R Benny Gerber

List of Publications by Year
in descending order

338 papers	14,242 citations	18436 62 h-index	33814 99 g-index
346 all docs	346 docs citations	346 times ranked	6470 citing authors

#	Article	IF	Citations
1	Experiments and Simulations of Ion-Enhanced Interfacial Chemistry on Aqueous NaCl Aerosols. Science, 2000, 288, 301-306.	6.0	615
2	Ab initio calculation of anharmonic vibrational states of polyatomic systems: Electronic structure combined with vibrational self-consistent field. Journal of Chemical Physics, 1999, 111, 1823-1829.	1.2	426
3	Vibrational wave functions and spectroscopy of (H2O)n,n=2,3,4,5: Vibrational selfâ€consistent field with correlation corrections. Journal of Chemical Physics, 1996, 105, 10332-10348.	1.2	381
4	Timeâ€dependent selfâ€consistent field approximation for intramolecular energy transfer. I. Formulation and application to dissociation of van der Waals molecules. Journal of Chemical Physics, 1982, 77, 3022-3030.	1.2	371
5	Noble-Gas Hydrides: New Chemistry at Low Temperatures. Accounts of Chemical Research, 2009, 42, 183-191.	7.6	241
6	Mo/llerâ€“Plesset perturbation theory applied to vibrational problems. Journal of Chemical Physics, 1996, 105, 11261-11267.	1.2	227
7	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. Advances in Chemical Physics, 2007, , 97-132.	0.3	189
8	FORMATION OF NOVEL RARE-GAS MOLECULES IN LOW-TEMPERATURE MATRICES. Annual Review of Physical Chemistry, 2004, 55, 55-78.	4.8	176
9	Anharmonic Vibrational Spectroscopy of Hydrogen-Bonded Systems Directly Computed from ab Initio Potential Surfaces:Â (H2O)n,n= 2, 3; Cl-(H2O)n,n= 1, 2; H+(H2O)n,n= 1, 2; H2Oâ‹¯CH3OH. Journal of Physical Chemistry A, 2000, 104, 2772-2779.	1.1	174
10	Simplified mechanism for new particle formation from methanesulfonic acid, amines, and water via experiments and ab initio calculations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 18719-18724.	3.3	173
11	Calculation of Vibrational Transition Frequencies and Intensities in Water Dimer:â€‰ Comparison of Different Vibrational Approaches. Journal of Physical Chemistry A, 2008, 112, 4324-4335.	1.1	165
12	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. Physical Chemistry Chemical Physics, 2013, 15, 9468.	1.3	163
13	Molecular scattering from surfaces: theoretical methods and results. Chemical Reviews, 1987, 87, 29-79.	23.0	162
14	A Gate to Organokrypton Chemistry:Â HKrCCH. Journal of the American Chemical Society, 2003, 125, 6876-6877.	6.6	160
15	Excited vibrational states of polyatomic molecules: the semiclassical self-consistent field approach. The Journal of Physical Chemistry, 1986, 90, 20-30.	2.9	157
16	Calculations predict a stable molecular crystal of N8. Nature Chemistry, 2014, 6, 52-56.	6.6	152
17	Degenerate perturbation theory corrections for the vibrational self-consistent field approximation: Method and applications. Journal of Chemical Physics, 2002, 117, 3541-3547.	1.2	142
18	HKrF in solid krypton. Journal of Chemical Physics, 2002, 116, 2508-2515.	1.2	133

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19	Anharmonic wave functions of proteins: quantum self-consistent field calculations of BPTI. Science, 1995, 268, 1319-1322.	6.0	119
20	Validity of timeâ€dependent selfâ€consistentâ€field (TDSCF) approximations for unimolecular dynamics: A test for photodissociation of the Xeâ€“HI cluster. Journal of Chemical Physics, 1990, 93, 6484-6490.	1.2	115
21	Reactions of Methanesulfonic Acid with Amines and Ammonia as a Source of New Particles in Air. Journal of Physical Chemistry B, 2016, 120, 1526-1536.	1.2	115
