# 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 | 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 |
| 2 | Highly Emissive Red Heterobimetallic Ir<sup>III</sup>/M<sup>I</sup> (M<sup>I</sup> = Cu<sup>I</sup>) Tj ETQq0 0 0 rgBT /Overlock Materials, 2022, 34, 1756-1769. | 6.7 | 16 |
| 3 | Developments in ultrafast spectroscopy. Physical Chemistry Chemical Physics, 2022, , . | 2.8 | 1 |
| 4 | Ultrafast processes: coordination chemistry and quantum theory. Physical Chemistry Chemical Physics, 2021, 23, 43-58. | 2.8 | 24 |
| 5 | 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 |
| 6 | Excited-state dynamics of [Mn(im)(CO)3(phen)]+: PhotoCORM, catalyst, luminescent probe?. Journal of Chemical Physics, 2021, 154, 154102. | 3.0 | 8 |
| 7 | Density Functional Theories and Coordination Chemistry. , 2020, , . | | 2 |
| 8 | 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 |
| 9 | Phosphorescent Cationic Heterodinuclear Ir<sup>III</sup>/M<sup>I</sup> Complexes (M=Cu<sup>I</sup>, Au<sup>I</sup>) with a Hybrid Janusâ€Type Nâ€Heterocyclic Carbene Bridge. Chemistry - A European Journal, 2020, 26, 11751-11766. | 3.3 | 4 |
| 10 | 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 |
| 11 | Chargeâ€Transfer versus Chargeâ€Separated Triplet Excited States of [Re<sup>I</sup>(dmp)(CO)<sub>3</sub>(His124)(Trp122)]<sup>+</sup> in Water and in Modified Pseudomonas aeruginosa Azurin Protein. Chemistry - A European Journal, 2019, 25, 2519-2526. | 3.3 | 8 |
| 12 | 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 |
| 13 | Excitedâ€State Reactivity of [Mn(im)(CO)<sub>3</sub>(phen)]<sup>+</sup>: A Structural Exploration. Journal of Computational Chemistry, 2019, 40, 72-81. | 3.3 | 7 |
| 14 | Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97. | 18.8 | 109 |
| 15 | 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 |
| 16 | Ligand substitution and conformational effects on the ultrafast luminescent decay of [Re(CO)<sub>3</sub>(phen)(L)]<sup>+</sup> (L = imidazole, pyridine): non-adiabatic quantum dynamics. Physical Chemistry Chemical Physics, 2018, 20, 1134-1141. | 2.8 | 22 |
| 17 | Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119. | 3.0 | 33 |
| 18 | Spin-Vibronic Mechanism for Intersystem Crossing. Chemical Reviews, 2018, 118, 6975-7025. | 47.7 | 592 |

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|---|---|---|---|
| 19 | New luminescent copper(I) complexes with extended Ï€-conjugation. Polyhedron, 2018, 140, 42-50. | 2.2 | 18 |
| 20 | Absorption Spectroscopy and Photophysics of a Re<sup>I</sup>â€dppz Probe for DNAâ€Mediated Charge Transport. Chemistry - A European Journal, 2018, 24, 14425-14435. | 3.3 | 9 |
| 21 | 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 |
| 22 | Electrochemical Generation and Spectroscopic Characterization of the Key Rhodium(III) Hydride Intermediates of Rhodium Poly(bipyridyl) H<sub>2</sub>-Evolving Catalysts. Inorganic Chemistry, 2018, 57, 11225-11239. | 4.0 | 21 |
| 23 | Ultrafast Excited-State Decays in [Re(CO)<sub>3</sub>(N,N)(L)]<sup>n+</sup>: Nonadiabatic Quantum Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 1293-1306. | 5.3 | 45 |
| 24 | 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 |
| 25 | 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 |
| 26 | Chemical bonding alteration upon electronic excitation in transition metal complexes. Coordination Chemistry Reviews, 2017, 344, 131-149. | 18.8 | 27 |
| 27 | 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 |
| 28 | 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 |
