DayÃ¡n PÃ¡ez-HernÃ¡ndez

List of Publications by Year
in descending order

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50 papers	771 citations	567281 15 h-index	580821 25 g-index
50 all docs	50 docs citations	50 times ranked	957 citing authors

#	Article	IF	Citations
1	Antiferromagnetic Coupling Supported by Metallophilic Interactions: Theoretical View. Inorganic Chemistry, 2022, 61, 1401-1417.	4.0	2
2	Theoretical study of 8â€hydroxyquinoline derivatives as potential antennas in lanthanide complexes: Photophysical properties and elucidation of energy transfer pathways. International Journal of Quantum Chemistry, 2022, 122, e26880.	2.0	5
3	Understanding the Deactivating/Activating Mechanisms in Three Optical Chemosensors Based on Crown Ether with Na⁺/K⁺ Selectivity Using Quantum Chemical Tools. ChemPhysChem, 2022, 23, .	2.1	1
4	Quantum Inelastic Scattering of ArHAr⁺, HeHHe⁺, and NeHNe⁺ with He on New Potential Energy Surfaces. ACS Earth and Space Chemistry, 2022, 6, 1924-1929.	2.7	5
5	Exploring rhenium (I) complexes as potential fluorophores for walled-cells (yeasts and bacteria): Photophysics, biocompatibility, and confocal microscopy. Dyes and Pigments, 2021, 184, 108876.	3.7	8
6	Fluorescence turn-on and turn-off mechanisms of a dual-selective chemosensor of Bi3+ and pH changes: Insights from a theoretical perspective. Dyes and Pigments, 2021, 185, 108934.	3.7	11
7	New Cationic fac-[Re(CO)3(deeb)B2]+ Complex, Where B2 Is a Benzimidazole Derivative, as a Potential New Luminescent Dye for Proteins Separated by SDS-PAGE. Frontiers in Chemistry, 2021, 9, 647816.	3.6	3
8	Insights into the selective sensing mechanism of a luminescent Cd(II)-based MOF chemosensor toward NACs: roles of the hostâ€"guest interactions and PET processes. Journal of Materials Science, 2021, 56, 13684-13704.	3.7	14
9	Magnetic properties of organolanthanide(ii) complexes, from the electronic structure and the crystal field effect. Dalton Transactions, 2021, 50, 9787-9795.	3.3	0
10	A theoretical chemistry-based strategy for the rational design of new luminescent lanthanide complexes: an approach from a multireference SOC-NEVPT2 method. Dalton Transactions, 2021, 50, 13561-13571.	3.3	5
11	The role of zero-field splitting and Ï€-stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. New Journal of Chemistry, 2021, 45, 11192-11201.	2.8	7
12	The role of substituted pyridine Schiff bases as ancillary ligands in the optical properties of a new series of fac-rhenium(<scp>i</scp>) tricarbonyl complexes: a theoretical view. RSC Advances, 2021, 11, 37181-37193.	3.6	2
13	Creation of an unexpected plane of enhanced covalency in cerium(III) and berkelium(III) terpyridyl complexes. Nature Communications, 2021, 12, 7230.	12.8	11
14	Radiative decay channel assessment to understand the sensing mechanism of a fluorescent turnâ€on Al³⁺ chemosensor. International Journal of Quantum Chemistry, 2020, 120, e26083.	2.0	16
15	Insights into the role of Dâ€Aâ€Ïâ€A type proâ€aromatic organic dyes with thieno[3,4â€b]pyrazine as A acceptor group into dyeâ€sensitized solarâ€cells. A TDâ€DFT/periodic DFT study. International Journal of Quantum Chemistry, 2020, 120, e26108.	2.0	6
16	Sensing mechanism elucidation of a chemosensor based on a <scp>metalâ€organic</scp> framework selective to explosive aromatic compounds. International Journal of Quantum Chemistry, 2020, 120, e26404.	2.0	14
17	The role of the excited state dynamic of the antenna ligand in the lanthanide sensitization mechanism. Dalton Transactions, 2020, 49, 7444-7450.	3.3	25
18	Structural Characterization, DFT Calculation, NCI, Scan-Rate Analysis and Antifungal Activity against Botrytis cinerea of (E)-2-{[(2-Aminopyridin-2-yl)imino]-methyl}-4,6-di-tert-butylphenol (Pyridine Schiff) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.8	6

