Sebastian Fernandez-Alberti

List of Publications by Year
in descending order

79	2,942	172207 29	174990 52
papers	citations	h-index	g-index

81	81	81	1959
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	23.0	231
2	Nonadiabatic Excited-State Molecular Dynamics: Modeling Photophysics in Organic Conjugated Materials. Accounts of Chemical Research, 2014, 47, 1155-1164.	7.6	201
3	Identification of unavoided crossings in nonadiabatic photoexcited dynamics involving multiple electronic states in polyatomic conjugated molecules. Journal of Chemical Physics, 2012, 137, 014512.	1.2	175
4	Nonadiabatic Excited-State Molecular Dynamics Modeling of Photoinduced Dynamics in Conjugated Molecules. Journal of Physical Chemistry B, 2011, 115, 5402-5414.	1.2	172
5	Self-Trapping of Excitons, Violation of Condon Approximation, and Efficient Fluorescence in Conjugated Cycloparaphenylenes. Nano Letters, 2014, 14, 6539-6546.	4.5	142
6	Nonadiabatic excited-state molecular dynamics: Treatment of electronic decoherence. Journal of Chemical Physics, 2013, 138, 224111.	1.2	127
7	A b initio quantum direct dynamics simulations of ultrafast photochemistry with Multiconfigurational Ehrenfest approach. Chemical Physics, 2017, 493, 200-218.	0.9	93
8	Evolutionary conservation of protein vibrational dynamics. Gene, 2008, 422, 7-13.	1.0	85
9	Nonadiabatic excited-state molecular dynamics: Numerical tests of convergence and parameters. Journal of Chemical Physics, 2012, 136, 054108.	1.2	84
10	Nonadiabatic Molecular Dynamics Simulations of the Energy Transfer between Building Blocks in a Phenylene Ethynylene Dendrimer. Journal of Physical Chemistry A, 2009, 113, 7535-7542.	1.1	76
11	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. Nature Communications, 2018, 9, 2316.	5.8	71
12	Exploring the Common Dynamics of Homologous Proteins. Application to the Globin Family. Biophysical Journal, 2005, 89, 3-13.	0.2	66
13	Unidirectional Energy Transfer in Conjugated Molecules: The Crucial Role of High-Frequency Câ‰¡C Bonds. Journal of Physical Chemistry Letters, 2010, 1, 2699-2704.	2.1	59
14	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 3020-3031.	2.1	59
15	Non-radiative relaxation of photoexcited chlorophylls: theoretical and experimental study. Scientific Reports, 2015, 5, 13625.	1.6	58
16	Shishiodoshi unidirectional energy transfer mechanism in phenylene ethynylene dendrimers. Journal of Chemical Physics, 2012, 137, 22A526.	1.2	56
17	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	2.3	56
18	Artifacts due to trivial unavoided crossings in the modeling of photoinduced energy transfer dynamics in extended conjugated molecules. Chemical Physics Letters, 2013, 590, 208-213.	1.2	53

#	Article	IF	Citations
19	Non-adiabatic excited state molecular dynamics of phenylene ethynylene dendrimer using a multiconfigurational Ehrenfest approach. Physical Chemistry Chemical Physics, 2016, 18, 10028-10040.	1.3	51
20	Analysis of State-Specific Vibrations Coupled to the Unidirectional Energy Transfer in Conjugated Dendrimers. Journal of Physical Chemistry A, 2012, 116, 9802-9810.	1.1	50
21	Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast Localization of Excitations. Journal of the American Chemical Society, 2015, 137, 11637-11644.	6.6	50
22	Conformational diversity analysis reveals three functional mechanisms in proteins. PLoS Computational Biology, 2017, 13, e1005398.	1.5	46
23	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	2.3	39
24	Instantaneous normal modes, resonances, and decay channels in the vibrational relaxation of the amide I mode of N-methylacetamide-D in liquid deuterated water. Journal of Chemical Physics, 2010, 132, 224501.	1.2	33
25	Conformational disorder in energy transfer: beyond FÃ¶rster theory. Physical Chemistry Chemical Physics, 2013, 15, 9245.	1.3	33
26	Controlling Charge Carrier Trapping and Recombination in BiVO₄ with the Oxygen Vacancy Oxidation State. Journal of Physical Chemistry Letters, 2021, 12, 3514-3521.	2.1	33
27	Interference of Interchromophoric Energy-Transfer Pathways in Ï€-Conjugated Macrocycles. Journal of Physical Chemistry Letters, 2016, 7, 4936-4944.	2.1	32
28	Protein Conformational Diversity Modulates Sequence Divergence. Molecular Biology and Evolution, 2013, 30, 79-87.	3.5	31
29	Internal Conversion and Vibrational Energy Redistribution in Chlorophyll A. Journal of Physical Chemistry B, 2016, 120, 49-58.	1.2	30
30	Photoinduced Intra- and Intermolecular Energy Transfer in ChlorophyllaDimer. Journal of Physical Chemistry B, 2017, 121, 5331-5339.	1.2	30
31	Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution. Physical Chemistry Chemical Physics, 2016, 18, 25080-25089.	1.3	29
32	Carbon nanorings with inserted acenes: breaking symmetry in excited state dynamics. Scientific Reports, 2016, 6, 31253.	1.6	26
33	An ab initio multiple cloning approach for the simulation of photoinduced dynamics in conjugated molecules. Physical Chemistry Chemical Physics, 2018, 20, 17762-17772.	1.3	26
34	Photoinduced dynamics in cycloparaphenylenes: planarization, electronâ€“phonon coupling, localization and intra-ring migration of the electronic excitation. Physical Chemistry Chemical Physics, 2017, 19, 30914-30924.	1.3	24
35	Computational Study of Photoexcited Dynamics in Bichromophoric Cross-Shaped Oligofluorene. Journal of Physical Chemistry A, 2014, 118, 10742-10753.	1.1	23
36	Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes. Journal of Physical Chemistry A, 2014, 118, 10372-10379.	1.1	23

