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	Affinity and Correlation in DNA. J, 2022, 5, 214-231.	0.6	0
2	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
3	Structure, shape, topology: entangled concepts in molecular chemistry. Foundations of Chemistry, 2020, 22, 279-307.	0.4	3
4	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
5	Quantum Mechanical Investigation of the G-Quadruplex Systems of Human Telomere. ACS Omega, 2018, 3, 9934-9944.	1.6	6
6	Chemical perspective in the study of living beings: a systemic complexity approach. Foundations of Chemistry, 2017, 19, 77-91.	0.4	2
7	Quantum mechanical investigation of G-quartet systems of DNA. New Journal of Chemistry, 2017, 41, 2574-2585.	1.4	7
8	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
9	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. RSC Advances, 2014, 4, 876-885.	1.7	26
10	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
11	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
12	Structured system in chemistry: comparison with mechanics and biology. Foundations of Chemistry, 2014, 16, 107-123.	0.4	10
13	l'approccio sistemico della chimica al concetto di vita. Epistemologia, 2014, , 22-36.	0.1	1
14	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
15	Theoretical investigation of hydrogen atom transfer in the hydrated Câ€“G base pair. Molecular Physics, 2013, 111, 201-214.	0.8	11
16	Theoretical Investigation of the Coupling between Hydrogenâ€Atom Transfer and Stacking Interaction in Adenineâ€“Thymine Dimers. ChemPhysChem, 2013, 14, 1256-1263.	1.0	15
17	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
18	Theoretical investigation of the hydrogen atom transfer in the hydrated Aâ€“T base pair. Chemical Physics, 2012, 394, 9-16.	0.9	17

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19	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
20	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
21	Properties of the Thiobase Pairs Hydrogen Bridges: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 2128-2134.	1.2	12
22	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
23	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
24	Non-stationary states in chemistry. Theoretical Chemistry Accounts, 2007, 117, 755-764.	0.5	4
25	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
26	Theoretical investigation of hydrogen transfer mechanism in the guanineâ€“cytosine base pair. Chemical Physics, 2006, 324, 438-446.	0.9	65
27	Theoretical investigation of hydrogen transfer mechanism in the adenineâ€“thymine base pair. Chemical Physics, 2005, 316, 1-8.	0.9	67
28	Quantum dynamics of proton-coupled electron transfer in model systems. Chemical Physics, 2004, 302, 309-322.	0.9	9
29	Electron Transfer between Quinones in Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 2004, 108, 3068-3077.	1.2	20
30	Electron transfer in the Dâ€“Bâ€“A model system: A vibronic analysis. Journal of Chemical Physics, 2002, 117, 1279-1289.	1.2	7
31	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
32	On the Photophysics of Molecules with Charge-Transfer Excitations between aromatic rings. Advances in Quantum Chemistry, 2000, 36, 283-300.	0.4	1
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	Vibronic Model Hamiltonian for the Study of the Near-IRâˆ’Visible Optical Properties of [(NH3)5Ruâˆ’(4,4â€²-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
35	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
36	Theory of Electroabsorption Spectroscopy in Pyrazine-Bridged Ru Dimers. Journal of the American Chemical Society, 1999, 121, 2594-2596.	6.6	20

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37	Interference effects in molecular system with curve crossing. Chemical Physics Letters, 1998, 290, 131-135.	1.2	4
38	Theory of the Stark Effect spectral lineshape for a delocalized mixed-valence complex. Inorganic Chemistry Communication, 1998, 1, 137-140.	1.8	12
39	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
40	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
41	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
42	Quantum dynamics of a model system with a conical intersection. Journal of Chemical Physics, 1997, 106, 934-941.	1.2	25
43	Dynamics around a multidimensional conical intersection: A mixed quantum-classical model. Journal of Chemical Physics, 1997, 107, 3498-3504.	1.2	10
44	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
45	Quantum mechanical and semiclassical dynamics at a conical intersection. Journal of Chemical Physics, 1996, 104, 5517-5527.	1.2	94
46	Quantum dynamics of proton transfer in the H3O+î—¸H2O complex. Chemical Physics Letters, 1995, 238, 137-142.	1.2	10
47	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
48	Time-dependent observables and diabatic curve crossing: a model study. Computational and Theoretical Chemistry, 1995, 330, 107-111.	1.5	2
49	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
50	Comment on the Calculation of Absorption Line Shapes for Mixed-Valence Dimers. The Journal of Physical Chemistry, 1994, 98, 11230-11232.	2.9	12
51	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
52	Two-Electron Transfer Through A Linear Chain. Molecular Crystals and Liquid Crystals, 1993, 234, 109-114.	0.3	0
53	Chemisorption of Ag on the Si(111) surface: a theoretical study. Surface Science, 1991, 244, 355-361.	0.8	15
54	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

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55	Vibrational energy migration along hydrocarbon chains: a model study. The Journal of Physical Chemistry, 1990, 94, 6959-6962.	2.9	7
56	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
57	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
58	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
59	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
60	Tunneling in the presence of fluctuations: the stochastic liouville equation approach. Chemical Physics, 1987, 115, 391-397.	0.9	3
61	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