

Dayán Páez-Hernández

List of Publications by Year in descending order

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50
papers

771
citations

567247

15
h-index

580810

25
g-index

50
all docs

50
docs citations

50
times ranked

957
citing authors

#	ARTICLE	IF	CITATIONS
1	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystal-Field Models. <i>Chemistry - A European Journal</i> , 2014, 20, 7994-8011.	3.3	85
2	Theoretical Method for an Accurate Elucidation of Energy Transfer Pathways in Europium(III) Complexes with Dipyridophenazine (dppz) Ligand: One More Step in the Study of the Molecular Antenna Effect. <i>Inorganic Chemistry</i> , 2017, 56, 9200-9208.	4.0	53
3	Study of the structure-bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays. <i>New Journal of Chemistry</i> , 2018, 42, 8851-8863.	2.8	41
4	Luminescent europium(III) and terbium(III) complexes of β^2 -diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. <i>New Journal of Chemistry</i> , 2019, 43, 15139-15152.	2.8	38
5	Novel fluorescent Schiff bases as Al ³⁺ sensors with high selectivity and sensitivity, and their bioimaging applications. <i>Materials Chemistry and Physics</i> , 2019, 233, 89-101.	4.0	37
6	Understanding the Selective-Sensing Mechanism of Al ³⁺ Cation by a Chemical Sensor Based on Schiff Base: A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6970-6977.	2.5	31
7	Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn ²⁺ : synthesis, theory and bioimaging applications. <i>RSC Advances</i> , 2019, 9, 30778-30789.	3.6	28
8	Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. <i>Inorganic Chemistry</i> , 2018, 57, 5120-5132.	4.0	27
9	Electronic Structure and Properties of Berkelium Iodates. <i>Journal of the American Chemical Society</i> , 2017, 139, 13361-13375.	13.7	25
10	Rare-Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2-cryptand)] [Sc(OC ₆ H ₄ CH ₂ CH ₂ CH ₂ OC ₆ H ₄) ₂ Me ₄] ₃ . <i>Chemistry - A European Journal</i> , 2018, 24, 18059-18067.	3.3	25
11	The role of the excited state dynamic of the antenna ligand in the lanthanide sensitization mechanism. <i>Dalton Transactions</i> , 2020, 49, 7444-7450.	3.3	25
12	Sensing mechanism elucidation of a europium(III) metal-organic framework selective to aniline: A theoretical insight by means of multiconfigurational calculations. <i>Journal of Computational Chemistry</i> , 2020, 41, 1956-1964.	3.3	24
13	Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin- β -Cyclodextrin Polymer, and Antifungal Effect. <i>Frontiers in Chemistry</i> , 2018, 6, 312.	3.6	23
14	Cyclic voltammetry, relativistic DFT calculations and biological test of cytotoxicity in walled-cell models of two classical rhenium(I) tricarbonyl complexes with 5-amine-1,10-phenanthroline. <i>Chemical Physics Letters</i> , 2019, 715, 231-238.	2.6	20
15	Spectral, theoretical characterization and antifungal properties of two phenol derivative Schiff bases with an intramolecular hydrogen bond. <i>New Journal of Chemistry</i> , 2015, 39, 7822-7831.	2.8	19
16	Radiative decay channel assessment to understand the sensing mechanism of a fluorescent turn-on Al ³⁺ chemosensor. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26083.	2.0	16
17	The role of the [CpM(CO) ₂] ⁺ chromophore in the optical properties of the [Cp ₂ ThMCP(CO) ₂] ⁺ complexes, where M = Fe, Ru and Os. A theoretical view. <i>Dalton Transactions</i> , 2015, 44, 20004-20010.	3.3	15
18	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. <i>Inorganic Chemistry</i> , 2019, 58, 3457-3465.	4.0	14