22	Vibrational deactivation of diatomic molecules by collisions with solid surfaces. Journal of Chemical Physics, 1981, 74, 4709-4725.	1.2	113
23	New Experimental and Theoretical Approach to the Heterogeneous Hydrolysis of NO2:Â Key Role of Molecular Nitric Acid and Its Complexesâ€. Journal of Physical Chemistry A, 2006, 110, 6886-6897.	1.1	113
24	A Small Neutral Molecule with Two Noble-Gas Atoms: HXeOXeH. Journal of the American Chemical Society, 2008, 130, 6114-6118.	6.6	111
25	Quantum Chemical Calculations on Novel Molecules from Xenon Insertion into Hydrocarbons. Journal of Physical Chemistry A, 2002, 106, 11950-11955.	1.1	107
26	Chlorine activation indoors and outdoors via surface-mediated reactions of nitrogen oxides with hydrogen chloride. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13647-13654.	3.3	107
27	Rotationally inelastic moleculeâ€“surface scattering in the sudden approximation. Journal of Chemical Physics, 1980, 73, 4397-4412.	1.2	106
28	Combined ab initio and anharmonic vibrational spectroscopy calculations for rare gas containing fluorohydrides, HRgF. Chemical Physics Letters, 2000, 331, 308-316.	1.2	105
29	Ab Initio and Improved Empirical Potentials for the Calculation of the Anharmonic Vibrational States and Intramolecular Mode Coupling ofN-Methylacetamide. Journal of Physical Chemistry A, 2002, 106, 8696-8707.	1.1	103
30	Exact timeâ€dependent quantum mechanical dissociation dynamics of I2He: Comparison of exact timeâ€dependent quantum calculation with the quantum timeâ€dependent selfâ€consistent field (TDSCF) approximation. Journal of Chemical Physics, 1987, 87, 2760-2765.	1.2	98
31	Vibrational Spectroscopy of the GÂ·â€‰Â·â€‰Â·C Base Pair:â€‰ Experiment, Harmonic and Anharmonic Calculations, and the Nature of the Anharmonic Couplings. Journal of Physical Chemistry A, 2005, 109, 6974-6984.	1.1	98
32	Dynamics of molecular reactions in solids: Photodissociation of HI in crystalline Xe. Journal of Chemical Physics, 1988, 89, 174-183.	1.2	96
33	Dynamics of molecular reactions in solids: Photodissociation of F2in crystalline Ar. Journal of Chemical Physics, 1990, 92, 3551-3558.	1.2	95
34	Transition from Hydrogen Bonding to Ionization in (HCl)n(NH3)n and (HCl)n(H2O)n Clusters:â€‰ Consequences for Anharmonic Vibrational Spectroscopy. Journal of Physical Chemistry A, 2001, 105, 8323-8332.	1.1	94
35	Anharmonic Vibrational Spectroscopy of Glycine:Â Testing of ab Initio and Empirical Potentials. Journal of Physical Chemistry A, 2000, 104, 10035-10044.	1.1	93
36	Ab Initio Vibrational Calculations for H2SO4 and H2SO4Â·H2O:â€‰ Spectroscopy and the Nature of the Anharmonic Couplings. Journal of Physical Chemistry A, 2005, 109, 6565-6574.	1.1	93

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37	Photochemical Reactions in Weakly Bound Clusters. Annual Review of Physical Chemistry, 1994, 45, 275-314.	4.8	92
38	Spectroscopically-tested, improved, semi-empirical potentials for biological molecules: Calculations for glycine, alanine and prolineElectronic supplementary information (ESI) available: Geometries (MP2) Tj ETQq0 0 0 rgBT /Overlock 10 T http://www.rsc.org/suppdata/cp/b3/b315326f/. Physical Chemistry Chemical Physics, 2004, 6, 2543.	1.3	92
39	Solvation effects on chemical reaction dynamics in clusters: Photodissociation of HI inXeNHI. Physical Review Letters, 1990, 64, 1453-1456.	2.9	91
40	Computational Studies of Atmospherically-Relevant Chemical Reactions in Water Clusters and on Liquid Water and Ice Surfaces. Accounts of Chemical Research, 2015, 48, 399-406.	7.6	89
