Gianni Cardini

List of Publications by Year in Descending Order

132 papers	2,993 citations	31 h-index	48 g-index
136 ext. papers	3,138 ext. citations	3.4 avg, IF	4.75 L-index

#	Paper	IF	Citations
132	Exploring the effect of Mg substitution on amorphous calcium phosphate nanoparticles. *Journal of Colloid and Interface Science*, **2022**, 606, 444-453	9.3	5
131	"Cyclopropylidene Effect" in the 1,3-Dipolar Cycloaddition of Nitrones to Alkylidene Cyclopropanes: A Computational Rationalization. *Journal of Physical Chemistry A*, **2021**, 125, 3892-3899	2.8	2
130	Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride. *Journal of Physical Chemistry A*, **2021**, 125, 6362-6373	2.8	1
129	Regioselective Deuteration of a 3,4-Dialkoxypyrroline N-Oxide and Synthesis of 8a-d-Indolizidines. *European Journal of Organic Chemistry*, **2020**, 2020, 3423-3429	3.2	
128	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. *Journal of Physical Chemistry B*, **2019**, 123, 4055-4064	3.4	8
127	Computational Investigation of the Selective Cleavage of Diastereotopic Cyclopropane Bonds in 5-Spirocyclopropane Isoxazolidines Rearrangement. *Journal of Organic Chemistry*, **2019**, 84, 6757-6764	4.2	4
126	Evidence of a Low-High Density Turning Point in Liquid Water at Ordinary Temperature under Pressure: A Molecular Dynamics Study. *Journal of Physical Chemistry Letters*, **2019**, 10, 6414-6418	6.4	6
125	DFT calculations of the IR and Raman spectra of anthraquinone dyes and lakes. *Journal of Raman Spectroscopy*, **2018**, 49, 668-683	2.3	12
124	Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states. *Journal of Chemical Physics*, **2018**, 149, 084101	3.9	
123	New atomistic model of pyrrole with improved liquid state properties and structure. *International Journal of Quantum Chemistry*, **2018**, 118, e25554	2.1	8
122	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. *Journal of Physical Chemistry A*, **2017**, 121, 8825-8834	2.8	9
121	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. *Journal of Chemical Theory and Computation*, **2017**, 13, 5874-5886	6.4	9
120	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. *Journal of Chemical Theory and Computation*, **2017**, 13, 5887-5899	6.4	8
119	Elastic Barrier Dynamical Freezing in Free Energy Calculations: A Way To Speed Up Nonequilibrium Molecular Dynamics Simulations by Orders of Magnitude. *Journal of Chemical Theory and Computation*, **2016**, 12, 1029-39	6.4	3
118	XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P4S3. *Journal of Physical Chemistry A*, **2016**, 120, 5136-44	2.8	9
117	Nonequilibrium work theorems applied to transitions between configurational domains. *Journal of Statistical Mechanics: Theory and Experiment*, **2016**, 2016, 123204	1.9	3
116	Computing Free Energy Differences of Configurational Basins. *Journal of Chemical Theory and Computation*, **2015**, 11, 3561-71	6.4	5

