Chantal Daniel

List of Publications by Year
in descending order

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		159585	175258
66	2,847	30	52
papers	citations	h-index	g-index

68	68	68	2736
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spin-Vibronic Mechanism for Intersystem Crossing. Chemical Reviews, 2018, 118, 6975-7025.	47.7	592
2	Photochemistry and photophysics of transition metal complexes: Quantum chemistry. Coordination Chemistry Reviews, 2015, 282-283, 19-32.	18.8	118
3	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	18.8	109
4	UVâ^'Visible Absorption Spectra of [Ru(E)(Eâ€˜)(CO)2(iPr-DAB)] (E = Eâ€˜ = SnPh3or Cl; E = SnPh3or Cl, Eâ€˜ =) Tj ETQq0 0 0 rgBT /Over Calculations. Journal of the American Chemical Society, 2001, 123, 11431-11440.	13.7	101
5	Spin-Vibronic Quantum Dynamics for Ultrafast Excited-State Processes. Accounts of Chemical Research, 2015, 48, 809-817.	15.6	96
6	Relativistic effects in spectroscopy and photophysics of heavy-metal complexes illustrated by spinâ€“orbit calculations of [Re(imidazole)(CO)3(phen)]+. Coordination Chemistry Reviews, 2011, 255, 975-989.	18.8	90
7	Photo-induced redox catalysis for proton reduction to hydrogen with homogeneous molecular systems using rhodium-based catalysts. Coordination Chemistry Reviews, 2015, 304-305, 20-37.	18.8	87
8	Spinâ€“Orbit Treatment of UVâ€“vis Absorption Spectra and Photophysics of Rhenium(I) Carbonylâ€“Bipyridine Complexes: MS-CASPT2 and TD-DFT Analysis. Journal of Physical Chemistry A, 2012, 116, 11319-11329.	2.5	74
9	A theoretical study of Ru(II) polypyridyl DNA intercalators. Journal of Inorganic Biochemistry, 2010, 104, 893-901.	3.5	70
10	Influence of the Halogen Ligand on the Near-UVâ^'Visible Spectrum of [Ru(X)(Me)(CO)2(Î±-diimine)] (X = Cl,) Tj ETQq0 0 0 rgBT /Overloc Chemistry, 2004, 43, 7978-7985.	4.0	60
11	Spectroscopy of Ru(II) polypyridyl complexes used as intercalators in DNA: Towards a theoretical study of the light switch effect. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 310-320.	3.9	57
12	Electronic absorption spectroscopy of [Ru(phen)2(bpy)]2+, [Ru(phen)2(dmbp)]2+, [Ru(tpy)(phen)(CH3CN)]2+ and [Ru(tpy)(dmp)(CH3CN)]2+A theoretical study. Coordination Chemistry Reviews, 2008, 252, 2493-2503.	18.8	56
13	Photophysical Properties of Ruthenium(II) Polypyridyl DNA Intercalators: Effects of the Molecular Surroundings Investigated by Theory. Chemistry - A European Journal, 2014, 20, 12901-12909.	3.3	54
14	Heteroleptic diimine copper(i) complexes with large extinction coefficients: synthesis, quantum chemistry calculations and physico-chemical properties. Dalton Transactions, 2013, 42, 14628.	3.3	53
15	Exploring the Mechanism of Ultrafast Intersystem Crossing in Rhenium(I) Carbonyl Bipyridine Halide Complexes: Key Vibrational Modes and Spinâ€“Vibronic Quantum Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 2335-2345.	5.3	52
16	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. Journal of Chemical Theory and Computation, 2019, 15, 5031-5045.	5.3	50
17	Spin-orbit induced radiationless transitions in organometallics: Quantum simulation of the intersystem crossing processes in the photodissociation of HCo(CO)4. Journal of Chemical Physics, 1997, 106, 1421-1428.	3.0	49
18	Theoretical evidence of photo-induced charge transfer from DNA to intercalated ruthenium (II) organometallic complexes. Chemical Physics Letters, 2013, 578, 133-137.	2.6	47

