# Felix Plasser

## List of Publications by Citations



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|---|---|---|---|
| 100 papers | 5,467 citations | 34 h-index | 73 g-index |
| 124 ext. papers | 6,635 ext. citations | 5.7 avg, IF | 6.37 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 100 | Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41 | 3.5 | 1047 |
| 99 | OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964 | 5.4 | 310 |
| 98 | New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. *Journal of Chemical Physics*, **2014**, 141, 024106 | 3.9 | 290 |
| 97 | Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 2777-89 | 6.4 | 284 |
| 96 | Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33 | 7.9 | 280 |
| 95 | Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361 | 68.1 | 181 |
| 94 | New tools for the systematic analysis and visualization of electronic excitations. II. Applications. *Journal of Chemical Physics*, **2014**, 141, 024107 | 3.9 | 172 |
| 93 | The multiradical character of one- and two-dimensional graphene nanoribbons. *Angewandte Chemie - International Edition*, **2013**, 52, 2581-4 | 16.4 | 168 |
| 92 | Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405 | 6.4 | 139 |
| 91 | Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, **2012**, 137, 22A514 | 3.9 | 139 |
| 90 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801 | 3.9 | 115 |
| 89 | Exciton analysis of many-body wave functions: Bridging the gap between the quasiparticle and molecular orbital pictures. *Physical Review A*, **2014**, 90, | 2.6 | 105 |
| 88 | Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. *Journal of Chemical Theory and Computation*, **2016**, 12, 1207-19 | 6.4 | 100 |
| 87 | Benchmarking Excited-State Calculations Using Exciton Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 710-725 | 6.4 | 97 |
| 86 | Excited-state diproton transfer in [2,2'-bipyridyl]-3,3'-diol: the mechanism is sequential, not concerted. *Journal of Physical Chemistry A*, **2009**, 113, 8490-9 | 2.8 | 96 |
| 85 | TheoDORE: A toolbox for a detailed and automated analysis of electronic excited state computations. *Journal of Chemical Physics*, **2020**, 152, 084108 | 3.9 | 95 |
| 84 | Quantitative wave function analysis for excited states of transition metal complexes. *Coordination Chemistry Reviews*, **2018**, 361, 74-97 | 23.2 | 81 |

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| 83 | Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. *Journal of Computational Chemistry*, **2015**, 36, 1609-20 | 3.5 | 78 |
| 82 | Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. *Journal of Physical Chemistry A*, **2016**, 120, 1625-36 | 2.8 | 70 |
| 81 | Electronically excited states and photodynamics: a continuing challenge. *Theoretical Chemistry Accounts*, **2012**, 131, 1 | 1.9 | 69 |
| 80 | Communication: Exciton analysis in time-dependent density functional theory: How functionals shape excited-state characters. *Journal of Chemical Physics*, **2015**, 143, 171101 | 3.9 | 68 |
| 79 | Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. *Chemical Science*, **2017**, 8, 5682-5691 | 9.4 | 61 |
| 78 | UV absorption spectrum of alternating DNA duplexes. Analysis of excitonic and charge transfer interactions. *Journal of Physical Chemistry A*, **2012**, 116, 11151-60 | 2.8 | 61 |
| 77 | The effect of hydrogen bonding on the excited-state proton transfer in 2-(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 9016-25 | 3.6 | 60 |
| 76 | Electronically excited states in poly(p-phenylenevinylene): vertical excitations and torsional potentials from high-level ab initio calculations. *Journal of Physical Chemistry A*, **2013**, 117, 2181-9 | 2.8 | 59 |
| 75 | Highly efficient surface hopping dynamics using a linear vibronic coupling model. *Physical Chemistry Chemical Physics*, **2018**, 21, 57-69 | 3.6 | 55 |
| 74 | A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. *Theoretical Chemistry Accounts*, **2014**, 133, 1 | 1.9 | 51 |
| 73 | Excitons in poly(para phenylene vinylene): a quantum-chemical perspective based on high-level ab initio calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 2548-63 | 3.6 | 47 |
| 72 | Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the ☒ State. *Journal of Physical Chemistry A*, **2015**, 119, 6232-43 | 2.8 | 46 |
| 71 | Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. *Photochemical and Photobiological Sciences*, **2013**, 12, 1440-52 | 4.2 | 43 |
| 70 | Ultrafast Excited-State Decays in [Re(CO)(N,N)(L)]: Nonadiabatic Quantum Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 1293-1306 | 6.4 | 42 |
| 69 | Study of the diradicaloid character in a prototypical pancake-bonded dimer: the stacked tetracyanoethylene (TCNE) anion dimer and the neutral K(2)TCNE(2) complex. *ChemPhysChem*, **2014**, 15, 165-76 | 3.2 | 39 |
| 68 | Toward an understanding of electronic excitation energies beyond the molecular orbital picture. *Physical Chemistry Chemical Physics*, **2020**, 22, 6058-6080 | 3.6 | 37 |
| 67 | Excited-states of a rhenium carbonyl diimine complex: solvation models, spin-orbit coupling, and vibrational sampling effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 27240-27250 | 3.6 | 36 |
| 66 | Universal Exciton Size in Organic Polymers is Determined by Nonlocal Orbital Exchange in Time-Dependent Density Functional Theory. *Journal of Physical Chemistry Letters*, **2017**, 8, 1205-1210 | 6.4 | 34 |