115	Annealed importance sampling with constant cooling rate. *Journal of Chemical Physics*, **2015**, 142, 074102	3.9	1
114	Simulations in generalized ensembles through noninstantaneous switches. *Physical Review E*, **2015**, 92, 043310	2.4	1
113	Identification of Di(oxymethylene)glycol in the Raman Spectrum of Formaldehyde Aqueous Solutions by ab Initio Molecular Dynamics Simulations and Quantum Chemistry Calculations. *Journal of Physical Chemistry A*, **2015**, 119, 9785-93	2.8	3
112	Structural and spectroscopic properties of methanediol in aqueous solutions from quantum chemistry calculations and ab initio molecular dynamics simulations. *Journal of Physical Chemistry A*, **2015**, 119, 290-8	2.8	9
111	Vibrational frequencies of fullerenes C60 and C70 under pressure studied with a quantum chemical model including spatial confinement effects. *Journal of Physical Chemistry A*, **2014**, 118, 5098-111	2.8	35
110	Nonequilibrium Candidate Monte Carlo Simulations with Configurational Freezing Schemes. *Journal of Chemical Theory and Computation*, **2014**, 10, 4273-83	6.4	9
109	Comment on "Fermi resonance in solid CO2 under pressure" [J. Chem. Phys. 138, 074501 (2013)]. *Journal of Chemical Physics*, **2014**, 140, 177101	3.9	5
108	Combining path-breaking with bidirectional nonequilibrium simulations to improve efficiency in free energy calculations. *Journal of Chemical Physics*, **2014**, 140, 064104	3.9	14
107	Path-breaking schemes for nonequilibrium free energy calculations. *Journal of Chemical Physics*, **2013**, 138, 214109	3.9	24
106	Hydrogen bond effects in the vibrational spectra of 1,3-propanediol in acetonitrile: ab initio and experimental study. *Journal of Chemical Physics*, **2012**, 137, 244501	3.9	8
105	Bifurcated hydrogen bond in lithium nitrate trihydrate probed by ab initio molecular dynamics. *Journal of Physical Chemistry A*, **2012**, 116, 2147-53	2.8	11
104	Raman and infrared spectra of minerals from ab initio molecular dynamics simulations: The spodumene crystal. *Journal of Molecular Structure*, **2011**, 993, 151-154	3.4	7
103	Wavelet Transform for Spectroscopic Analysis: Application to Diols in Water. *Journal of Chemical Theory and Computation*, **2011**, 7, 1109-18	6.4	20
102	Structural and vibrational properties of arsenic sulfides: alacranite (As8S9). *Journal of Physical Chemistry A*, **2011**, 115, 4558-62	2.8	14
101	Spectroscopic properties with a combined approach of ab initio molecular dynamics and wavelet analysis. *Journal of Molecular Structure*, **2011**, 993, 438-442	3.4	16
100	Hydrogen Bond Dynamics of Methyl Acetate in Methanol. *Journal of Physical Chemistry Letters*, **2010**, 1, 2951-2955	6.4	33
99	Nitromethane decomposition under high static pressure. *Journal of Physical Chemistry B*, **2010**, 114, 9420-8	3.4	51
98	Spectroscopy and monitoring of high pressure phenomena. *Journal of Molecular Structure*, **2009**, 924-926, 2-8	3.4	3

97	Solvation dynamics and adsorption on Ag hydrosols of oxazole: a Raman and computational study. *Journal of Physical Chemistry A*, **2009**, 113, 15198-205	2.8	13
96	Ab Initio Molecular Dynamics Study of Mg(2+) and Ca(2+) Ions in Liquid Methanol. *Journal of Chemical Theory and Computation*, **2008**, 4, 156-63	6.4	15
95	Role of Surface Metal Clusters in SERS Spectra of Ligands Adsorbed on Ag Colloidal Nanoparticles. *Journal of Physical Chemistry C*, **2008**, 112, 762-767	3.8	23
94	Mechanism of the Ethylene Polymerization at Very High Pressure. *Journal of Chemical Theory and Computation*, **2008**, 4, 646-51	6.4	17
93	Anharmonic infrared and Raman spectra in Car-Parrinello molecular dynamics simulations. *Journal of Chemical Physics*, **2008**, 128, 224514	3.9	37
92	DFT investigation on the SERS band at ~1025 cm^{-1} of pyridine adsorbed on silver. *Chemical Physics Letters*, **2007**, 436, 179-183	2.5	20
91	A density functional study of the SERS spectra of pyridine adsorbed on silver clusters. *Theoretical Chemistry Accounts*, **2007**, 117, 451-458	1.9	40
90	Problems in molecular dynamics of condensed phases. *Theoretical Chemistry Accounts*, **2007**, 117, 1105-1120	1.9	5
89	Free volume from molecular dynamics simulations and its relationships to the positron annihilation lifetime spectroscopy. *Theoretical Chemistry Accounts*, **2007**, 118, 443-448	1.9	6
88	The solvation dynamics of Na+ and K+ ions in liquid methanol. *Theoretical Chemistry Accounts*, **2007**, 118, 417-423	1.9	19
87	Ab initio molecular dynamics study of aqueous formaldehyde and methanediol. *Molecular Physics*, **2007**, 105, 2203-2210	1.7	34
86	Ab initio molecular dynamics study of the hydrolysis reaction of diborane. *Physical Chemistry Chemical Physics*, **2007**, 9, 3857-63	3.6	7
85	Lithium hydroxide phase transition under high pressure: an ab initio molecular dynamics study. *ChemPhysChem*, **2006**, 7, 141-7	3.2	18
84	A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols. *Physical Chemistry Chemical Physics*, **2006**, 8, 171-8	3.6	35
83	Solid-state phase transition induced by pressure in LiOH x H2O. *Journal of Physical Chemistry B*, **2006**, 110, 13539-46	3.4	10
82	Structure and dynamics of Br- ion in liquid methanol. *Journal of Physical Chemistry B*, **2006**, 110, 14923-8	3.4	22
81	Solvation dynamics of Li+ and Cl- ions in liquid methanol. *Journal of Physical Chemistry B*, **2005**, 109, 7475-81	3.4	29
80	Insights into positron annihilation lifetime spectroscopy by molecular dynamics simulations. *European Physical Journal D*, **2005**, 32, 289-297	1.3	14