41	Impact, Trapping, and Accommodation of Hydroxyl Radical and Ozone at Aqueous Salt Aerosol Surfaces. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2003, 107, 12690-12699.	1.2	88
42	New particle formation and growth from methanesulfonic acid, trimethylamine and water. Physical Chemistry Chemical Physics, 2015, 17, 13699-13709.	1.3	88
43	Mixed quantum wave packet/classical trajectory treatment of the photodissociation process ArHClâ†'Ar+H+Cl. Journal of Chemical Physics, 1992, 97, 7242-7250.	1.2	86
44	Direct calculation of anharmonic vibrational states of polyatomic molecules using potential energy surfaces calculated from density functional theory. Journal of Chemical Physics, 2000, 112, 2598-2604.	1.2	84
45	Vibrational spectroscopy and matrix-site geometries of HArF, HKrF, HXeCl, and HXeI in rare-gas solids. Journal of Chemical Physics, 2002, 116, 5521-5529.	1.2	76
46	The future of airborne sulfur-containing particles in the absence of fossil fuel sulfur dioxide emissions. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13514-13519.	3.3	76
47	Vibrational wave functions and energy levels of large anharmonic clusters: A vibrational SCF study of (Ar)13. Journal of Chemical Physics, 1996, 105, 10682-10690.	1.2	75
48	First compounds with argonâ€"carbon and argonâ€"silicon chemical bonds. Journal of Chemical Physics, 2003, 119, 6415-6417.	1.2	75
49	Ionization of N₂O₄ in Contact with Water: Mechanism, Time Scales and Atmospheric Implications. Journal of the American Chemical Society, 2009, 131, 12180-12185.	6.6	72
50	Photooxidation of Ammonia on TiO₂ as a Source of NO and NO₂ under Atmospheric Conditions. Journal of the American Chemical Society, 2013, 135, 8606-8615.	6.6	72
51	Theoretical study of decomposition pathways for HArF and HKrF. Chemical Physics Letters, 2002, 364, 628-633.	1.2	71
52	A remedy for zeroâ€point energy problems in classical trajectories: A combined semiclassical/classical molecular dynamics algorithm. Journal of Chemical Physics, 1992, 96, 2034-2038.	1.2	70
53	Dynamics of Vibrational Overtone Excitations of H2SO4, H2SO4â^'H2O:Â Hydrogenâ^'Hopping and Photodissociation Processes. Journal of the American Chemical Society, 2006, 128, 9594-9595.	6.6	70
54	Distributions of energy spacings and wave function properties in vibrationally excited states of polyatomic molecules. I. Numerical experiments on coupled Morse oscillators. Journal of Chemical Physics, 1982, 76, 5397-5404.	1.2	69

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55	Anharmonic vibrational spectroscopy of the glycineâ€“water complex: Calculations for ab initio, empirical, and hybrid quantum mechanics/molecular mechanics potentials. Journal of Chemical Physics, 2001, 115, 1340-1348.	1.2	68
56	Vibrational levels and tunneling dynamics by the optimal coordinates, self-consistent field method: a study of hydrocyanic acid .dblarw. hydroisocyanic acid. The Journal of Physical Chemistry, 1986, 90, 3606-3612.	2.9	67
57	Quantum Molecular Dynamics of Ultrafast Processes in Large Polyatomic Systems. Chemical Reviews, 1999, 99, 1583-1606.	23.0	66
58	Early Structural Evolution of Native Cytochrome c after Solvent Removal. ChemBioChem, 2008, 9, 2417-2423.	1.3	66
59	Anharmonic Vibrational Spectroscopy of the F-(H2O)nComplexes,n= 1, 2. Journal of Physical Chemistry A, 2003, 107, 4952-4956.	1.1	65
60	Vibrational states and structure of Ar3: The role of threeâ€body forces. Journal of Chemical Physics, 1991, 94, 6728-6736.	1.2	64
61	Hybrid quantum/semiclassical wave packet method for molecular dynamics: Application to photolysis of Ar...HCl. Journal of Chemical Physics, 1993, 98, 427-436.	1.2	63
