal of the American Chemical Society, 2007, 129, 7224-7225.	6.6	31
39	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
40	[Am(C₅Me₄H)₃]: An Organometallic Americium Complex. Angewandte Chemie - International Edition, 2019, 58, 11695-11699.	7.2	29
41	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
42	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
43	Electronic structure and O K-edge XAS spectroscopy of U3O8. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 81-87.	0.8	26
44	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
45	Isolation and characterization of a californium metallocene. Nature, 2021, 599, 421-424.	13.7	25
46	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
47	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
48	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
49	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
50	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
51	Revisiting complexation thermodynamics of transplutonium elements up to einsteinium. Chemical Communications, 2018, 54, 10578-10581.	2.2	20
52	Computer-Assisted Design of Macrocyclic Chelators for Actinium-225 Radiotherapeutics. Inorganic Chemistry, 2021, 60, 623-632.	1.9	20
53	Solubility model of metal complex in ionic liquids from first principle calculations. RSC Advances, 2019, 9, 18506-18526.	1.7	19
54	Ligand induced shape transformation of thorium dioxide nanocrystals. Physical Chemistry Chemical Physics, 2018, 20, 17563-17573.	1.3	18

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55	Iron-iminopyridine complexes as charge carriers for non-aqueous redox flow battery applications. Energy Storage Materials, 2021, 37, 576-586.	9.5	18
56	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
57	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
58	Probing Ni[S₂PR₂]₂ Electronic Structure to Generate Insight Relevant to Minor Actinide Extraction Chemistry. Inorganic Chemistry, 2012, 51, 7551-7560.	1.9	16
59	A Pseudotetrahedral Uranium(V) Complex. Inorganic Chemistry, 2018, 57, 8106-8115.	1.9	16
60	[Am(C 5 Me 4 H) 3]: An Organometallic Americium Complex. Angewandte Chemie, 2019, 131, 11821-11825.	1.6	16
61	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
62	Kinetics of alkali-based photocathode degradation. AIP Advances, 2016, 6, .	0.6	15
63	Complexation of Lanthanides and Heavy Actinides with Aqueous Sulfur-Donating Ligands. Inorganic Chemistry, 2021, 60, 6125-6134.	1.9	15
64	Influence of Substituents on the Electronic Structure of Mono- and Bis(phosphido) Thorium(IV) Complexes. Inorganic Chemistry, 2018, 57, 7270-7278.	1.9	13
65	Water on Actinide Dioxide Surfaces: A Review of Recent Progress. Applied Sciences (Switzerland), 2020, 10, 4655.	1.3	13
66	Complexation and redox chemistry of neptunium, plutonium and americium with a hydroxylaminato ligand. Chemical Science, 2021, 12, 13343-13359.	3.7	13
67	Linked Picolinamide Nickel Complexes as Redox Carriers for Nonaqueous Flow Batteries. ChemSusChem, 2019, 12, 1304-1309.	3.6	11
68	A Comparative Review of Metalâ€Based Charge Carriers in Nonaqueous Flow Batteries. ChemSusChem, 2021, 14, 1214-1228.	3.6	11
69	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
70	Plutonium coordination and redox chemistry with the CyMe₄-BTPhen polydentate N-donor extractant ligand. Chemical Communications, 2018, 54, 12582-12585.	2.2	10
71	Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. ACS Omega, 2018, 3, 14766-14778.	1.6	10
72	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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73	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
74	Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. Frontiers in Physics, 2019, 6, .	1.0	9
75	Computational screening of two-dimensional coatings for semiconducting photocathodes. Physical Review Materials, 2020, 4, .	0.9	8
76	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
77	An Allyl Uranium(IV) Sandwich Complex: Are Ï• Bonding Interactions Possible?. Chemistry - A European Journal, 2022, , e202200114.	1.7	7
78	Tight-Binding Modeling of Uranium in an Aqueous Environment. Journal of Chemical Theory and Computation, 2020, 16, 3073-3083.	2.3	6
79	Expanding the potential of redox carriers for flow battery applications. Journal of Materials Chemistry A, 2020, 8, 17808-17816.	5.2	5
80	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
81	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
82	SCC-DFTB Parameters for Feâ€“C Interactions. Journal of Physical Chemistry A, 2020, 124, 9674-9682.	1.1	3
83	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
84	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
85	Halide anion discrimination by a tripodal hydroxylamine ligand in gas and condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 19868-19878.	1.3	1
86	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
87	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
88	Electronic Structure and Spectroscopy of f-Element Tris(cyclopentadienyl) Complexes. ACS Symposium Series, 0, , 285-327.	0.5	1
89	RÃ¼cktitelbild: [Am(C₅Me₄H)₃]: An Organometallic Americium Complex (Angew. Chem. 34/2019). Angewandte Chemie, 2019, 131, 12050-12050.	1.6	0
90	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

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91	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:msub></mml:mrow></mml:math> heterointerfaces. Physical Review B, 2021, 104, .	3.7	0
92	Synthesis, solid-state, solution, and theoretical characterization of an â€œin-cageâ€•scandium-NOTA complex. Dalton Transactions, 0, , .	1.6	0