Giovanni Granucci

List of Publications by Year
in descending order

92	5,326	136950 32	82547 72
papers	citations	h-index	g-index

96	96	96	3313
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational design of singlet fission biradicaloid chromophores. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 427, 113807.	3.9	4
2	Sampling initial positions and momenta for nuclear trajectories from quantum mechanical distributions. Journal of Chemical Physics, 2021, 154, 074115.	3.0	6
3	Photoisomerization dynamics of spiropyran: A surface-hopping investigation. Journal of Chemical Physics, 2021, 154, 124312.	3.0	3
4	Multiscale Models for Light-Driven Processes. Annual Review of Physical Chemistry, 2021, 72, 489-513.	10.8	29
5	Singlet fission in covalent dimers of methylene-locked 1,3-diphenyl-isobenzofuran: semiclassical simulations of nonadiabatic dynamics. Journal of Materials Chemistry A, 2021, 9, 21897-21909.	10.3	5
6	Surface Hopping Dynamics with the Frenkel Exciton Model in a Semiempirical Framework. Journal of Chemical Theory and Computation, 2021, 17, 7373-7383.	5.3	13
7	Strong Coupling with Light Enhances the Photoisomerization Quantum Yield of Azobenzene. CheM, 2020, 6, 250-265.	11.7	59
8	Surface Hopping Dynamics for Azobenzene Photoisomerization: Effects of Packing Density on Surfaces, Fluorination, and Excitation Wavelength. Journal of Physical Chemistry C, 2020, 124, 26287-26295.	3.1	7
9	Delocalization effects in singlet fission: Comparing models with two and three interacting molecules. Journal of Chemical Physics, 2020, 152, 244125.	3.0	12
10	Photochemistry in the strong coupling regime: A trajectory surface hopping scheme. Journal of Computational Chemistry, 2020, 41, 2033-2044.	3.3	25
11	Unveiling the photophysics of thiourea from CASPT2/CASSCF potential energy surfaces and singlet/triplet excited state molecular dynamics simulations. Computational and Theoretical Chemistry, 2019, 1151, 36-42.	2.5	2
12	Nonadiabatic dynamics simulations of singlet fission in 2,5-bis(fluorene-9-ylidene)-2,5-dihydrothiophene crystals. Physical Chemistry Chemical Physics, 2019, 21, 692-701.	2.8	9
13	Diabatization by Localization in the Framework of Configuration Interaction Based on Floating Occupation Molecular Orbitals (FOMOâˆ’CI). ChemPhotoChem, 2019, 3, 933-944.	3.0	19
14	Excited state dynamics of some nonsteroidal anti-inflammatory drugs: A surface-hopping investigation. Computational and Theoretical Chemistry, 2019, 1152, 20-27.	2.5	13
15	Energy Selection in Nonadiabatic Transitions. Journal of Physical Chemistry A, 2018, 122, 678-689.	2.5	2
16	Azobenzene as a photoregulator covalently attached to RNA: a quantum mechanics/molecular mechanics-surface hopping dynamics study. Chemical Science, 2018, 9, 4671-4681.	7.4	20
17	Manipulating azobenzene photoisomerization through strong lightâ€“molecule coupling. Nature Communications, 2018, 9, 4688.	12.8	111
18	Testing new chromophores for singlet fission: A computational protocol applied to 2,3-diamino-1,4-benzoquinone. Chemical Physics, 2018, 515, 635-642.	1.9	5

#	Article	IF	Citations
19	Electronic Excitation and Decay. Theoretical Chemistry and Computational Modelling, 2018, , 79-118.	0.2	0
20	Introduction to Photochemistry. Theoretical Chemistry and Computational Modelling, 2018, , 1-24.	0.2	0
21	Fast Nonadiabatic Dynamics. Theoretical Chemistry and Computational Modelling, 2018, , 141-177.	0.2	1
22	Charge and Energy Transfer Processes. Theoretical Chemistry and Computational Modelling, 2018, , 179-213.	0.2	0
23	Decoding the Molecular Basis for the Population Mechanism of the Triplet Phototoxic Precursors in UVA Lightâ€Activated Pyrimidine Anticancer Drugs. Chemistry - A European Journal, 2017, 23, 2619-2627.	3.3	49
24	Can in silico calculations assess phototoxicity of non-steroidal anti-inflammatory drugs?. Toxicology Letters, 2017, 280, S282.	0.8	0
25	Photoisomerization of Self-Assembled Monolayers of Azobiphenyls: Simulations Highlight the Role of Packing and Defects. Journal of Physical Chemistry Letters, 2016, 7, 4027-4031.	4.6	34
26	Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects. Journal of Physical Chemistry Letters, 2016, 7, 3591-3596.	4.6	42
27	Surface hopping investigation of benzophenone excited state dynamics. Physical Chemistry Chemical Physics, 2016, 18, 10499-10506.	2.8	28
28	Potential energy surfaces for the HBr+ + CO2 â† Br + HOCO+ reaction in the HBr+â€‰2Î3/2 and 2Î1/2 spin-orbit states. Journal of Chemical Physics, 2015, 142, 104302.	3.0	6
29	Can Azobenzene Photoisomerize When Chemisorbed on a Gold Surface? An Analysis of Steric Effects Based on Nonadiabatic Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 5962-5974.	3.1	21
30	Interplay of radiative and nonradiative transitions in surface hopping with radiation-molecule interactions. Journal of Chemical Physics, 2014, 140, 044113.	3.0	26
31	The photo-orientation of azobenzene in viscous solutions, simulated by a stochastic model. Physical Chemistry Chemical Physics, 2014, 16, 25081-25092.	2.8	8
32	Simulation of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si109.gif" overflow="scroll"><mml:mrow><mml:mi>Ï€</mml:mi><mml:mo>â†'</mml:mo><mml:msup><mml:mrow><mml:mi>Ï€</mml:mi></mml: photodynamics of azobenzene: Decoherence and solvent effects. Computational and Theoretical Chemistry, 2014, 1040-1041, 126-135.	2.5	43
33	Competing ultrafast intersystem crossing and internal conversion: a time resolved picture for the deactivation of 6-thioguanine. Chemical Science, 2014, 5, 1336.	7.4	126
34	An overview of nonadiabatic dynamics simulations methods, with focus on the direct approach versus the fitting of potential energy surfaces. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	158
35	Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33.	14.6	370
36	Dynamics of acetone photodissociation: a surface hopping study. Physical Chemistry Chemical Physics, 2013, 15, 20651.	2.8	32