62	Quantum dynamics of large polyatomic systems using a classically based separable potential method. Journal of Chemical Physics, 1995, 102, 6046-6056.	1.2	63
63	Vibrational Spectra of Î±-Glucose, Î²-Glucose, and Sucrose: Anharmonic Calculations and Experiment. Journal of Physical Chemistry A, 2011, 115, 5859-5872.	1.1	63
64	Vibrational states of very floppy clusters: Approximate separability and the choice of good curvilinear coordinates for XeHe2, I2He. Journal of Chemical Physics, 1989, 91, 1813-1823.	1.2	62
65	Photodissociation dynamics of HCl in solid Ar: Cage exit, nonadiabatic transitions, and recombination. Journal of Chemical Physics, 1997, 106, 6574-6587.	1.2	62
66	Effects of solvation by a single atom on photodissociation: Classical and quantum/classical studies of HCl photolysis in Arâ‹…â‹…â‹…HCl. Journal of Chemical Physics, 1992, 97, 3297-3306.	1.2	60
67	The dynamics of water evaporation from partially solvated cytochrome c in the gas phase. Physical Chemistry Chemical Physics, 2007, 9, 4690.	1.3	60
68	Dynamics of dissociation and energy transfer in molecular collisions with solid surfaces. The Journal of Physical Chemistry, 1986, 90, 4483-4491.	2.9	58
69	On the number of significant mode-mode anharmonic couplings in vibrational calculations: Correlation-corrected vibrational self-consistent field treatment of di-, tri-, and tetrapeptides. Journal of Chemical Physics, 2008, 128, 165105.	1.2	58
70	A quantitative approximation for the quantum dynamics of hydrogen transfer: Transition state dynamics and decay in ClHClâ‡. Journal of Chemical Physics, 1994, 101, 1975-1987.	1.2	57
71	Quantum-Mechanical Inversion of the Differential Cross Section: Determination of the He-Ne Potential. Physical Review Letters, 1978, 41, 236-239.	2.9	56
72	Theoretical study of anharmonic vibrational spectra of HNO3, HNO3â€“H2O, HNO4: Fundamental, overtone and combination excitations. Chemical Physics, 2005, 313, 213-224.	0.9	56

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73	Role of Rotational and Translational Local Modes in Vibrational Relaxation in Solids: A Study of NH and ND in Solid Ar. Physical Review Letters, 1977, 39, 1000-1004.	2.9	54
74	Nonadiabatic dynamics and electronic energy relaxation of Cl(2P) atoms in solid Ar. Journal of Chemical Physics, 1996, 105, 4626-4635.	1.2	54
75	Conformational evolution of ubiquitin ions in electrospray mass spectrometry: molecular dynamics simulations at gradually increasing temperatures. Physical Chemistry Chemical Physics, 2008, 10, 3077.	1.3	54
76	Ultraviolet spectroscopy of water clusters: Excited electronic states and absorption line shapes of (H2O)n, n=2â€“6. Journal of Chemical Physics, 1998, 109, 8747-8750.	1.2	53
77	Mid-IRspectra of different conformers of phenylalanine in the gas phase. Physical Chemistry Chemical Physics, 2008, 10, 1248-1256.	1.3	53
78	The Role of Oxalic Acid in New Particle Formation from Methanesulfonic Acid, Methylamine, and Water. Environmental Science & Technology, 2017, 51, 2124-2130.	4.6	53
79	Photodissociation of ICN in solid and in liquid Ar: Dynamics of the cage effect and of excitedâ€state isomerization. Journal of Chemical Physics, 1994, 100, 4242-4252.	1.2	52
80	Photodissociation of HBr adsorbed on the surface and embedded in large Arn clusters. Journal of Chemical Physics, 2000, 113, 329-338.	1.2	52
81	Molecular dynamics simulations of reactions in solids: Photodissociation of Cl2in crystalline Xe. Journal of Chemical Physics, 1989, 91, 1611-1617.	1.2	51
82	Atom scattering studies of liquid structure and dynamics: Collisions of Xe with a model of squalane. Journal of Chemical Physics, 1994, 100, 8408-8417.	1.2	51