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19	Sensing mechanism elucidation of a europium(<scp>III</scp>) <scp>metalâ€“organic</scp> framework selective to aniline: A theoretical insight by means of multiconfigurational calculations. Journal of Computational Chemistry, 2020, 41, 1956-1964.	3.3	24
20	New Sensitive and Selective Chemical Sensors for Ni²⁺ and Cu²⁺ Ions: Insights into the Sensing Mechanism through DFT Methods. Journal of Physical Chemistry A, 2020, 124, 6493-6503.	2.5	9
21	Theoretical examination of covalency in berkelium(<scp>IV</scp>) carbonate complexes. International Journal of Quantum Chemistry, 2020, 120, e26254.	2.0	8
22	A new approach to the mechanism for the acetalization of benzaldehyde over MOF catalysts. New Journal of Chemistry, 2020, 44, 14865-14871.	2.8	5
23	Understanding the Selective-Sensing Mechanism of Al³⁺ Cation by a Chemical Sensor Based on Schiff Base: A Theoretical Approach. Journal of Physical Chemistry A, 2019, 123, 6970-6977.	2.5	31
24	Structure, Spectroscopy, and Theoretical Analysis of Zero- and Three-Dimensional Lithium Plutonium Fluorides: Li4PuF8 and LiPuF5. Inorganic Chemistry, 2019, 58, 14790-14799.	4.0	11
25	Luminescent europium(<scp>iii</scp>) and terbium(<scp>iii</scp>) complexes of Î²-diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. New Journal of Chemistry, 2019, 43, 15139-15152.	2.8	38
26	Novel fluorescent Schiff bases as Al3+ sensors with high selectivity and sensitivity, and their bioimaging applications. Materials Chemistry and Physics, 2019, 233, 89-101.	4.0	37
27	Spin-filter transport and magnetic properties in a binuclear Cu(ii) expanded porphyrin based molecular junction. Dalton Transactions, 2019, 48, 8418-8426.	3.3	12
28	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd^{III} Complexes with Regular and Mismatched DNA Sequences. Journal of Physical Chemistry B, 2019, 123, 3219-3231.	2.6	5
29	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. Inorganic Chemistry, 2019, 58, 3457-3465.	4.0	14
30	Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn²⁺: synthesis, theory and bioimaging applications. RSC Advances, 2019, 9, 30778-30789.	3.6	28
31	Electronic, Magnetic, and Theoretical Characterization of (NH₄)₄UF₈, a Simple Molecular Uranium(IV) Fluoride. Inorganic Chemistry, 2019, 58, 637-647.	4.0	12
32	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. Chemical Physics Letters, 2019, 715, 231-238.	2.6	20
33	The role of Cr, Mo and W in the electronic delocalization and the metalâ€“ring interaction in metallocene complexes. New Journal of Chemistry, 2018, 42, 5334-5344.	2.8	8
34	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re₆(Î¼₃-Q)₈X₆]^{4â^'} clusters. New Journal of Chemistry, 2018, 42, 5471-5478.	2.8	12
35	Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. Inorganic Chemistry, 2018, 57, 5120-5132.	4.0	27
36	Study of the structureâ€“bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays. New Journal of Chemistry, 2018, 42, 8851-8863.	2.8	41

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37	Three new types of transition metal carboranylamidinate complexes. Dalton Transactions, 2018, 47, 6666-6671.	3.3	8
38	Ab initio calculations of heavy-actinide hexahalide compounds: do these heavy actinides behave like their isoelectronic lanthanide analogues?. Physical Chemistry Chemical Physics, 2018, 20, 4038-4049.	2.8	5
39	Rareâ€Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2â€cryptand)][Sc(OC₆H₂tBu₂â€2,6â€Meâ€4)₃]. Chemistry - A European Journal, 2018, 24, 18059-18067.	3.3	25
40	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. New Journal of Chemistry, 2018, 42, 11013-11022.	2.8	5
41	A theoretical study of the super exchange mechanism and magneto-structural relationships in the [Mn(<scp>iii</scp>)₂(Î¼-F)F₄(Me₃tacn)₂](PF₆) coordination compound. New Journal of Chemistry, 2018, 42, 13847-13855.	2.8	3
42	Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin-Î²-Cyclodextrin Polymer, and Antifungal Effect. Frontiers in Chemistry, 2018, 6, 312.	3.6	23
43	Modeling the electronic states and magnetic properties derived from the f¹ configuration in lanthanocene and actinocene compounds. Dalton Transactions, 2017, 46, 4834-4843.	3.3	8
44	Electronic Structure and Properties of Berkelium Iodates. Journal of the American Chemical Society, 2017, 139, 13361-13375.	13.7	25
45	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. Inorganic Chemistry, 2017, 56, 9200-9208.	4.0	53
46	Spectral, theoretical characterization and antifungal properties of two phenol derivative Schiff bases with an intramolecular hydrogen bond. New Journal of Chemistry, 2015, 39, 7822-7831.	2.8	19
47	The role of the [CpM(CO)₂]^{â^'} chromophore in the optical properties of the [Cp₂ThMCp(CO)₂]⁺ complexes, where M = Fe, Ru and Os. A theoretical view. Dalton Transactions, 2015, 44, 20004-20010.	3.3	15
48	Aromatic Lateral Substituents Influence the Excitation Energies of Hexaaza Lanthanide Macrocyclic Complexes: A Wave Function Theory and Density Functional Study. Journal of Physical Chemistry A, 2015, 119, 9931-9940.	2.5	10
49	Predicting the electronic structure and magnetic properties of UO2+, UO 2 (CO)5+and UO 2 (Ar)5+using wavefunction based methods. Journal of Electron Spectroscopy and Related Phenomena, 2014, 197, 1-6.	1.7	4
50	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystalâ€Field Models. Chemistry - A European Journal, 2014, 20, 7994-8011.	3.3	85