79	Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: implications for charge transfer. *Journal of Chemical Physics*, **2005**, 122, 074504	3.9	36
78	Charge separation and polymerization of hydrocarbons at an ultrahigh pressure. *Physical Review B*, **2004**, 70,	3.3	23
77	High pressure reactivity of propene by first principles molecular dynamics calculations. *Journal of Chemical Physics*, **2004**, 120, 5327-33	3.9	20
76	Ab initiomolecular dynamics study of the potential energy surface for the CH 3Cl+F□reaction. *Rendiconti Lincei*, **2004**, 15, 99-113	1.7	1
75	Surface-enhanced Raman spectra of pyridine and pyrazolide on silver colloids: chemical and electromagnetic effects. *Theoretical Chemistry Accounts*, **2004**, 111, 264-269	1.9	44
74	SERS and DFT Study on 4-Methylpyridine Adsorbed on Silver Colloids and Electrodes. *Journal of Physical Chemistry B*, **2004**, 108, 17007-17011	3.4	57
73	The Absorption Spectrum of Anisole and the Anisole/CO2 1:1-Cluster. The Influence of Intermolecular Interaction on Intramolecular Vibrations. *Zeitschrift Fur Physikalische Chemie*, **2004**, 218, 123-154	3.1	12
72	Substitution and Elimination Reaction of F- with C2H5Cl: An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2003**, 107, 2540-2547	2.8	25
71	Car□Parrinello molecular dynamics on the SN2 reaction Cl□CH3Br in water. *Computational and Theoretical Chemistry*, **2003**, 630, 141-149		23
70	Hydrogen bond dynamics in liquid methanol. *Journal of Chemical Physics*, **2003**, 119, 6655-6662	3.9	163
69	An ab initio molecular dynamics study of the SN2 reaction F□CH3Cl-□H3F+Cl□*Journal of Chemical Physics*, **2003**, 118, 2767	3.9	9
68	Intramolecular solvation effects in the SN2 reaction Cl□Cl(CH2)nCN. *Journal of Chemical Physics*, **2003**, 119, 9063-9072	3.9	6
67	Dynamical and structural correlation in supercooled liquids: A molecular dynamics investigation of m-toluidine. *Journal of Chemical Physics*, **2003**, 119, 357-363	3.9	11
66	Thermal effects on the Cl□ClCH2CN reaction by Car-Parrinello molecular dynamics. *Journal of Chemical Physics*, **2002**, 117, 2199-2204	3.9	6
65	Density Functional Study on the Adsorption of Pyrazole onto Silver Colloidal Particles. *Journal of Physical Chemistry B*, **2002**, 106, 6875-6880	3.4	77
64	The Infrared and Raman Spectra of Fullerene C70. DFT Calculations and Correlation with C60. *Journal of Physical Chemistry A*, **2002**, 106, 1815-1823	2.8	80
63	Molecular dynamics of glass-forming liquids: Structure and dynamics of liquid metatoluidine. *Journal of Chemical Physics*, **2002**, 116, 6205-6215	3.9	17
62	Microsolvation effect on chemical reactivity: The case of the Cl□CH3Br SN2 reaction. *Journal of Chemical Physics*, **2001**, 114, 4089-4098	3.9	40