83	Anharmonic Vibrational Spectroscopy Calculations for Novel Rare-Gas-Containing Compounds:Â HXeH, HXeCl, HXeBr, and HXeOH. Journal of Physical Chemistry A, 2000, 104, 7944-7949.	1.1	51
84	Vibrational spectroscopy of (SO42â^')â^™(H2O)n clusters, n=1â€“5: Harmonic and anharmonic calculations and experiment. Journal of Chemical Physics, 2007, 127, 094305.	1.2	51
85	Anharmonic vibrational spectroscopy calculations with electronic structure potentials: comparison of MP2 and DFT for organic molecules. Theoretical Chemistry Accounts, 2008, 120, 273-279.	0.5	51
86	Quantumâ€Mechanical Treatments of Rotationally Inelastic Moleculeâ€Surface Scattering. Israel Journal of Chemistry, 1982, 22, 321-328.	1.0	49
87	Î”Mj transitions in homonuclear molecule scattering off corrugated surfaces. Square and rectangular lattice symmetry and purely repulsive interaction. Journal of Chemical Physics, 1984, 80, 3845-3858.	1.2	49
88	Phonon sudden theory of Debyeâ€“Waller attenuation. Temperature dependence of rotational energy transfer in molecule/surface scattering. Journal of Chemical Physics, 1985, 82, 1567-1576.	1.2	49
89	Photochemical Processes Induced by Vibrational Overtone Excitations:Â Dynamics Simulations forcis-HONO,trans-HONO, HNO3, and HNO3â^'H2Oâ€. Journal of Physical Chemistry A, 2006, 110, 5342-5354.	1.1	49
90	Absorption Spectra and Photolysis of Methyl Peroxide in Liquid and Frozen Water. Journal of Physical Chemistry A, 2012, 116, 6068-6077.	1.1	49

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91	Atom scattering from isolated adsorbates on surfaces: Rainbows, diffraction interferences, and trapping resonances. Journal of Chemical Physics, 1988, 88, 7209-7220.	1.2	48
92	Structure of Large Nitrateâˆ™Water Clusters at Ambient Temperatures: Simulations with Effective Fragment Potentials and Force Fields with Implications for Atmospheric Chemistry. Journal of Physical Chemistry A, 2009, 113, 12805-12814.	1.1	47
93	Lifetimes of compounds made of noble-gas atoms with water. Chemical Physics Letters, 2009, 482, 30-33.	1.2	42
94	Hygroscopic Growth and Deliquescence of NaCl Nanoparticles Mixed with Surfactant SDS. Journal of Physical Chemistry B, 2010, 114, 2435-2449.	1.2	42
95	High resolution absolute absorption cross sections of the BÌ*f* ¹Aâ€²â€“XÌ*f* ¹Aâ€² transition of the CH₂OO biradical. Physical Chemistry Chemical Physics, 2015, 17, 32539-32546.	1.3	42
96	Proton Transfer in Mixed Clusters of Methanesulfonic Acid, Methylamine, and Oxalic Acid: Implications for Atmospheric Particle Formation. Journal of Physical Chemistry A, 2017, 121, 2377-2385.	1.1	42
97	Particle formation and growth from oxalic acid, methanesulfonic acid, trimethylamine and water: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 28286-28301.	1.3	42
98	Dynamics of photoinduced reactions in hydrogen-bonded clusters: classical studies of the photodissociation of hydrogen chloride dimer. The Journal of Physical Chemistry, 1993, 97, 12516-12522.	2.9	41
99	Photodissociation and recombination of F2 molecule in Ar54 cluster: Nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6660-6672.	1.2	41
100	Lifetime and decomposition pathways of a chemically bound helium compound. Journal of Chemical Physics, 2001, 115, 7341-7343.	1.2	41
101	Raman spectra of long chain hydrocarbons: anharmonic calculations, experiment and implications for imaging of biomembranes. Physical Chemistry Chemical Physics, 2011, 13, 12724.	1.3	41
102	Quantum diffusion of hydrogen on metal surfaces. Journal of Chemical Physics, 1986, 84, 5181-5195.	1.2	40
