Giovanni Villani

List of Publications by Year
in descending order

61	896	567144 15	526166 27
papers	citations	h-index	g-index

62	62	62	579
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum mechanical and semiclassical dynamics at a conical intersection. Journal of Chemical Physics, 1996, 104, 5517-5527.	1.2	94
2	Theoretical investigation of hydrogen transfer mechanism in the adenineâ€“thymine base pair. Chemical Physics, 2005, 316, 1-8.	0.9	67
3	Theoretical investigation of hydrogen transfer mechanism in the guanineâ€“cytosine base pair. Chemical Physics, 2006, 324, 438-446.	0.9	65
4	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	64
5	Role of vibronic coupling and correlation effects on the optical properties of mixed-valent and monovalent dimer compounds: the Creutz-Taube ion and its monovalent analogs. The Journal of Physical Chemistry, 1995, 99, 10484-10491.	2.9	58
6	Theoretical Investigation of Hydrogen Atom Transfer in the Cytosine-Guanine Base Pair and Its Coupling with Electronic Rearrangement. Concerted vs Stepwise Mechanism. Journal of Physical Chemistry B, 2010, 114, 9653-9662.	1.2	30
7	Theoretical investigation of hydrogen atom transfer in the adenineâ€“thymine base pair and its coupling with the electronic rearrangement. Concerted vs. stepwise mechanism. Physical Chemistry Chemical Physics, 2010, 12, 2664.	1.3	26
8	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. RSC Advances, 2014, 4, 876-885.	1.7	26
9	Quantum dynamics of a model system with a conical intersection. Journal of Chemical Physics, 1997, 106, 934-941.	1.2	25
10	A Basic Electronic Model for the Study of Optical Properties of Delocalized and Partially Localized Donorâ^'Bridgeâ^'Acceptor Systems. Inorganic Chemistry, 1998, 37, 2799-2805.	1.9	22
11	Theory of Electroabsorption Spectroscopy in Pyrazine-Bridged Ru Dimers. Journal of the American Chemical Society, 1999, 121, 2594-2596.	6.6	20
12	Electron Transfer between Quinones in Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 2004, 108, 3068-3077.	1.2	20
13	Third-Harmonic Generation in Mixed-Valent Ruâ^'Pyrazine Chains:Â A Theoretical Study. Journal of Physical Chemistry A, 1997, 101, 9439-9444.	1.1	17
14	Theoretical investigation of the hydrogen atom transfer in the hydrated Aâ€“T base pair. Chemical Physics, 2012, 394, 9-16.	0.9	17
15	A time-dependent quantum dynamics investigation of the guanine-cytosine system: A six-dimensional model. Journal of Chemical Physics, 2008, 128, 114306.	1.2	16
16	Chemisorption of Ag on the Si(111) surface: a theoretical study. Surface Science, 1991, 244, 355-361.	0.8	15
17	Theoretical investigation of the coupling between the hydrogen transfer and the base pair opening in the adenineâ€“thymine system. Chemical Physics, 2007, 336, 143-149.	0.9	15
18	Theoretical Investigation of the Coupling between Hydrogenâ€Atom Transfer and Stacking Interaction in Adenineâ€“Thymine Dimers. ChemPhysChem, 2013, 14, 1256-1263.	1.0	15

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19	Control of the yield of photophysical/photochemical processes by excitation with properly delayed ultrashort phase-locked light pulses: a model study on the pyrazine S2 â†' S 1 internal conversion. Chemical Physics, 1995, 196, 447-454.	0.9	14
20	Optical dynamics in monodimensional aggregates with excitonâ€"phonon coupling: a numerical investigation on the time-evolution of the optical doorway state. Chemical Physics, 1993, 172, 285-294.	0.9	13
21	Transition probability due to a conical intersection: On the role of the initial conditions and of the geometric setup of the crossing surfaces. Journal of Chemical Physics, 1999, 111, 916-922.	1.2	13
22	Comment on the Calculation of Absorption Line Shapes for Mixed-Valence Dimers. The Journal of Physical Chemistry, 1994, 98, 11230-11232.	2.9	12
23	Theory of the Stark Effect spectral lineshape for a delocalized mixed-valence complex. Inorganic Chemistry Communication, 1998, 1, 137-140.	1.8	12
24	Properties of the Thiobase Pairs Hydrogen Bridges: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 2128-2134.	1.2	12
25	Crown Ether Encapsulation Effects on the Optical Properties of Delocalized and Partially Localized Bridged Ruthenium Dimers. Inorganic Chemistry, 1998, 37, 4460-4465.	1.9	11
26	Quantum dynamics at a conical intersection: The role of the variation of oscillator frequencies in the diabatic transition. Journal of Chemical Physics, 1998, 109, 9002-9009.	1.2	11
27	Theoretical investigation of the coupling between hydrogen atoms transfer and stacking interaction in guanineâ€"cytosine dimers. Physical Chemistry Chemical Physics, 2013, 15, 19242.	1.3	11
28	Theoretical investigation of hydrogen atom transfer in the hydrated Câ€"G base pair. Molecular Physics, 2013, 111, 201-214.	0.8	11
29	Quantum dynamics of proton transfer in the H3O+î—¸H2O complex. Chemical Physics Letters, 1995, 238, 137-142.	1.2	10
30	Dynamics around a multidimensional conical intersection: A mixed quantum-classical model. Journal of Chemical Physics, 1997, 107, 3498-3504.	1.2	10
31	Coupling Between Hydrogen Atoms Transfer and Stacking Interaction in Adenine-Thymine/Guanine-Cytosine Complexes: A Theoretical Study. Journal of Physical Chemistry B, 2014, 118, 5439-5452.	1.2	10
32	Structured system in chemistry: comparison with mechanics and biology. Foundations of Chemistry, 2014, 16, 107-123.	0.4	10
33	A model study of the wavepacket dynamics around a Jahnâ€"Teller conical intersection in a symmetric charge-transfer system. Chemical Physics, 2000, 259, 201-210.	0.9	9
34	Quantum dynamics of proton-coupled electron transfer in model systems. Chemical Physics, 2004, 302, 309-322.	0.9	9
35	Theoretical investigation of DNA oligomer systems. Modification of the hydrogen atoms transfer in a base pair due to time-dependent interaction with stacked base pairs. Chemical Physics, 2006, 325, 389-396.	0.9	9
36	Control of the yield of competing unimolecular reactions through double-resonance coherent trapping. The Journal of Physical Chemistry, 1988, 92, 4348-4351.	2.9	8