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37	Photoexcited Energy Transfer in a Weakly Coupled Dimer. Journal of Physical Chemistry B, 2015, 119, 7242-7252.	1.2	23
38	Evolutionary Conserved Positions Define Protein Conformational Diversity. PLoS Computational Biology, 2016, 12, e1004775.	1.5	23
39	Intermolecular conical intersections in molecular aggregates. Nature Nanotechnology, 2021, 16, 63-68.	15.6	22
40	Ultrafast Non-FÃ¶rster Intramolecular Donorâ€“Acceptor Excitation Energy Transfer. Journal of Physical Chemistry Letters, 2017, 8, 1688-1694.	2.1	20
41	Nonadiabatic Excited-State Molecular Dynamics Methodologies: Comparison and Convergence. Journal of Physical Chemistry Letters, 2021, 12, 2970-2982.	2.1	20
42	Vibrational dynamics of polyatomic molecules in solution: assignment, time evolution and mixing of instantaneous normal modes. Theoretical Chemistry Accounts, 2011, 128, 769-782.	0.5	19
43	Modeling of internal conversion in photoexcited conjugated molecular donors used in organic photovoltaics. Energy and Environmental Science, 2014, 7, 1175.	15.6	19
44	Unraveling the quantum dynamics origin of high photocatalytic activity in nitrogen-doped anatase TiO₂: time-domain ab initio analysis. Journal of Materials Chemistry A, 2020, 8, 25235-25244.	5.2	19
45	Monitoring molecular vibronic coherences in a bichromophoric molecule by ultrafast X-ray spectroscopy. Chemical Science, 2021, 12, 5286-5294.	3.7	16
46	Energy transfer and spatial scrambling of an exciton in a conjugated dendrimer. Physical Chemistry Chemical Physics, 2018, 20, 29648-29660.	1.3	15
47	Photoinduced non-adiabatic energy transfer pathways in dendrimer building blocks. Journal of Chemical Physics, 2019, 150, 124301.	1.2	15
48	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2021, 17, 3629-3643.	2.3	15
49	Pockets as structural descriptors of EGFR kinase conformations. PLoS ONE, 2017, 12, e0189147.	1.1	15
50	Depleted Oxygen Defect State Enhancing Tungsten Trioxide Photocatalysis: A Quantum Dynamics Perspective. Journal of Physical Chemistry Letters, 2022, 13, 5571-5580.	2.1	15
51	Let Digons be Bygones: The Fate of Excitons in Curved Ï€-Systems. Journal of Physical Chemistry Letters, 2018, 9, 7123-7129.	2.1	14
52	Vibrational energy redistribution during donorâ€“acceptor electronic energy transfer: criteria to identify subsets of active normal modes. Physical Chemistry Chemical Physics, 2020, 22, 18454-18466.	1.3	14
53	Nonadiabatic excited-state molecular dynamics: On-the-fly limiting of essential excited states. Chemical Physics, 2016, 481, 84-90.	0.9	13
54	Phonon bottleneck and long-lived excited states in Ï€-conjugated pyrene hoop. Physical Chemistry Chemical Physics, 2017, 19, 9478-9484.	1.3	12