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37	Theoretical Study of the Chemiluminescence of the Al + H₂O Reaction. Journal of Physical Chemistry A, 2013, 117, 67-74.	2.5	13
38	Surface hopping dynamics of direct trans â†' cis photoswitching of an azobenzene derivative in constrained adsorbate geometries. Journal of Chemical Physics, 2012, 137, 234701.	3.0	18
39	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.	3.0	173
40	Potential energy surface for dissociation including spinâ€“orbit effects. Molecular Physics, 2012, 110, 2599-2609.	1.7	6
41	Surface hopping trajectory simulations with spin-orbit and dynamical couplings. Journal of Chemical Physics, 2012, 137, 22A501.	3.0	122
42	Semiempirical Hamiltonian for Simulation of Azobenzene Photochemistry. Journal of Physical Chemistry A, 2012, 116, 98-110.	2.5	62
43	Stochastic model for photoinduced anisotropy. Journal of Computational Chemistry, 2012, 33, 1015-1022.	3.3	3
44	Photodynamics and Time-Resolved Fluorescence of Azobenzene in Solution: A Mixed Quantum-Classical Simulation. Journal of the American Chemical Society, 2011, 133, 5109-5123.	13.7	140
45	Gradients for configuration interaction energies with spinâ€orbit coupling in a semiempirical framework. Journal of Computational Chemistry, 2011, 32, 2690-2696.	3.3	24
46	Unusual photochemical dynamics of a bridged azobenzene derivative. Journal of Chemical Physics, 2010, 133, 124305.	3.0	52
47	Potential energy surfaces of the first three singlet states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si64.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Chemical Physics Letters, 2010, 500, 202-206.	2.6	10
48	Including quantum decoherence in surface hopping. Journal of Chemical Physics, 2010, 133, 134111.	3.0	309
49	Absorption Oscillator Strengths for Vibronic Transitions of npÏ€ Rydberg Series in NO. Journal of Physical Chemistry A, 2010, 114, 8450-8456.	2.5	9
50	Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics. Journal of Physical Chemistry B, 2010, 114, 12116-12128.	2.6	53
51	Photodynamics of azobenzene in a hindering environment. Chemical Physics, 2008, 347, 492-502.	1.9	31
52	The photoisomerization of a peptidic derivative of azobenzene: A nonadiabatic dynamics simulation of a supramolecular system. Chemical Physics, 2008, 349, 325-333.	1.9	28
53	Oscillator strength and polarization of the forbidden nâ†'Ï€* band of trans-azobenzene: A computational study. Journal of Chemical Physics, 2008, 128, 194312.	3.0	48
54	Critical appraisal of the fewest switches algorithm for surface hopping. Journal of Chemical Physics, 2007, 126, 134114.	3.0	524

