Basile F E Curchod

List of Publications by Year
in descending order

94 papers	7,828 citations	108046 37 h-index	54771 88 g-index
102 all docs	102 docs citations	102 times ranked	10316 citing authors

#	Article	IF	Citations
1	Photo-isomerization of the isolated photoactive yellow protein chromophore: what comes before the primary step?. Physical Chemistry Chemical Physics, 2022, 24, 1305-1309.	1.3	2
2	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
3	A Photochemical Reaction in Different Theoretical Representations. Journal of Physical Chemistry A, 2022, 126, 1263-1281.	1.1	8
4	Photochemistry of the pyruvate anion produces CO2, CO, CH3â€“, CH3, and a low energy electron. Nature Communications, 2022, 13, 937.	5.8	8
5	Extended Conjugation Attenuates the Quenching of Aggregationâ€Induced Emitters by Photocyclization Pathways. Angewandte Chemie - International Edition, 2022, 61, .	7.2	12
6	Chemistry without the Bornâ€“Oppenheimer approximation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200375.	1.6	6
7	Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds. ACS Earth and Space Chemistry, 2022, 6, 207-217.	1.2	14
8	Thermodynamic equilibrium between locally excited and charge-transfer states through thermally activated charge transfer in 1-(pyren-2â€²-yl)-o-carborane. Chemical Science, 2022, 13, 5205-5219.	3.7	20
9	Suppressing dimer formation by increasing conformational freedom in multi-carbazole thermally activated delayed fluorescence emitters. Journal of Materials Chemistry C, 2021, 9, 189-198.	2.7	25
10	Caveat when using ADC(2) for studying the photochemistry of carbonyl-containing molecules. Physical Chemistry Chemical Physics, 2021, 23, 12945-12949.	1.3	15
11	Comparing (stochastic-selection) ab initio multiple spawning with trajectory surface hopping for the photodynamics of cyclopropanone, fulvene, and dithiane. Journal of Chemical Physics, 2021, 154, 104110.	1.2	18
12	Nonadiabatic Kinetics in the Intermediate Coupling Regime: Comparing Molecular Dynamics to an Energy-Grained Master Equation. Journal of Physical Chemistry A, 2021, 125, 3473-3488.	1.1	5
13	Study of the Decoherence Correction Derived from the Exact Factorization Approach for Nonadiabatic Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 3852-3862.	2.3	27
14	AIMSWISSâ€”Ab initio multiple spawning with informed stochastic selections. Journal of Chemical Physics, 2021, 154, 211106.	1.2	9
15	Dynamics near a conical intersectionâ€”A diabolical compromise for the approximations of ab initio multiple spawning. Journal of Chemical Physics, 2021, 155, 174119.	1.2	5
16	Excited-state dynamics of molecules with classically driven trajectories and Gaussians. Molecular Physics, 2020, 118, e1665199.	0.8	11
17	Tracking the ultraviolet-induced photochemistry of thiophenone during and after ultrafast ring opening. Nature Chemistry, 2020, 12, 795-800.	6.6	44
18	Geometric and electronic structure probed along the isomerisation coordinate of a photoactive yellow protein chromophore. Nature Communications, 2020, 11, 2827.	5.8	11

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19	On the Theoretical Determination of Photolysis Properties for Atmospheric Volatile Organic Compounds. Journal of Physical Chemistry Letters, 2020, 11, 5418-5425.	2.1	25
20	Modulation of charge transfer by N-alkylation to control photoluminescence energy and quantum yield. Chemical Science, 2020, 11, 6990-6995.	3.7	9
21	A molecular perspective on Tully models for nonadiabatic dynamics. Physical Chemistry Chemical Physics, 2020, 22, 15183-15196.	1.3	49
22	SSAIMSâ€"Stochastic-Selection Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry A, 2020, 124, 6133-6143.	1.1	13
23	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2020, , 75-121.		3
24	Synthesis of Organic Super-Electron-Donors by Reaction of Nitrous Oxide with N-Heterocyclic Olefins. Journal of the American Chemical Society, 2019, 141, 17112-17116.	6.6	39
25	Cover Image, Volume 8, Issue 5. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1443.	6.2	1
26	Photoelectron Spectroscopy of the Hexafluorobenzene Cluster Anions: (C₆F₆)_n^{â€“} (n = 1â€“5) and I^{â€“}(C₆F₆). Journal of Physical Chemistry A, 2019, 123, 1602-1612.	1.1	25
27	Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses. Journal of Physical Chemistry Letters, 2019, 10, 742-747.	2.1	10
28	Electron-nuclear entanglement in the time-dependent molecular wavefunction. Computational and Theoretical Chemistry, 2019, 1151, 99-106.	1.1	14
29	Different flavors of nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1417.	6.2	65
30	Steering the outcome of a photochemical reactionâ€"An in silico experiment on the H2CSO sulfine using few-femtosecond dump pulses. Journal of Chemical Physics, 2019, 150, 101101.	1.2	3
31	Exploring ultraviolet photoinduced charge-transfer dynamics in a model dinucleotide of guanine and thymine. Physical Chemistry Chemical Physics, 2019, 21, 14407-14417.	1.3	12
32	Azoâ€MICs: Redoxâ€Active Mesoionic Carbene Ligands Derived from Azoimidazolium Dyes. Angewandte Chemie, 2019, 131, 1778-1781.	1.6	8
33	Excited-State Molecular Dynamics Triggered by Light Pulsesâ€"Ab Initio Multiple Spawning vs Trajectory Surface Hopping. Journal of Physical Chemistry A, 2019, 123, 3582-3591.	1.1	27
34	Capturing the interplay between spinâ€"orbit coupling and non-Condon effects on the photoabsorption spectra of Ru and Os dyes. Journal of Materials Chemistry C, 2019, 7, 6564-6570.	2.7	2
35	Azoâ€MICs: Redoxâ€Active Mesoionic Carbene Ligands Derived from Azoimidazolium Dyes. Angewandte Chemie - International Edition, 2019, 58, 1764-1767.	7.2	18
36	Ab Initio Nonadiabatic Quantum Molecular Dynamics. Chemical Reviews, 2018, 118, 3305-3336.	23.0	459