| 29 | Electronic and Photophysical Properties of [Re (L)(CO)<sub>3</sub>(phen)]<sup>+</sup> and [Ru(L)<sub>2</sub>(bpy)<sub>2</sub>]<sup>2+</sup> (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 |
| 30 | Description of excited states in [Re(Imidazole)(CO)<sub>3</sub>(Phen)]<sup>+</sup> 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 |
| 31 | 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 |
| 32 | Spin-Vibronic Quantum Dynamics for Ultrafast Excited-State Processes. Accounts of Chemical Research, 2015, 48, 809-817. | 15.6 | 96 |
| 33 | Spectroscopy and Photophysics Involving Transition Metal Complexes, Theoretical Perspectives. , 2015, , . | | 0 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Photochemistry and photophysics of transition metal complexes: Quantum chemistry. Coordination Chemistry Reviews, 2015, 282-283, 19-32. | 18.8 | 118 |
| 38 | Structural and optical properties of new cyclometalated Ru(II) derived compounds. Journal of Organometallic Chemistry, 2014, 760, 248-259. | 1.8 | 15 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | 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 |
| 45 | Inorganic photoisomerization: the case study of rhenium(i) complexes. Dalton Transactions, 2012, 41, 13191. | 3.3 | 28 |
| 46 | 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 |
| 47 | Spinâ€“orbit absorption spectroscopy of transition metal hydrides: A TDâ€ĐFT and MSâ€CASPT2 study of HM(CO)<sub>5</sub> (M = Mn, Re). International Journal of Quantum Chemistry, 2012, 112, 2085-2097. | 2.0 | 22 |
| 48 | 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 |
| 49 | A theoretical study of Ru(II) polypyridyl DNA intercalators. Journal of Inorganic Biochemistry, 2010, 104, 893-901. | 3.5 | 70 |
| 50 | 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 |
| 51 | 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 |
| 52 | A coupled cluster study of the electronic spectroscopy and photochemistry of Cr(CO)6. Physical Chemistry Chemical Physics, 2007, 9, 6115. | 2.8 | 46 |
| 53 | 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 |
| 54 | Theoretical analysis of low-lying charge transfer states in [Ru(X) (Me)(CO)2(Me-DAB)] (Xï£¾Cl, I;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Quantum Chemistry, 2006, 106, 2458-2469. | 2.0 | 25 |

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|---|---|---|---|
| 55 | 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 |
| 56 | The electronic spectroscopy of transition metal carbonyls: The tough case of Cr(CO)6. Chemical Physics Letters, 2006, 421, 378-382. | 2.6 | 38 |
| 57 | 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 |
| 58 | Influence of the Halogen Ligand on the Near-UVâˆ’Visible Spectrum of [Ru(X)(Me)(CO)2(Î±-diimine)] (X = Cl,) Tj ETQq0 0 0 rgBT /Overlo Chemistry, 2004, 43, 7978-7985. | 4.0 | 60 |
| 59 | UVâˆ’Visible Absorption Spectra of [Ru(E)(Eâ€˜)(CO)2(iPr-DAB)] (E = Eâ€˜ = SnPh3or Cl; E = SnPh3or Cl, Eâ€˜ =) Tj ETQq1 1 0.784314 Calculations. Journal of the American Chemical Society, 2001, 123, 11431-11440. | 13.7 | 101 |
| 60 | 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 |
| 61 | Electronic spectroscopy of HRe(CO)5: a CASSCF/CASPT2 and TD-DFT study. Chemical Physics Letters, 2001, 342, 617-624. | 2.6 | 28 |
| 62 | Spinâˆ’Orbit Coupling Effects on the Metalâˆ’Hydrogen Bond Homolysis of M(H)(CO)3(H-DAB) (M = Mn, Re;) Tj ETQq0 0 0 rgBT /Overloc | 2.5 | 34 |
| 63 | The Spectroscopy of HMn(CO)5:Â A CASSCF/MRCI and CASPT2 ab Initio Study. Inorganic Chemistry, 1998, 37, 1387-1391. | 4.0 | 20 |
| 64 | 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 |
| 65 | 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 |
| 66 | 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 |