103	Photodissociation dynamics ofF2in solid Kr: Theory versus experiment. Physical Review Letters, 1991, 66, 1295-1297.	2.9	40
104	A Vibrational Eigenfunction of a Protein:â€‰ Anharmonic Coupled-Mode Ground and Fundamental Excited States of BPTI. Journal of Physical Chemistry B, 1997, 101, 1700-1706.	1.2	40
105	Photodissociation of HCl adsorbed on the surface of an Ar12 cluster: Nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1999, 110, 11047-11053.	1.2	40
106	Photodissociation of oriented HXeI molecules generated from HIâ€“Xen clusters. Journal of Chemical Physics, 2003, 119, 224-231.	1.2	40
107	Catalytic Role for Water in the Atmospheric Production of ClNO. Journal of Physical Chemistry A, 2010, 114, 4609-4618.	1.1	40
108	Resonances in the photolysis of HCl in Ar-CHl: Imaging of a resonance wave function in the photofragment angular distribution. Physical Review Letters, 1993, 71, 931-934.	2.9	39

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109	Vibrational Spectroscopy of Peptides and Peptideâ^'Water Complexes:â€‰ Anharmonic Coupled-Mode Calculations. Journal of Physical Chemistry B, 1997, 101, 8595-8606.	1.2	39
110	Vibrational spectroscopy and the development of new force fields for biological molecules. Biopolymers, 2003, 68, 370-382.	1.2	39
111	Complexes of HNO3 and NO3â^' with NO2 and N2O4, and their potential role in atmospheric HONO formation. Physical Chemistry Chemical Physics, 2008, 10, 6019.	1.3	39
112	Threeâ€dimensional quantum wave packet study of the Arâ€"HCl photodissociation: A comparison between timeâ€dependent selfâ€consistentâ€field and exact treatments. Journal of Chemical Physics, 1995, 103, 3463-3473.	1.2	38
113	Photodissociation, electronic relaxation and recombination of HCl in Arn(HCl) clusters Non-adiabatic molecular dynamics simulations. Faraday Discussions, 1997, 108, 243-254.	1.6	38
114	Acceleration of Correlation-corrected Vibrational Self-consistent Field Calculation Times for Large Polyatomic Molecules. Theoretical Chemistry Accounts, 2006, 117, 69-72.	0.5	38
115	A statistical wave function model for Câ€"H/Câ€"D overtone linewidths: Application to C6H6, C6D6, C6HD5, C6HF5. Journal of Chemical Physics, 1984, 81, 3393-3399.	1.2	37
116	Direct calculation of anharmonic vibrational states of polyatomic molecules using density functional theory: spectroscopic tests of recently developed functionals. Chemical Physics Letters, 2000, 324, 206-212.	1.2	37
117	Photochemistry of Thin Solid Films of the Neonicotinoid Imidacloprid on Surfaces. Environmental Science & Technology, 2017, 51, 2660-2668.	4.6	37
118	Delayed and direct cage exit in photodissociation ofCl2in solid Ar. Physical Review Letters, 1992, 69, 856-859.	2.9	36
119	Dynamics simulations of atmospherically relevant molecular reactions. International Reviews in Physical Chemistry, 2009, 28, 207-222.	0.9	36
120	Ultrafast quantum dynamics and resonance Raman spectroscopy of photoexcited I2(B) in large argon and xenon clusters. Journal of Chemical Physics, 1996, 104, 9332-9339.	1.2	35
121	Ab initio and semi-empirical Molecular Dynamics simulations of chemical reactions in isolated molecules and in clusters. Physical Chemistry Chemical Physics, 2014, 16, 9760-9775.	1.3	35
122	Scattering from disordered surfaces in the sudden approximation. Journal of Chemical Physics, 1983, 78, 4277-4287.	1.2	34
123	The sudden approximation for scattering from noncrystalline surfaces: Applications to models of adsorbed impurities and to mixed overlayers. Journal of Chemical Physics, 1986, 84, 5955-5961.	1.2	34