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55	The electronic mean field configuration interaction method: II â€“ Improving guess geminals. Chemical Physics Letters, 2007, 450, 151-155.	2.6	8
56	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 228-240.	3.9	422
57	Excited state dynamics with the direct trajectory surface hopping method: azobenzene and its derivatives as a case study. Theoretical Chemistry Accounts, 2007, 117, 1131-1143.	1.4	78
58	The Chromophore of asFP595:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 9348-9353.	2.6	21
59	Semiempirical molecular dynamics investigation of the excited state lifetime of ethylene. Chemical Physics Letters, 2005, 401, 276-281.	2.6	68
60	Photodissociation of formic acid: A trajectory surface hopping study. Chemical Physics Letters, 2005, 412, 35-40.	2.6	20
61	Photodissociation Dynamics of Chlorine Peroxide Adsorbed on Ice. Journal of Physical Chemistry B, 2005, 109, 7941-7947.	2.6	13
62	Are azobenzenophanes rotation-restricted?. Journal of Chemical Physics, 2005, 123, 174317.	3.0	56
63	A computational study of the excited states of bilirubin IX. Physical Chemistry Chemical Physics, 2005, 7, 2594.	2.8	19
64	Alignment of molecules in pulsed resonant laser fields. Journal of Chemical Physics, 2004, 120, 7438-7445.	3.0	21
65	QM/MM connection atoms for the multistate treatment of organic and biological molecules. Theoretical Chemistry Accounts, 2004, 111, 270-279.	1.4	30
66	The Photoisomerization Mechanism of Azobenzene: A Semiclassical Simulation of Nonadiabatic Dynamics. Chemistry - A European Journal, 2004, 10, 2327-2341.	3.3	277
67	A Theoretical Study for the Valenceâ^'Rydberg Interaction in Diatomic Molecules. Application to the NO Î² Band System. Journal of Physical Chemistry A, 2004, 108, 11279-11284.	2.5	10
68	Semiclassical simulation of photochemical reactions in condensed phase. Computational and Theoretical Chemistry, 2003, 621, 119-126.	1.5	37
69	Conical Intersections in Solution:â€‰ A QM/MM Study Using Floating Occupation Semiempirical Configuration Interaction Wave Functions. Journal of Physical Chemistry A, 2003, 107, 3822-3830.	2.5	162
70	Rabi oscillations in the dissociative continuum: Rotation and alignment effects. Journal of Chemical Physics, 2002, 116, 1022-1029.	3.0	14
71	Non-Coulombic states of N24+and O24+ions probed by laser-induced multi-ionization of N2and O2. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, L145-L151.	1.5	6
72	Intermolecular photochemical proton transfer in solution: new insights and perspectives. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 154, 3-11.	3.9	113

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73	Direct semiclassical simulation of photochemical processes with semiempirical wave functions. Journal of Chemical Physics, 2001, 114, 10608-10615.	3.0	386
74	Theoretical study of the photodissociation dynamics of ClOOCl. Physical Chemistry Chemical Physics, 2001, 3, 4266-4279.	2.8	23
75	Theoretical study of the photochemistry of Cl2O. Journal of Chemical Physics, 2001, 115, 1251-1263.	3.0	20
76	Molecular gradients for semiempirical CI wavefunctions with floating occupation molecular orbitals. Chemical Physics Letters, 2000, 325, 79-85.	2.6	116
77	Quantum and semiclassical dynamics of the Franckâ€“Condon wave packet on the coupled potential surfaces of the conical intersection. Chemical Physics, 2000, 259, 193-200.	1.9	11
78	Atomic charges for molecular dynamics calculations. Computational and Theoretical Chemistry, 2000, 507, 17-23.	1.5	9
79	A Theoretical Investigation of Excited-State Acidity of Phenol and Cyanophenols. Journal of the American Chemical Society, 2000, 122, 12243-12253.	13.7	145
80	Derivation of an Optimized Potential Model for Phase Equilibria (OPPE) for Sulfides and Thiols. Journal of Physical Chemistry B, 2000, 104, 4745-4753.	2.6	64
81	A new method for deriving atomic charges and dipoles forn, -alkanes: investigation of transferability and geometry dependence. Molecular Physics, 1999, 97, 1117-1128.	1.7	13
82	Simulations of Condensed Phase Photochemistry:â€‰ Cage Effect and Internal Conversion in Azoalkanes and Nitrosamines. Journal of Physical Chemistry A, 1999, 103, 3364-3371.	2.5	29
83	A chemical application of the algebraic concept of internal space. Journal of Chemical Physics, 1998, 108, 2538-2544.	3.0	3
84	Theoretical study of $m Na(4p^2P)+Na(3s^2S)$ and $m Cd(5p^3P_0)+Na(3s^2S)$ collisions and their role in the energy transfer between Cd * and Na. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 39, 261-265.	1.0	2
85	Nonadiabatic transitions and interference in photodissociation dynamics. Chemical Physics, 1997, 219, 21-30.	1.9	10
86	A surface hopping study of energy transfer in Na + Cdâ^—* collisions. Chemical Physics Letters, 1996, 255, 65-70.	2.6	5
87	Quantum mechanical and semiclassical dynamics at a conical intersection. Journal of Chemical Physics, 1996, 104, 5517-5527.	3.0	94
88	Coherent excitation of wavepackets in two electronic states. Interference effects at an avoided crossing. Chemical Physics Letters, 1995, 246, 228-234.	2.6	13
89	The energetics of fragmentation of the naphthalene cation. Chemical Physics, 1995, 191, 165-175.	1.9	22
90	Benzeneâ€”O2 interaction potential from ab initio calculations. Chemical Physics Letters, 1993, 205, 331-336.	2.6	31

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91	Electronic structure of compounds with Fe-C bonds. Computational and Theoretical Chemistry, 1993, 283, 111-116.	1.5	2
92	Electronic structure, vibrational spectrum and photochemistry of the Fe+H2 system. Chemical Physics, 1992, 167, 121-130.	1.9	15