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19	Sensing mechanism elucidation of a chemosensor based on a metal-organic framework selective to explosive aromatic compounds. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26404.	2.0	14
20	Insights into the selective sensing mechanism of a luminescent Cd(II)-based MOF chemosensor toward NACs: roles of the host-guest interactions and PET processes. <i>Journal of Materials Science</i> , 2021, 56, 13684-13704.	3.7	14
21	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the $[\text{Re}(\text{I}^{\frac{1}{4}}\text{-Q})\text{X}_6]^{4+}$ clusters. <i>New Journal of Chemistry</i> , 2018, 42, 5471-5478.	2.8	12
22	Spin-filter transport and magnetic properties in a binuclear Cu(ii) expanded porphyrin based molecular junction. <i>Dalton Transactions</i> , 2019, 48, 8418-8426.	3.3	12
23	Electronic, Magnetic, and Theoretical Characterization of $(\text{NH}_4)_4\text{UF}_8$, a Simple Molecular Uranium(IV) Fluoride. <i>Inorganic Chemistry</i> , 2019, 58, 637-647.	4.0	12
24	Structure, Spectroscopy, and Theoretical Analysis of Zero- and Three-Dimensional Lithium Plutonium Fluorides: Li_4PuF_8 and LiPuF_5 . <i>Inorganic Chemistry</i> , 2019, 58, 14790-14799.	4.0	11
25	Fluorescence turn-on and turn-off mechanisms of a dual-selective chemosensor of Bi^{3+} and pH changes: Insights from a theoretical perspective. <i>Dyes and Pigments</i> , 2021, 185, 108934.	3.7	11
26	Creation of an unexpected plane of enhanced covalency in cerium(III) and berkelium(III) terpyridyl complexes. <i>Nature Communications</i> , 2021, 12, 7230.	12.8	11
27	Aromatic Lateral Substituents Influence the Excitation Energies of Hexaaza Lanthanide Macrocyclic Complexes: A Wave Function Theory and Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9931-9940.	2.5	10
28	New Sensitive and Selective Chemical Sensors for Ni^{2+} and Cu^{2+} Ions: Insights into the Sensing Mechanism through DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6493-6503.	2.5	9
29	Modeling the electronic states and magnetic properties derived from the f^1 configuration in lanthanocene and actinocene compounds. <i>Dalton Transactions</i> , 2017, 46, 4834-4843.	3.3	8
30	The role of Cr, Mo and W in the electronic delocalization and the metal-ring interaction in metallocene complexes. <i>New Journal of Chemistry</i> , 2018, 42, 5334-5344.	2.8	8
31	Three new types of transition metal carboranylamidinate complexes. <i>Dalton Transactions</i> , 2018, 47, 6666-6671.	3.3	8
32	Theoretical examination of covalency in berkelium(IV) carbonate complexes. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26254.	2.0	8
33	Exploring rhenium (I) complexes as potential fluorophores for walled-cells (yeasts and bacteria): Photophysics, biocompatibility, and confocal microscopy. <i>Dyes and Pigments</i> , 2021, 184, 108876.	3.7	8
34	The role of zero-field splitting and π -stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. <i>New Journal of Chemistry</i> , 2021, 45, 11192-11201.	2.8	7
35	Insights into the role of D-A-A type pro-aromatic organic dyes with thieno[3,4-b]pyrazine as A acceptor group into dye-sensitized solar cells. A TD-DFT/periodic DFT study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26108.	2.0	6
36	Structural Characterization, DFT Calculation, NCI, Scan-Rate Analysis and Antifungal Activity against <i>Botrytis cinerea</i> of (E)-2-[(2-Aminopyridin-2-yl)imino]-methyl]-4,6-di-tert-butylphenol (Pyridine Schiff) Tj ETQq0 0 OrgBT / Overlock 10 TF		

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37	<i>Ab initio</i> calculations of heavy-actinide hexahalide compounds: do these heavy actinides behave like their isoelectronic lanthanide analogues?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4038-4049.	2.8	5
38	Tuning the molecular antenna effect using donor and acceptor substituents on the optical properties of the [(C5F5)2ThMCp2]2+ and [(C5F5)2ThMCpL2]+ complexes, where M = Fe, Ru and Os and L = CO and C5H5N. <i>New Journal of Chemistry</i> , 2018, 42, 11013-11022.	2.8	5
39	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd ^{III} Complexes with Regular and Mismatched DNA Sequences. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3219-3231.	2.6	5
40	A theoretical chemistry-based strategy for the rational design of new luminescent lanthanide complexes: an approach from a multireference SOC-NEVPT2 method. <i>Dalton Transactions</i> , 2021, 50, 13561-13571.	3.3	5
41	A new approach to the mechanism for the acetalization of benzaldehyde over MOF catalysts. <i>New Journal of Chemistry</i> , 2020, 44, 14865-14871.	2.8	5
42	Theoretical study of 8-hydroxyquinoline derivatives as potential antennas in lanthanide complexes: Photophysical properties and elucidation of energy transfer pathways. <i>International Journal of Quantum Chemistry</i> , 2022, 122, e26880.	2.0	5
43	Quantum Inelastic Scattering of ArHAr ⁺ , HeHHe ⁺ , and NeHNe ⁺ with He on New Potential Energy Surfaces. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 1924-1929.	2.7	5
44	Predicting the electronic structure and magnetic properties of UO ₂ ⁺ , UO ₂ (CO) ₅ ⁺ and UO ₂ (Ar) ₅ ⁺ using wavefunction based methods. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2014, 197, 1-6.	1.7	4
45	A theoretical study of the super exchange mechanism and magneto-structural relationships in the [Mn(ⁱⁱⁱ) ₂ (^{1/4} -F) ₄ (Me) ₃ tacn) ₂](PF ₆) ₆ 2.8 coordination compound. <i>New Journal of Chemistry</i> , 2018, 42, 13847-13855.	2.8	3
46	New Cationic fac-[Re(CO) ₃ (deeb)B ₂] ⁺ Complex, Where B ₂ Is a Benzimidazole Derivative, as a Potential New Luminescent Dye for Proteins Separated by SDS-PAGE. <i>Frontiers in Chemistry</i> , 2021, 9, 647816.	3.6	3
47	The role of substituted pyridine Schiff bases as ancillary ligands in the optical properties of a new series of <i>fac</i> -rhenium(ⁱ) tricarbonyl complexes: a theoretical view. <i>RSC Advances</i> , 2021, 11, 37181-37193.	3.6	2
48	Antiferromagnetic Coupling Supported by Metallophilic Interactions: Theoretical View. <i>Inorganic Chemistry</i> , 2022, 61, 1401-1417.	4.0	2
49	Understanding the Deactivating/Activating Mechanisms in Three Optical Chemosensors Based on Crown Ether with Na ⁺ /K ⁺ Selectivity Using Quantum Chemical Tools. <i>ChemPhysChem</i> , 2022, 23, .	2.1	1
50	Magnetic properties of organolanthanide(ii) complexes, from the electronic structure and the crystal field effect. <i>Dalton Transactions</i> , 2021, 50, 9787-9795.	3.3	0