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55	Modification of Optical Properties and Excited-State Dynamics by Linearizing Cyclic Paraphenylene Chromophores. Journal of Physical Chemistry C, 2018, 122, 16639-16648.	1.5	12
56	Unraveling Direct and Indirect Energy Transfer Pathways in a Light-Harvesting Dendrimer. Journal of Physical Chemistry C, 2020, 124, 22383-22391.	1.5	12
57	Vibronic Quantum Beating between Electronic Excited States in a Heterodimer. Journal of Physical Chemistry B, 2020, 124, 3992-4001.	1.2	12
58	Protein Fluctuations and Cavity Changes Relationship. Journal of Chemical Theory and Computation, 2018, 14, 998-1008.	2.3	10
59	Fatty Acid and Retinol-Binding Protein: Unusual Protein Conformational and Cavity Changes Dictated by Ligand Fluctuations. Journal of Chemical Information and Modeling, 2019, 59, 3545-3555.	2.5	10
60	Evaluating the effect of mutations and ligand binding on transthyretin homotetramer dynamics. PLoS ONE, 2017, 12, e0181019.	1.1	9
61	Network analysis of dynamically important residues in protein structures mediating ligand-binding conformational changes. European Biophysics Journal, 2019, 48, 559-568.	1.2	9
62	Electronic Excited State Specific IR Spectra for Phenylene Ethynylene Dendrimer Building Blocks. Journal of Physical Chemistry C, 2013, 117, 26517-26528.	1.5	8
63	Electronic Energy Relaxation in a Photoexcited Fully Fused Edge-Sharing Carbon Nanobelt. Journal of Physical Chemistry Letters, 2020, 11, 4711-4719.	2.1	8
64	Experimental and theoretical study of energy transfer in a chromophore triad: What makes modeling dynamics successful?. Journal of Chemical Physics, 2020, 153, 244114.	1.2	8
65	Photoexcitation dynamics in perylene diimide dimers. Journal of Chemical Physics, 2020, 153, 244117.	1.2	8
66	Photoinduced Dynamics with Constrained Vibrational Motion: FrozeNM Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7289-7298.	2.3	7
67	Structural and dynamics evidence for scaffold asymmetric flexibility of the human transthyretin tetramer. PLoS ONE, 2017, 12, e0187716.	1.1	7
68	Photoinduced Energy Transfer in Linear Guestâ€“Host Chromophores: A Computational Study. Journal of Physical Chemistry A, 2021, 125, 5303-5313.	1.1	5
69	Ultrafast coherent photoexcited dynamics in a trimeric dendrimer probed by X-ray stimulated-Raman signals. Chemical Science, 2022, 13, 6373-6384.	3.7	5
70	On the analysis and comparison of conformer-specific essential dynamics upon ligand binding to a protein. Journal of Chemical Physics, 2015, 142, 245101.	1.2	4
71	Exploring Conformational Space with Thermal Fluctuations Obtained by Normal-Mode Analysis. Journal of Chemical Information and Modeling, 2020, 60, 3068-3080.	2.5	4
72	Photoexcited energy relaxation and vibronic couplings in Ï€-conjugated carbon nanorings. Physical Chemistry Chemical Physics, 2020, 22, 15321-15332.	1.3	4

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73	Dynamics fingerprints of active conformers of epidermal growth factor receptor kinase. Journal of Computational Chemistry, 2018, 39, 2472-2480.	1.5	3
74	Exciton Spatial Dynamics and Self-Trapping in Carbon Nanocages. Journal of Physical Chemistry Letters, 2021, 12, 224-231.	2.1	3
75	Intrinsically Disordered Region Modulates Ligand Binding in Glutaredoxin 1 from Trypanosoma Brucei. Journal of Physical Chemistry B, 2021, 125, 13366-13375.	1.2	3
76	Excitation Energy Transfer between bodipy Dyes in a Symmetric Molecular Excitonic Seesaw. Journal of Physical Chemistry A, 2021, 125, 8404-8416.	1.1	2
77	Analysis of changes of cavity volumes in predefined directions of protein motions and cavity flexibility. Journal of Computational Chemistry, 2022, 43, 391-401.	1.5	2
78	Back-and-Forth Energy Transfer during Electronic Relaxation in a Chlorinâ€“Perylene Dyad. Journal of Physical Chemistry Letters, 2021, 12, 10394-10401.	2.1	1
79	Vibronic Photoexcitation Dynamics of Perylene Diimide: Computational Insights. Journal of Physical Chemistry A, 2022, 126, 733-741.	1.1	1