61	The fast dynamics of benzene in the liquid phase. Part II. A molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2001**, 3, 2803-2810	3.6	48
60	The fast dynamics of benzene in the liquid phase. Part I. Optical Kerr effect experimental investigation. *Physical Chemistry Chemical Physics*, **2001**, 3, 2795-2802	3.6	56
59	The Vibrational Spectrum of Fullerene C60. *Journal of Physical Chemistry A*, **2001**, 105, 11192-11196	2.8	114
58	CarParrinello molecular dynamics of the SN2 reaction Cl + Cl2CH2. *Physical Chemistry Chemical Physics*, **2001**, 3, 4870-4873	3.6	13
57	Ab-initio molecular dynamics study of theSN2 reaction Cl ClCH2CN. *Physical Chemistry Chemical Physics*, **2001**, 3, 2559-2566	3.6	20
56	Excited state photoelectron spectroscopy of anisole. *Physical Chemistry Chemical Physics*, **2001**, 3, 5358-5368	3.6	27
55	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the TryptophanHistidine Pair. *Journal of Physical Chemistry B*, **2000**, 104, 1108-1114	3.4	40
54	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. *Journal of Physical Chemistry A*, **2000**, 104, 5351-5357	2.8	57
53	Conformational Distribution of Gas-phase Glycerol. *Journal of Physical Chemistry A*, **2000**, 104, 11220-11228	2.8	32
52	Simulated structure, dynamics, and vibrational spectra of liquid benzene. *Journal of Chemical Physics*, **2000**, 113, 6851-6863	3.9	57
51	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. *Journal of Chemical Physics*, **1999**, 111, 4218-4229	3.9	65
50	Glycerol condensed phases Part I. A molecular dynamics study. *Physical Chemistry Chemical Physics*, **1999**, 1, 871-877	3.6	103
49	An ab initio molecular dynamics study of the SN2 reaction ClCH3Br-ClH3Cl+Br *Journal of Chemical Physics*, **1999**, 111, 10887-10894	3.9	28
48	Glycerol condensed phases Part II.A molecular dynamics study of the conformational structure and hydrogen bonding. *Physical Chemistry Chemical Physics*, **1999**, 1, 879-885	3.6	120
47	Density functional calculation of structure and vibrational spectra of polyenes. *Journal of Chemical Physics*, **1999**, 110, 3241-3250	3.9	34
46	Intermolecular interactions in the N2-N2 dimer. *Molecular Physics*, **1998**, 95, 477-481	1.7	14
45	Low-Frequency Vibrations ofall-trans-Retinal:Far-Infrared and Raman Spectra and Density Functional Calculations. *Journal of Physical Chemistry A*, **1998**, 102, 2131-2136	2.8	49
44	A molecular dynamics simulation of the vibrational properties of the Ar1(N2)x crystal. *Journal of Chemical Physics*, **1998**, 109, 6382-6389	3.9	3

43	A molecular dynamics study of the CO2/NaCl(001) system. *Journal of Chemical Physics*, **1997**, 106, 5693-5705	3.9	6
42	A molecular dynamics study of translation-rotation coupling in the NaCN plastic crystal. *Journal of Chemical Physics*, **1997**, 107, 8041-8050	3.9	8
41	Orientational ordering in the mixed crystal Ar1−x(N2)x: A molecular dynamics study. *Journal of Chemical Physics*, **1997**, 106, 8196-8203	3.9	7
40	Calculation of elastic coherent neutron scattering spectra from molecular dynamics data: The NaCN plastic crystal. *Chemical Physics Letters*, **1997**, 274, 335-340	2.5	
39	A comparison between the rigid and flexible model of cyclohexane in the plastic phase by molecular dynamic simulations. *Chemical Physics*, **1995**, 193, 101-108	2.3	9
38	On the vibrational assignment of fullerene C60. *Journal of Chemical Physics*, **1994**, 101, 11079-11081	3.9	46
37	A molecular dynamics simulation of the plastic phase (I) of cyclopentane. *Chemical Physics*, **1994**, 189, 17-23	2.3	4
36	Infrared Spectrum of Two Fullerene Derivatives: C60O and C61H2. *The Journal of Physical Chemistry* , **1994**, 98, 9966-9971		30
35	Molecular dynamics simulation of the plastic phase of 2-methyl-2-nitropropane. *Chemical Physics*, **1993**, 178, 93-103	2.3	2
34	Sideband modeling in molecular crystals N2 and CO2. *Journal of Chemical Physics*, **1992**, 96, 5703-5711	3.9	12
33	Anharmonic lattice dynamics and computer simulation for simple model systems. *Physical Review B*, **1992**, 45, 2113-2125	3.3	17
32	An intra-molecular potential for S8. *Journal of Molecular Structure*, **1992**, 266, 229-234	3.4	4
31	A molecular dynamics simulation of crystalline S8. *Chemical Physics*, **1992**, 165, 313-322	2.3	14
30	Vibrational frequencies of C70. *Chemical Physics Letters*, **1992**, 195, 347-351	2.5	30
29	A molecular dynamics study of the isotopic substitution effects on the lineshape of an internal mode in a molecular crystal. *Chemical Physics Letters*, **1992**, 200, 552-558	2.5	3
28	Vibrational properties of Xe–fullerene adducts. A molecular dynamics approach. *Chemical Physics Letters*, **1992**, 200, 39-45	2.5	22
27	Molecular dynamics simulation of crystalline imidazole. *Chemical Physics*, **1991**, 156, 71-77	2.3	4
26	Molecular dynamics simulation of the vibrational properties of a disordered N2O crystal. II. The symmetric stretching mode. *Journal of Chemical Physics*, **1991**, 94, 2502-2508	3.9	13