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37	A walk through the approximations of ab initio multiple spawning. Journal of Chemical Physics, 2018, 148, 134110.	1.2	44
38	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		3
39	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		7
40	On the importance of initial conditions for excited-state dynamics. Faraday Discussions, 2018, 212, 307-330.	1.6	38
41	When the exact factorization meets conical intersections.... European Physical Journal B, 2018, 91, 1.	0.6	24
42	CT-MQC â€“ a coupled-trajectory mixed quantum/classical method including nonadiabatic quantum coherence effects. European Physical Journal B, 2018, 91, 1.	0.6	37
43	On the Dynamics through a Conical Intersection. Journal of Physical Chemistry Letters, 2017, 8, 831-837.	2.1	50
44	Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs. Journal of Physical Chemistry A, 2017, 121, 265-276.	1.1	48
45	Pushing the Limits of EOM-CCSD with Projector-Based Embedding for Excitation Energies. Journal of Physical Chemistry Letters, 2017, 8, 5559-5565.	2.1	43
46	Spin Changes Accompany Ultrafast Structural Interconversion in the Ground State of a Cobalt Nitrosyl Complex. Angewandte Chemie - International Edition, 2017, 56, 13713-13716.	7.2	14
47	Ultrafast isomerization in acetylene dication after carbon K-shell ionization. Nature Communications, 2017, 8, 453.	5.8	31
48	Synthesis and Characterization of a Series of Bis-homoleptic Cycloruthenates with Terdentate Ligands as a Family of Panchromatic Dyes. Inorganic Chemistry, 2017, 56, 9903-9912.	1.9	5
49	Criegee Intermediateâ€“Alcohol Reactions, A Potential Source of Functionalized Hydroperoxides in the Atmosphere. ACS Earth and Space Chemistry, 2017, 1, 664-672.	1.2	104
50	Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3909-3917.	1.1	15
51	Spin Changes Accompany Ultrafast Structural Interconversion in the Ground State of a Cobalt Nitrosyl Complex. Angewandte Chemie, 2017, 129, 13901-13904.	1.6	5
52	Communication: GAIMSâ€”Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. Journal of Chemical Physics, 2016, 144, 101102.	1.2	93
53	Communication: XFAIMSâ€”eXternal Field Ab Initio Multiple Spawning for electron-nuclear dynamics triggered by short laser pulses. Journal of Chemical Physics, 2016, 145, 191104.	1.2	31
54	Rich Athermal Groundâ€State Chemistry Triggered by Dynamics through a Conical Intersection. Angewandte Chemie, 2016, 128, 15217-15220.	1.6	12