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19	A coupled cluster study of the electronic spectroscopy and photochemistry of Cr(CO)6. Physical Chemistry Chemical Physics, 2007, 9, 6115.	2.8	46
20	Ultrafast Excited-State Decays in [Re(CO)₃(N,N)(L)]ⁿ⁺: Nonadiabatic Quantum Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 1293-1306.	5.3	45
21	Spinâ€“orbit effects in square-planar Pt(<scp>ii</scp>) complexes with bidentate and terdentate ligands: theoretical absorption/emission spectroscopy. Dalton Transactions, 2014, 43, 17806-17819.	3.3	41
22	Excited-states of a rhenium carbonyl diimine complex: solvation models, spinâ€“orbit coupling, and vibrational sampling effects. Physical Chemistry Chemical Physics, 2017, 19, 27240-27250.	2.8	40
23	Quantum Chemical Interpretation of Ultrafast Luminescence Decay and Intersystem Crossings in Rhenium(I) Carbonyl Bipyridine Complexes. Journal of Chemical Theory and Computation, 2015, 11, 99-110.	5.3	39
24	The electronic spectroscopy of transition metal carbonyls: The tough case of Cr(CO)6. Chemical Physics Letters, 2006, 421, 378-382.	2.6	38
25	Spinâ€“orbit induced radiationless transitions in organometallics: Quantum simulation of the 1Eâ†'3A1 intersystem crossing process in HCo(CO)4. Journal of Chemical Physics, 1995, 102, 905-912.	3.0	37
26	Photoreactivity of Cr(CO)4(2,2â€˜-Bipyridine): Quantum Chemistry and Photodissociation Dynamics. Journal of Physical Chemistry A, 2001, 105, 1107-1114.	2.5	37
27	Spinâ€“orbit coupled excited states in transition metal complexes: A configuration interaction treatment of HCo(CO)4. Journal of Chemical Physics, 1994, 100, 6591-6596.	3.0	36
28	Spinâ˜'Orbit Coupling Effects on the Metalâ˜'Hydrogen Bond Homolysis of M(H)(CO)3(H-DAB) (M = Mn, Re;) Tj ETQq0 0 0 rgBT /Overloc	2.5	34
29	Luminescent Dinuclear Copper(I) Complexes as Potential Thermally Activated Delayed Fluorescence (TADF) Emitters: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 1413-1421.	2.5	34
30	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	3.0	33
31	Structural and spectroscopic properties of Ir(III) complexes with phenylpyridine ligands: Absorption spectra without and with spinâ€“orbit-coupling. Computational and Theoretical Chemistry, 2014, 1040-1041, 219-229.	2.5	31
32	Description of excited states in [Re(Imidazole)(CO)₃(Phen)]⁺ including solvent and spinâ€•orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. Journal of Computational Chemistry, 2016, 37, 2454-2466.	3.3	30
33	Ultrafast Intersystem Crossing vs Internal Conversion in Î±-Diimine Transition Metal Complexes: Quantum Evidence. Journal of Physical Chemistry Letters, 2018, 9, 5189-5195.	4.6	30
34	Electronic spectroscopy of HRe(CO)5: a CASSCF/CASPT2 and TD-DFT study. Chemical Physics Letters, 2001, 342, 617-624.	2.6	28
35	Inorganic photoisomerization: the case study of rhenium(i) complexes. Dalton Transactions, 2012, 41, 13191.	3.3	28
36	Chemical bonding alteration upon electronic excitation in transition metal complexes. Coordination Chemistry Reviews, 2017, 344, 131-149.	18.8	27