25	Vibrational relaxation and dephasing of Fermi resonance states in molecular crystals. *Journal of Chemical Physics*, **1991**, 95, 2523-2536	3.9	11
24	Computer simulation of the dynamics of the plastic phase of succinonitrile. *Journal of Chemical Physics*, **1991**, 95, 679-685	3.9	35
23	Application of normal mode analysis in molecular dynamics simulation of model alkanes. *Chemical Physics*, **1990**, 146, 147-153	2.3	17
22	Molecular dynamics simulation of the vibrational properties of a disordered N2O crystal. I. Lattice frequencies. *Journal of Chemical Physics*, **1990**, 93, 1973-1980	3.9	9
21	Vibrational relaxation and dephasing of two-phonon bound states in molecular crystals. *Physical Review B*, **1990**, 42, 2307-2324	3.3	26
20	Pressure tuning of Fermi resonance in crystal CO2. *Journal of Chemical Physics*, **1989**, 91, 3869-3876	3.9	19
19	Structure and dynamics of carbon dioxide clusters: A molecular dynamics study. *Journal of Chemical Physics*, **1989**, 90, 4441-4449	3.9	66
18	Characterization of a Langmuir-Blodgett monolayer using molecular dynamics calculations. *Chemical Physics Letters*, **1988**, 145, 493-498	2.5	46
17	Biphonons in crystal N2O. *Chemical Physics*, **1988**, 119, 241-251	2.3	16
16	Characterization of structural and dynamical behavior in monolayers of long-chain molecules using molecular-dynamics calculations. *Physical Review Letters*, **1988**, 60, 2152-2155	7.4	110
15	Molecular Dynamics Study of A Model Langmuir-Blodgett Film. *Materials Research Society Symposia Proceedings*, **1988**, 141, 411		3
14	Recursive computation of many-phonon densities of states. *Physical Review Letters*, **1987**, 59, 2196-2198	7.4	8
13	Molecular dynamics and anharmonic effects in the phonon spectra of solid carbon dioxide. *Chemical Physics*, **1987**, 117, 355-366	2.3	13
12	Molecular dynamics and head-tail disorder in the Raman spectrum of crystalline N2O. *Chemical Physics Letters*, **1987**, 142, 570-574	2.5	18
11	Anharmonic interactions and Fermi resonance in crystals CS2. *Chemical Physics*, **1987**, 117, 341-353	2.3	20
10	Analytical approximations to virial coefficients for pure and mixed systems. *Molecular Physics*, **1986**, 57, 841-856	1.7	4
9	Solid and liquid carbon monoxide studied with the use of constant-pressure molecular dynamics. *Physical Review B*, **1986**, 33, 3441-3447	3.3	11
8	Dispersion of surface phonons in xenon overlayers physisorbed on the Ag(111) surface. *Physical Review B*, **1985**, 32, 4261-4263	3.3	6

7	Molecular dynamics in crystalline alpha -nitrogen. *Physical Review B*, **1985**, 32, 2489-2496	3.3	20
6	Gas□urface potentials and the dynamics of overlayers. *Faraday Discussions of the Chemical Society*, **1985**, 80, 227-238		13
5	Dynamics of a monolayer of nitrogen physisorbed on graphite. *Surface Science*, **1985**, 154, 231-253	1.8	21
4	Dynamics of registered solid xenon overlayers on graphite. *Physical Review B*, **1984**, 30, 7177-7181	3.3	9
3	Virial coefficients of gas monolayers. *Chemical Physics Letters*, **1982**, 87, 18-22	2.5	1
2	Crystalline structures of condensed films at liquid interfaces. *Chemical Physics Letters*, **1982**, 93, 533-537	2.5	3
1	A molecular dynamics study of translation-rotation coupling in the NaCN plastic crystal		2