Dayn Pez-Hernndez

List of Publications by Year in Descending Order

48 papers	499 citations	14 h-index	19 g-index
50 ext. papers	634 ext. citations	4.2 avg, IF	4.15 L-index

#	Paper	IF	Citations
48	Antiferromagnetic Coupling Supported by Metallophilic Interactions: Theoretical View.. *Inorganic Chemistry*, **2022**, 61, 1401-1417	5.1	0
47	Creation of an unexpected plane of enhanced covalency in cerium(III) and berkelium(III) terpyridyl complexes. *Nature Communications*, **2021**, 12, 7230	17.4	0
46	The role of substituted pyridine Schiff bases as ancillary ligands in the optical properties of a new series of -rhenium(i) tricarbonyl complexes: a theoretical view.. *RSC Advances*, **2021**, 11, 37181-37193	3.7	1
45	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. *Journal of Materials Science*, **2021**, 56, 13684-13704	4.3	4
44	Exploring rhenium (I) complexes as potential fluorophores for walled-cells (yeasts and bacteria): Photophysics, biocompatibility, and confocal microscopy. *Dyes and Pigments*, **2021**, 184, 108876	4.6	7
43	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	4.6	5
42	New Cationic -[Re(CO)(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	5	3
41	Magnetic properties of organolanthanide(II) complexes, from the electronic structure and the crystal field effect. *Dalton Transactions*, **2021**, 50, 9787-9795	4.3	
40	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	4.3	2
39	The role of zero-field splitting and stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. *New Journal of Chemistry*, **2021**, 45, 11192-11201	3.6	5
38	The role of the excited state dynamic of the antenna ligand in the lanthanide sensitization mechanism. *Dalton Transactions*, **2020**, 49, 7444-7450	4.3	14
37	Structural Characterization, DFT Calculation, NCI, Scan-Rate Analysis and Antifungal Activity against of ()-2-{[(2-Aminopyridin-2-yl)imino]-methyl}-4,6-di--butylphenol (Pyridine Schiff Base). *Molecules*, **2020**, 25,	4.8	5
36	Sensing mechanism elucidation of a europium(III) metal-organic framework selective to aniline: A theoretical insight by means of multiconfigurational calculations. *Journal of Computational Chemistry*, **2020**, 41, 1956-1964	3.5	14
35	New Sensitive and Selective Chemical Sensors for Ni and Cu Ions: Insights into the Sensing Mechanism through DFT Methods. *Journal of Physical Chemistry A*, **2020**, 124, 6493-6503	2.8	3
34	A new approach to the mechanism for the acetalization of benzaldehyde over MOF catalysts. *New Journal of Chemistry*, **2020**, 44, 14865-14871	3.6	3
33	Radiative decay channel assessment to understand the sensing mechanism of a fluorescent turn-on Al3+ chemosensor. *International Journal of Quantum Chemistry*, **2020**, 120, e26083	2.1	3
32	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. *International Journal of Quantum Chemistry*, **2020**, 120, e26108	2.1	5

31	Sensing mechanism elucidation of a chemosensor based on a metal-organic framework selective to explosive aromatic compounds. *International Journal of Quantum Chemistry*, **2020**, 120, e26404	2.1	4
30	Theoretical examination of covalency in berkelium(IV) carbonate complexes. *International Journal of Quantum Chemistry*, **2020**, 120, e26254	2.1	4
29	Luminescent europium(III) and terbium(III) complexes of □diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. *New Journal of Chemistry*, **2019**, 43, 15139-15152	3.6	24
28	Novel fluorescent Schiff bases as Al3+ sensors with high selectivity and sensitivity, and their bioimaging applications. *Materials Chemistry and Physics*, **2019**, 233, 89-101	4.4	20
27	Spin-filter transport and magnetic properties in a binuclear Cu(ii) expanded porphyrin based molecular junction. *Dalton Transactions*, **2019**, 48, 8418-8426	4.3	9
26	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd Complexes with Regular and Mismatched DNA Sequences. *Journal of Physical Chemistry B*, **2019**, 123, 3219-3231	3.4	3
25	Understanding the Selective-Sensing Mechanism of Al Cation by a Chemical Sensor Based on Schiff Base: A Theoretical Approach. *Journal of Physical Chemistry A*, **2019**, 123, 6970-6977	2.8	21
24	Structure, Spectroscopy, and Theoretical Analysis of Zero- and Three-Dimensional Lithium Plutonium Fluorides: LiPuF and LiPuF. *Inorganic Chemistry*, **2019**, 58, 14790-14799	5.1	7
23	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. *Inorganic Chemistry*, **2019**, 58, 3457-3465	5.1	8
22	Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn: synthesis, theory and bioimaging applications.. *RSC Advances*, **2019**, 9, 30778-30789	3.7	16
21	Electronic, Magnetic, and Theoretical Characterization of (NH)UF, a Simple Molecular Uranium(IV) Fluoride. *Inorganic Chemistry*, **2019**, 58, 637-647	5.1	9
20	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	2.5	15
19	The role of Cr, Mo and W in the electronic delocalization and the metal□ing interaction in metallocene complexes. *New Journal of Chemistry*, **2018**, 42, 5334-5344	3.6	6
18	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re6(□3-Q)8X6]4□clusters. *New Journal of Chemistry*, **2018**, 42, 5471-5478	3.6	11
17	Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. *Inorganic Chemistry*, **2018**, 57, 5120-5132	5.1	21
16	Study of the structure□bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays. *New Journal of Chemistry*, **2018**, 42, 8851-8863	3.6	25
15	Three new types of transition metal carboranylamidinate complexes. *Dalton Transactions*, **2018**, 47, 6666-6671	4.5	4
14	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	3.6	5

13	A theoretical study of the super exchange mechanism and magneto-structural relationships in the [Mn(III)2(F)F4(Me3tacn)2](PF6) coordination compound. *New Journal of Chemistry*, **2018**, 42, 13847-13855	3.6	1
12	Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin- Cyclodextrin Polymer, and Antifungal Effect. *Frontiers in Chemistry*, **2018**, 6, 312	5	13
11	Rare-Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2-cryptand)][Sc(OC H tBu -2,6-Me-4)]. *Chemistry - A European Journal*, **2018**, 24, 18059-18067	4.8	19
10	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	3.6	4
9	Modeling the electronic states and magnetic properties derived from the f configuration in lanthanocene and actinocene compounds. *Dalton Transactions*, **2017**, 46, 4834-4843	4.3	6
8	Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375	16.4	18
7	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	5.1	40
6	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	3.6	15
5	The role of the [CpM(CO)2](-) chromophore in the optical properties of the [Cp2ThMCp(CO)2](+) complexes, where M = Fe, Ru and Os. A theoretical view. *Dalton Transactions*, **2015**, 44, 20004-10	4.3	13
4	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, 9931-40	2.8	6
3	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
2	Magnetic properties and electronic structure of neptunyl(VI) complexes: wavefunctions, orbitals, and crystal-field models. *Chemistry - A European Journal*, **2014**, 20, 7994-8011	4.8	73
1	Theoretical study of 8-hydroxyquinoline derivatives as potential antennas in lanthanide complexes: Photophysical properties and elucidation of energy transfer pathways. *International Journal of Quantum Chemistry*,e26880	2.1	1