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| 65 | 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 | 6.4 | 34 |
| 64 | Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. *Journal of Chemical Theory and Computation*, **2017**, 13, 5846-5860 | 6.4 | 33 |
| 63 | Entanglement entropy of electronic excitations. *Journal of Chemical Physics*, **2016**, 144, 194107 | 3.9 | 33 |
| 62 | Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. *Journal of Chemical Theory and Computation*, **2017**, 13, 5343-5353 | 6.4 | 32 |
| 61 | Exciton size and binding energy limitations in one-dimensional organic materials. *Journal of Chemical Physics*, **2015**, 143, 244905 | 3.9 | 31 |
| 60 | High-level ab initio computations of the absorption spectra of organic iridium complexes. *Journal of Physical Chemistry A*, **2015**, 119, 1023-36 | 2.8 | 29 |
| 59 | Description of excited states in [Re(Imidazole)(CO)3 (Phen)](+) including solvent and spin-orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. *Journal of Computational Chemistry*, **2016**, 37, 2454-66 | 3.5 | 27 |
| 58 | Semiclassical dynamics simulations of charge transport in stacked □systems. *Journal of Chemical Physics*, **2011**, 134, 034309 | 3.9 | 27 |
| 57 | Ultrafast Intersystem Crossing vs Internal Conversion in □Diimine Transition Metal Complexes: Quantum Evidence. *Journal of Physical Chemistry Letters*, **2018**, 9, 5189-5195 | 6.4 | 24 |
| 56 | Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. *Journal of Chemical Physics*, **2014**, 141, 074105 | 3.9 | 24 |
| 55 | Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. *Journal of Physical Chemistry Letters*, **2017**, 8, 1086-1092 | 6.4 | 23 |
| 54 | Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. *Journal of Chemical Physics*, **2017**, 147, 184109 | 3.9 | 23 |
| 53 | Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. *Scientific Reports*, **2018**, 8, 17273 | 4.9 | 23 |
| 52 | The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110 | 3.9 | 22 |
| 51 | Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. *Journal of Chemical Theory and Computation*, **2018**, 14, 6139-6148 | 6.4 | 22 |
| 50 | Interstate vibronic coupling constants between electronic excited states for complex molecules. *Journal of Chemical Physics*, **2018**, 148, 124119 | 3.9 | 21 |
| 49 | Der Multiradikalcharakter ein- und zweidimensionaler Graphen-Nanob□der. *Angewandte Chemie*, **2013**, 125, 2641-2644 | 3.6 | 21 |
| 48 | The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. *Journal of Chemical Theory and Computation*, **2019**, 15, 3470-3480 | 6.4 | 19 |