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55	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. Journal of Chemical Physics, 2016, 145, 034103.	1.2	40
56	Surface functionalization of dinuclear clathrochelates via Pd-catalyzed cross-coupling reactions: facile synthesis of polypyridyl metalloligands. Dalton Transactions, 2016, 45, 8422-8427.	1.6	12
57	Rich Athermal Groundâ€State Chemistry Triggered by Dynamics through a Conical Intersection. Angewandte Chemie - International Edition, 2016, 55, 14993-14996.	7.2	29
58	GPU-Accelerated State-Averaged Complete Active Space Self-Consistent Field Interfaced with Ab Initio Multiple Spawning Unravels the Photodynamics of Provitamin D₃. Journal of Physical Chemistry Letters, 2016, 7, 2444-2449.	2.1	55
59	Synthesis, characterization and ab initio investigation of a panchromatic ullazineâ€“porphyrin photosensitizer for dye-sensitized solar cells. Journal of Materials Chemistry A, 2016, 4, 2332-2339.	5.2	47
60	Tuning the oxidation potential of 2-phenylpyridine-based iridium complexes to improve the performance of bluish and white OLEDs. Journal of Materials Chemistry C, 2016, 4, 3738-3746.	2.7	27
61	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. Physical Chemistry Chemical Physics, 2015, 17, 14719-14730.	1.3	57
62	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€State Proton Transfer of 4â€Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133.	1.0	9
63	Qualitatively Incorrect Features in the TDDFT Spectrum of Thiophene-Based Compounds. Journal of Physical Chemistry Letters, 2015, 6, 13-21.	2.1	62
64	FIrpic: archetypal blue phosphorescent emitter for electroluminescence. Dalton Transactions, 2015, 44, 8318-8329.	1.6	170
65	Nonadiabatic Molecular Dynamics Based on Trajectories. Entropy, 2014, 16, 62-85.	1.1	46
66	Derivation of spin-orbit couplings in collinear linear-response TDDFT: A rigorous formulation. Journal of Chemical Physics, 2014, 140, 144103.	1.2	47
67	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. Nature Chemistry, 2014, 6, 242-247.	6.6	3,982
68	Structureâ€“property relationships based on Hammett constants in cyclometalated iridium(<scp>iii</scp>) complexes: their application to the design of a fluorine-free FIrPic-like emitter. Dalton Transactions, 2014, 43, 5667-5679.	1.6	96
69	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, .	0.8	6
70	Trajectoryâ€Based Nonadiabatic Dynamics with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1314-1340.	1.0	168
71	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739.	3.2	154
72	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648.	3.2	49

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73	Towards Compatibility between Ruthenium Sensitizers and Cobalt Electrolytes in Dyeâ€Sensitized Solar Cells. Angewandte Chemie - International Edition, 2013, 52, 8731-8735.	7.2	61
74	On trajectory-based nonadiabatic dynamics: Bohmian dynamics versus trajectory surface hopping. Journal of Chemical Physics, 2013, 138, 184112.	1.2	62
75	The Charge Transfer Problem in Density Functional Theory Calculations of Aqueously Solvated Molecules. Journal of Physical Chemistry B, 2013, 117, 12189-12201.	1.2	92
76	Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221.	0.3	6
77	Excited State Dynamics with Quantum Trajectories. Chimia, 2012, 66, 174.	0.3	5
78	Acid-Induced Degradation of Phosphorescent Dopants for OLEDs and Its Application to the Synthesis of Tris-heteroleptic Iridium(III) Bis-cyclometalated Complexes. Inorganic Chemistry, 2012, 51, 215-224.	1.9	165
79	Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444.	1.3	25
80	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. Chemistry of Materials, 2012, 24, 2330-2338.	3.2	63
81	Influence of Halogen Atoms on a Homologous Series of Bis-Cyclometalated Iridium(III) Complexes. Inorganic Chemistry, 2012, 51, 799-811.	1.9	107
82	A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. Angewandte Chemie - International Edition, 2012, 51, 8030-8033.	7.2	20
83	Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 3231.	1.3	64
84	The Cause for Tremendous Acceleration of Chloride Substitution via Base Catalysis in the Chloro Pentaammine Cobalt(III) Ion. Inorganic Chemistry, 2011, 50, 8728-8740.	1.9	13
85	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.3	5
86	Nonadiabatic molecular dynamics with solvent effects: A LR-TDDFT QM/MM study of ruthenium (II) tris (bipyridine) in water. Chemical Physics, 2011, 391, 101-109.	0.9	101
87	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.3	22
88	Local control theory in trajectory-based nonadiabatic dynamics. Physical Review A, 2011, 84, .	1.0	22
89	Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409.	1.7	50
90	Nonadiabatic coupling vectors for excited states within time-dependent density functional theory in the Tammâ€“Dancoff approximation and beyond. Journal of Chemical Physics, 2010, 133, 194104.	1.2	105

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91	Mixed quantum-classical dynamics with time-dependent external fields: A time-dependent density-functional-theory approach. Physical Review A, 2010, 81, .	1.0	49
92	On nonadiabatic coupling vectors in time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 196101.	1.2	80
93	Extended Conjugation Attenuates the Quenching of Aggregationâ€Induced Emitters by Photocyclization Pathways. Angewandte Chemie, 0, , .	1.6	0
94	From phosphorescence to delayed fluorescence in one step: tuning photophysical properties by quaternisation of an sp²-hybridised nitrogen atom. Journal of Materials Chemistry C, 0, , .	2.7	1