

Dayn Pez-Hernandez

List of Publications by Citations

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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	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	4.8	73
47	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	5.1	40
46	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	3.6	25
45	Luminescent europium(III) and terbium(III) complexes of β -diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. <i>New Journal of Chemistry</i> , 2019 , 43, 15139-15152	3.6	24
44	Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. <i>Inorganic Chemistry</i> , 2018 , 57, 5120-5132	5.1	21
43	Understanding the Selective-Sensing Mechanism of Al Cation by a Chemical Sensor Based on Schiff Base: A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6970-6977	2.8	21
42	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	4.4	20
41	Rare-Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2-cryptand)][Sc(OC H tBu -2,6-Me-4)]. <i>Chemistry - A European Journal</i> , 2018 , 24, 18059-18067	4.8	19
40	Electronic Structure and Properties of Berkelium Iodates. <i>Journal of the American Chemical Society</i> , 2017 , 139, 13361-13375	16.4	18
39	Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn: synthesis, theory and bioimaging applications.. <i>RSC Advances</i> , 2019 , 9, 30778-30789	3.7	16
38	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	3.6	15
37	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	2.5	15
36	The role of the excited state dynamic of the antenna ligand in the lanthanide sensitization mechanism. <i>Dalton Transactions</i> , 2020 , 49, 7444-7450	4.3	14
35	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	3.5	14
34	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, 20004-10	4.3	13
33	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	5	13
32	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re ₆ (B-Q) ₈ X ₆] ₄ clusters. <i>New Journal of Chemistry</i> , 2018 , 42, 5471-5478	3.6	11

31	Spin-filter transport and magnetic properties in a binuclear Cu(II) expanded porphyrin based molecular junction. <i>Dalton Transactions</i> , 2019 , 48, 8418-8426	4.3	9
30	Electronic, Magnetic, and Theoretical Characterization of (NH) ₄ UF ₆ , a Simple Molecular Uranium(IV) Fluoride. <i>Inorganic Chemistry</i> , 2019 , 58, 637-647	5.1	9
29	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. <i>Inorganic Chemistry</i> , 2019 , 58, 3457-3465	5.1	8
28	Structure, Spectroscopy, and Theoretical Analysis of Zero- and Three-Dimensional Lithium Plutonium Fluorides: LiPuF and LiPuF ₃ . <i>Inorganic Chemistry</i> , 2019 , 58, 14790-14799	5.1	7
27	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	4.6	7
26	Modeling the electronic states and magnetic properties derived from the f configuration in lanthanocene and actinocene compounds. <i>Dalton Transactions</i> , 2017 , 46, 4834-4843	4.3	6
25	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, 9931-40	2.8	6
24	The role of Cr, Mo and W in the electronic delocalization and the metal-ligand interaction in metallocene complexes. <i>New Journal of Chemistry</i> , 2018 , 42, 5334-5344	3.6	6
23	Structural Characterization, DFT Calculation, NCI, Scan-Rate Analysis and Antifungal Activity against of ()-2-[[[2-Aminopyridin-2-yl]imino]-methyl]-4,6-di- <i>n</i> -butylphenol (Pyridine Schiff Base). <i>Molecules</i> , 2020 , 25,	4.8	5
22	Ab initio 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	3.6	5
21	Insights into the role of D-A- π type pro-aromatic organic dyes with thieno[3,4- <i>b</i>]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	2.1	5
20	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	4.6	5
19	The role of zero-field splitting and π -backing 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	3.6	5
18	Three new types of transition metal carboranylamidinate complexes. <i>Dalton Transactions</i> , 2018 , 47, 6666-6671	4.5	4
17	Predicting the electronic structure and magnetic properties of UO ₂ 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
16	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	2.1	4
15	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	4.3	4
14	Theoretical examination of covalency in berkelium(IV) carbonate complexes. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26254	2.1	4

13	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	3.6	4
12	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd Complexes with Regular and Mismatched DNA Sequences. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 3219-3231	3.4	3
11	New Sensitive and Selective Chemical Sensors for Ni and Cu Ions: Insights into the Sensing Mechanism through DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6493-6503	2.8	3
10	A new approach to the mechanism for the acetalization of benzaldehyde over MOF catalysts. <i>New Journal of Chemistry</i> , 2020 , 44, 14865-14871	3.6	3
9	Radiative decay channel assessment to understand the sensing mechanism of a fluorescent turn-on Al3+ chemosensor. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26083	2.1	3
8	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. <i>Frontiers in Chemistry</i> , 2021 , 9, 647816	5	3
7	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	4.3	2
6	A theoretical study of the super exchange mechanism and magneto-structural relationships in the [Mn(III)2(FF)F4(Me3tacn)2](PF6) coordination compound. <i>New Journal of Chemistry</i> , 2018 , 42, 13847-13855	3.6	1
5	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> , e26880	2.1	1
4	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.. <i>RSC Advances</i> , 2021 , 11, 37181-37193	3.7	1
3	Creation of an unexpected plane of enhanced covalency in cerium(III) and berkelium(III) terpyridyl complexes. <i>Nature Communications</i> , 2021 , 12, 7230	17.4	0
2	Antiferromagnetic Coupling Supported by Metallophilic Interactions: Theoretical View.. <i>Inorganic Chemistry</i> , 2022 , 61, 1401-1417	5.1	0
1	Magnetic properties of organolanthanide(II) complexes, from the electronic structure and the crystal field effect. <i>Dalton Transactions</i> , 2021 , 50, 9787-9795	4.3	