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37	Theoretical analysis of low-lying charge transfer states in [Ru(X) (Me)(CO)2(Me-DAB)] (Xï£¾Cl, I;) Tj ETQq1 1 0.784314 rgBT /Overlo Quantum Chemistry, 2006, 106, 2458-2469.	2.0	25
38	Ultrafast processes: coordination chemistry and quantum theory. Physical Chemistry Chemical Physics, 2021, 23, 43-58.	2.8	24
39	Spinâ€“orbit effects on the electronic spectroscopy of transition metal dihydrides H2M(CO)4 (M=Fe,) Tj ETQq1 1 0.784314 rgBT /Ov	1.9	23
40	Intriguing Effects of Halogen Substitution on the Photophysical Properties of 2,9-(Bis)halo-Substituted Phenanthrolinecopper(I) Complexes. Inorganic Chemistry, 2019, 58, 7730-7745.	4.0	23
41	Spinâ€“orbit absorption spectroscopy of transition metal hydrides: A TDâ€DFT and MSâ€CASPT2 study of HM(CO)₅ (M = Mn, Re). International Journal of Quantum Chemistry, 2012, 112, 2085-2097.	2.0	22
42	Ligand substitution and conformational effects on the ultrafast luminescent decay of [Re(CO)₃(phen)(L)]⁺ (L = imidazole, pyridine): non-adiabatic quantum dynamics. Physical Chemistry Chemical Physics, 2018, 20, 1134-1141.	2.8	22
43	Ab initio study of the electronic singlet excited-state properties of tryptophan in the gas phase: The role of alanyl side-chain conformations. Chemical Physics, 2010, 374, 104-110.	1.9	21
44	Electrochemical Generation and Spectroscopic Characterization of the Key Rhodium(III) Hydride Intermediates of Rhodium Poly(bipyridyl) H₂-Evolving Catalysts. Inorganic Chemistry, 2018, 57, 11225-11239.	4.0	21
45	The Spectroscopy of HMn(CO)5:Â A CASSCF/MRCI and CASPT2 ab Initio Study. Inorganic Chemistry, 1998, 37, 1387-1391.	4.0	20
46	A computational mechanistic investigation of hydrogen production in water using the [RhIII(dmbpy)2Cl2]+/[RuII(bpy)3]2+/ascorbic acid photocatalytic system. Physical Chemistry Chemical Physics, 2015, 17, 10497-10509.	2.8	19
47	Nonâ€Symmetrical Sterically Challenged Phenanthroline Ligands and Their Homoleptic Copper(I) Complexes with Improved Excitedâ€State Properties. Chemistry - A European Journal, 2020, 26, 11887-11899.	3.3	19
48	New luminescent copper(I) complexes with extended Ï€-conjugation. Polyhedron, 2018, 140, 42-50.	2.2	18
49	Absorption Spectroscopy, Emissive Properties, and Ultrafast Intersystem Crossing Processes in Transition Metal Complexes: TD-DFT and Spin-Orbit Coupling. Topics in Current Chemistry, 2015, 368, 377-413.	4.0	17
50	Electronic and Photophysical Properties of [Re (L)(CO)₃(phen)]⁺ and [Ru(L)₂(bpy)₂]²⁺ (L = imidazole), Building Units for Long-Range Electron Transfer in Modified Blue Copper Proteins. Journal of Physical Chemistry A, 2016, 120, 6934-6943.	2.5	17
51	Highly Emissive Red Heterobimetallic Ir^{III}/M^I (M^I = Cu^I) Tj ETQq1 1 0.784314 rgBT Materials, 2022, 34, 1756-1769.	6.7	16
52	Structural and optical properties of new cyclometalated Ru(II) derived compounds. Journal of Organometallic Chemistry, 2014, 760, 248-259.	1.8	15
53	A multi state-CASPT2 vs. TD-DFT study of the electronic excited states of RCo(CO)4 (R=H, CH3) organometallic complexes. Chemical Physics Letters, 2006, 417, 545-549.	2.6	10
54	Structures and spectral properties of heteroleptic copper (I) complexes: A theoretical study based on density functional theory. Comptes Rendus Chimie, 2012, 15, 255-266.	0.5	9

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55	Absorption Spectroscopy and Photophysics of a Re^Iâ€dppz Probe for DNAâ€Mediated Charge Transport. Chemistry - A European Journal, 2018, 24, 14425-14435.	3.3	9
56	Chargeâ€Transfer versus Chargeâ€Separated Triplet Excited States of [Re^I(dmp)(CO)₃(His124)(Trp122)]⁺ in Water and in Modified Pseudomonas aeruginosa Azurin Protein. Chemistry - A European Journal, 2019, 25, 2519-2526.	3.3	8
57	Excited-state dynamics of [Mn(im)(CO)3(phen)]+: PhotoCORM, catalyst, luminescent probe?. Journal of Chemical Physics, 2021, 154, 154102.	3.0	8
58	Excitedâ€State Reactivity of [Mn(im)(CO)₃(phen)]⁺: A Structural Exploration. Journal of Computational Chemistry, 2019, 40, 72-81.	3.3	7
59	Substituent effects on the photophysical properties of 2,9â€substituted phenanthroline copper(I) complexes: a theoretical investigation. ChemPhysChem, 2021, 22, 509-515.	2.1	7
60	Comprehensive investigation of the electronic excitation of W(CO)6 by photoabsorption and theoretical analysis in the energy region from 3.9 to 10.8 eV. Beilstein Journal of Nanotechnology, 2017, 8, 2208-2218.	2.8	5
61	Phosphorescent Cationic Heterodinuclear Ir^{III}/M^I Complexes (M=Cu^I, Au^I) with a Hybrid Janusâ€Type Nâ€Heterocyclic Carbene Bridge. Chemistry - A European Journal, 2020, 26, 11751-11766.	3.3	4
62	Metalâ€“metal bonding in 1st, 2nd and 3rd row transition metal complexes: a topological analysis. Journal of Molecular Modeling, 2017, 23, 163.	1.8	2
63	Density Functional Theories and Coordination Chemistry. , 2020, , .		2
64	Developments in ultrafast spectroscopy. Physical Chemistry Chemical Physics, 2022, , .	2.8	1
65	Spectroscopy and Photophysics Involving Transition Metal Complexes, Theoretical Perspectives. , 2015, , .		0
66	Are luminescent Ru2+ chelated complexes selective coordinative sensors for the detection of heavy cations?. Physical Chemistry Chemical Physics, 2022, 24, 2309-2317.	2.8	0