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| 47 | Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. *Cellulose*, **2017**, 24, 3671-3687 | 5.5 | 18 |
| 46 | Electronic excitation processes in single-strand and double-strand DNA: a computational approach. *Topics in Current Chemistry*, **2015**, 356, 1-37 | | 17 |
| 45 | Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. *Journal of Chemical Physics*, **2016**, 145, 021103 | 3.9 | 17 |
| 44 | Dynamics of benzene excimer formation from the parallel-displaced dimer. *Physical Chemistry Chemical Physics*, **2019**, 21, 13916-13924 | 3.6 | 16 |
| 43 | Designing Singlet Fission Candidates from Donor/Acceptor Copolymers. *Chemistry of Materials*, **2020**, 32, 6515-6524 | 9.6 | 16 |
| 42 | 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, 6934-43 | 2.8 | 16 |
| 41 | Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. *Journal of Chemical Physics*, **2017**, 146, 064106 | 3.9 | 15 |
| 40 | Synthesis, spectroscopy, and computational analysis of photoluminescent bis(aminophenyl)-substituted thiophene derivatives. *ChemPhysChem*, **2013**, 14, 1016-24 | 3.2 | 15 |
| 39 | Charge-transfer states in triazole linked donor-acceptor materials: strong effects of chemical modification and solvation. *Physical Chemistry Chemical Physics*, **2017**, 19, 18055-18067 | 3.6 | 14 |
| 38 | Challenges in Simulating Light-Induced Processes in DNA. *Molecules*, **2017**, 22, 49 | 4.8 | 13 |
| 37 | Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. *Journal of Physical Chemistry Letters*, **2021**, 12, 2712-2720 | 6.4 | 13 |
| 36 | A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. *Journal of Materials Chemistry C*, **2020**, 8, 7793-7804 | 7.1 | 12 |
| 35 | Color Fine-Tuning of Optical Materials Through Rational Design. *ChemPhysChem*, **2017**, 18, 549-563 | 3.2 | 11 |
| 34 | Visualisation of Electronic Excited-State Correlation in Real Space. *ChemPhotoChem*, **2019**, 3, 702-706 | 3.3 | 11 |
| 33 | Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. *Journal of Chemical Theory and Computation*, **2017**, 13, 2612-2622 | 6.4 | 10 |
| 32 | Effect of symmetric and asymmetric substitution on the optoelectronic properties of 9,10-dicyanoanthracene. *Molecular Systems Design and Engineering*, **2019**, 4, 951-961 | 4.6 | 10 |
| 31 | Red-shifted delayed fluorescence at the expense of photoluminescence quantum efficiency - an intramolecular charge-transfer molecule based on a benzodithiophene-4,8-dione acceptor. *Physical Chemistry Chemical Physics*, **2019**, 21, 10580-10586 | 3.6 | 10 |
| 30 | Optical absorption properties of metal-organic frameworks: solid state molecular perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 19512-19521 | 3.6 | 8 |