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37	Proton and Electron Transfer Mechanisms in the Formation of Neutral and Charged Quinhydrone-Like Complexes: A Multilayered Computational Study. Journal of Chemical Theory and Computation, 2014, 10, 4883-4895.	2.3	8
38	Excitation and decay of a Câ€“H overtone attached to a linear hydrocarbon chain: A simple quantumâ€mechanical model. Journal of Chemical Physics, 1988, 88, 5186-5195.	1.2	7
39	Vibrational energy migration along hydrocarbon chains: a model study. The Journal of Physical Chemistry, 1990, 94, 6959-6962.	2.9	7
40	Vibronic Model Hamiltonian for the Study of the Near-IRâˆ'Visible Optical Properties of [(NH3)5Ruâˆ'(4,4â€˜-bipyridine)âˆ'Ru(NH3)5]m+ (m = 4, 5):â€‰ Charge Localization and Electroabsorption Spectra. Journal of Physical Chemistry A, 2000, 104, 9591-9599.	1.1	7
41	Electron transfer in the Dâ€“Bâ€“A model system: A vibronic analysis. Journal of Chemical Physics, 2002, 117, 1279-1289.	1.2	7
42	Quantum mechanical investigation of G-quartet systems of DNA. New Journal of Chemistry, 2017, 41, 2574-2585.	1.4	7
43	Decay of local stretching overtones for terminal groups attached to a hydrocarbon chain: A theoretical investigation based on a Morseâ€harmonic model. Journal of Chemical Physics, 1989, 90, 3559-3565.	1.2	6
44	Quantum Mechanical Investigation of the G-Quadruplex Systems of Human Telomere. ACS Omega, 2018, 3, 9934-9944.	1.6	6
45	Interference effects in molecular system with curve crossing. Chemical Physics Letters, 1998, 290, 131-135.	1.2	4
46	Non-stationary states in chemistry. Theoretical Chemistry Accounts, 2007, 117, 755-764.	0.5	4
47	Effect of Methylation on the Properties of the H-Bridges in DNA. A Systematic Theoretical Study on the Couples of Base Pairs. Journal of Physical Chemistry B, 2015, 119, 7931-7943.	1.2	4
48	Tunneling in the presence of fluctuations: the stochastic liouville equation approach. Chemical Physics, 1987, 115, 391-397.	0.9	3
49	Structure, shape, topology: entangled concepts in molecular chemistry. Foundations of Chemistry, 2020, 22, 279-307.	0.4	3
50	Time-dependent observables and diabatic curve crossing: a model study. Computational and Theoretical Chemistry, 1995, 330, 107-111.	1.5	2
51	Chemical perspective in the study of living beings: a systemic complexity approach. Foundations of Chemistry, 2017, 19, 77-91.	0.4	2
52	Proton tunnelling in a strong electromagnetic field at low frequency: a simple model for the weak-temperature limit. Lettere Al Nuovo Cimento Rivista Internazionale Della SocietÃ Italiana Di Fisica, 1985, 43, 65-68.	0.4	1
53	Hydrogen tunneling from a high-energy Cî—¸H overtone: A study of the dependence of the yield on the excitation frequency. Spectrochimica Acta Part A: Molecular Spectroscopy, 1990, 46, 653-655.	0.1	1
54	On the Photophysics of Molecules with Charge-Transfer Excitations between aromatic rings. Advances in Quantum Chemistry, 2000, 36, 283-300.	0.4	1

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55	Absorption and electroabsorption spectra of [(NH3)5Ruâ€“pyrazine]2+ and [(NH3)5Ruâ€“pyrazineâ€“H]3+ by a vibronic model Hamiltonian. Physical Chemistry Chemical Physics, 2001, 3, 2576-2580.	1.3	1
56	The orbital: a pivotal concept in the relationship between chemistry and physics? A comment to the work by Fortin and coauthors. Foundations of Chemistry, 2018, 20, 89-97.	0.4	1
57	A Time-Dependent Quantum Approach to Allostery and a Comparison With Light-Harvesting in Photosynthetic Phenomenon. Frontiers in Molecular Biosciences, 2020, 7, 156.	1.6	1
58	l'approccio sistemico della chimica al concetto di vita. Epistemologia, 2014, , 22-36.	0.1	1
59	A numerical investigation on the effects of bond hole pairs-phonon coupling in copper-oxygen high Tc superconductors. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1651-1652.	0.6	0
60	Two-Electron Transfer Through A Linear Chain. Molecular Crystals and Liquid Crystals, 1993, 234, 109-114.	0.3	0
61	Affinity and Correlation in DNA. J, 2022, 5, 214-231.	0.6	0