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| 29 | Surface Hopping Dynamics on Vibronic Coupling Models. *Accounts of Chemical Research*, **2021**, 54, 3760-3771 | 24.3 | 8 |
| 28 | Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donor-Acceptor Copolymers. *Journal of Physical Chemistry Letters*, **2020**, 11, 9788-9794 | 6.4 | 7 |
| 27 | Visualisation of Chemical Shielding Tensors (VIST) to Elucidate Aromaticity and Antiaromaticity. *European Journal of Organic Chemistry*, **2021**, 2021, 2529-2539 | 3.2 | 7 |
| 26 | Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. *Chemical Science*, **2020**, 11, 7685-7693 | 9.4 | 6 |
| 25 | Multi-Tier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N2 Splitting. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1506-1518 | 2.3 | 6 |
| 24 | Annihilation Dynamics of Molecular Excitons Measured at a Single Perturbative Excitation Energy. *Journal of Physical Chemistry Letters*, **2020**, 11, 7776-7781 | 6.4 | 6 |
| 23 | Exploitation of Baird Aromaticity and Clar's Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. *Chemistry*, **2021**, 3, 532-549 | 2.1 | 6 |
| 22 | Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donor–Acceptor Copolymers. *Chemistry of Materials*, **2021**, 33, 2567-2575 | 9.6 | 5 |
| 21 | Excited-State Reactivity of [Mn(im)(CO) (phen)] : A Structural Exploration. *Journal of Computational Chemistry*, **2019**, 40, 72-81 | 3.5 | 5 |
| 20 | UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. *Molecular Physics*, **2017**, 115, 2469-2477 | 1.7 | 4 |
| 19 | Computational Assessment of MLCT versus MC Stabilities in First-to-Third-Row d Pseudo-Octahedral Transition Metal Complexes. *Journal of Computational Chemistry*, **2019**, 40, 2377-2390 | 3.5 | 4 |
| 18 | OpenMolcas: From Source Code to Insight | | 4 |
| 17 | Excited-state symmetry breaking in 9,10-dicyanoanthracene-based quadrupolar molecules: the effect of donor-acceptor branch length. *Physical Chemistry Chemical Physics*, **2021**, 23, 15150-15158 | 3.6 | 4 |
| 16 | Highly sensitive 26Al measurements by Ion-Laser-InterAction Mass Spectrometry. *International Journal of Mass Spectrometry*, **2021**, 465, 116576 | 1.9 | 4 |
| 15 | Functional group introduction and aromatic unit variation in a set of π-conjugated macrocycles: revealing the central role of local and global aromaticity. *Organic Chemistry Frontiers*, **2021**, 8, 4730-4745 | 5.2 | 4 |
| 14 | A complementary approach to conjugated -acyliminium formation through photoredox-catalyzed intermolecular radical addition to allenamides and allencarbamates. *Beilstein Journal of Organic Chemistry*, **2020**, 16, 1983-1990 | 2.5 | 3 |
| 13 | Pushing the Limits of the Donor-Acceptor Copolymer Strategy for Intramolecular Singlet Fission. *Journal of Physical Chemistry Letters*, **2021**, 12, 7270-7277 | 6.4 | 3 |
| 12 | Solution processed CZTS solar cells using amine–thiol systems: understanding the dissolution process and device fabrication. *Journal of Materials Chemistry C*, **2020**, 8, 10309-10318 | 7.1 | 2 |

# List of Publications

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|---|---|---|---|
| 11 | The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in push-pull chromophores. *Physical Chemistry Chemical Physics*, **2021**, 23, 26135-26150 | 3.6 | 2 |
| 10 | Excited-state dynamics of [Mn(im)(CO)(phen)]: PhotoCORM, catalyst, luminescent probe?. *Journal of Chemical Physics*, **2021**, 154, 154102 | 3.9 | 2 |
| 9 | Multi-Reference Configuration Interaction **2020**, 277-297 | | 1 |
| 8 | Electronically excited states and photodynamics: a continuing challenge **2012**, 147-160 | | 1 |
| 7 | Mechanistic insight into the fluorescence activity of forensic fingerprinting reagents. *Journal of Chemical Physics*, **2021**, 154, 124313 | 3.9 | 1 |
| 6 | [2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). *Open Research Europe*,1, 111 | | 1 |
| 5 | Spin-density calculation via the graphical unitary group approach. *Molecular Physics*, | 1.7 | 1 |
| 4 | Sterically demanding macrocyclic Eu(iii) complexes for selective recognition of phosphate and real-time monitoring of enzymatically generated adenosine monophosphate.. *Chemical Science*, **2022**, 13, 3386-3394 | 9.4 | 0 |
| 3 | Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. *Chemical Science*, **2021**, 12, 13373-13378 | 9.4 | 0 |
| 2 | [2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). *Open Research Europe*,1, 111 | | 0 |
| 1 | Donor–Acceptor–Donor–Hot Exciton–Triads for High Reverse Intersystem Crossing in OLEDs. *Advanced Optical Materials*,2200509 | 8.1 | 0 |