124	Photodissociation dynamics of CH3I adsorbed on MgO(100): Theory and experiment. Journal of Chemical Physics, 1992, 97, 5168-5176.	1.2	34
125	Anharmonic Vibrational Self-Consistent Field Calculations as an Approach to Improving Force Fields for Monosaccharides. Journal of Physical Chemistry B, 1999, 103, 3476-3488.	1.2	34
126	Ultrafast Solvent-Induced Spin-Flip and Nonadiabatic Coupling: ClF in Argon Solids. Physical Review Letters, 2002, 89, 108301.	2.9	34

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127	Calculation of anharmonic vibrational spectroscopy of small biological molecules. PhysChemComm, 2002, 5, 142.	0.8	34
128	Predicted stability of the organo-xenon compound HXeCCH above the cryogenic range. Chemical Physics Letters, 2008, 460, 23-26.	1.2	34
129	NO_x Reactions on Aqueous Surfaces with Gaseous HCl: Formation of a Potential Precursor to Atmospheric Cl Atoms. Journal of Physical Chemistry Letters, 2012, 3, 3405-3410.	2.1	34
130	Direct inversion method for obtaining anisotropic potentials from rotationally inelastic and elastic cross sections. Journal of Chemical Physics, 1980, 72, 3596-3603.	1.2	33
131	Cross sections for He scattering from surface imperfections: Vacancies and CO adsorbates on Pt(111). Journal of Chemical Physics, 1988, 88, 3722-3731.	1.2	33
132	Molecularâ€dynamics simulations of the photodissociation of ICl adsorbed on a MgO(001) surface. Journal of Chemical Physics, 1990, 93, 887-893.	1.2	33
133	Quantum dynamics simulations of nonadiabatic processes in manyâ€atom systems: Photoexcited Ba(Ar)10 and Ba(Ar)20 clusters. Journal of Chemical Physics, 1996, 104, 5803-5814.	1.2	33
134	Vibrational self-consistent field approach to anharmonic spectroscopy of molecules in solids: Application to iodine in argon matrix. Journal of Chemical Physics, 2001, 115, 2695-2701.	1.2	33
135	Nitrogen dioxide at the airâ€“water interface: trapping, absorption, and solvation in the bulk and at the surface. Physical Chemistry Chemical Physics, 2013, 15, 204-212.	1.3	33
136	Isomerization and Decomposition of a Criegee Intermediate in the Ozonolysis of Alkenes: Dynamics Using a Multireference Potential. Angewandte Chemie - International Edition, 2014, 53, 265-268.	7.2	33
137	Dynamics of energy flow from CH overtone excitations: Theoretical and experimental studies of CH3Câ‰¡CH. Journal of Chemical Physics, 1988, 88, 7434-7447.	1.2	32
138	Spectroscopy, polarization and nonadiabatic dynamics of electronically excited Ba(Ar)n clusters: Theory and experiment. Journal of Chemical Physics, 1996, 104, 3651-3663.	1.2	32
139	Matrix-isolation and ab initio study of HXeCCH complexed with acetylene. Chemical Physics Letters, 2009, 481, 83-87.	1.2	32
140	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	1.1	32
141	First-principles anharmonic quantum calculations for peptide spectroscopy: VSCF calculations and comparison with experiments. Physical Chemistry Chemical Physics, 2016, 18, 1607-1614.	1.3	32
142	Amineâ€“Amine Exchange in Aminiumâ€“Methanesulfonate Aerosols. Journal of Physical Chemistry C, 2014, 118, 29431-29440.	1.5	31
143	Reaction of a charge-separated ONONO2 species with water in the formation of HONO: an MP2 Molecular Dynamics study. Physical Chemistry Chemical Physics, 2014, 16, 4483.	1.3	31
144	Subpicosecond spin-flip induced by the photodissociation dynamics of ClF in an Ar matrix. Physical Chemistry Chemical Physics, 2002, 4, 5554-5562.	1.3	30

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145	Vibrational Spectroscopy of Protonated Imidazole and its Complexes with Water Molecules:Â Ab Initio Anharmonic Calculations and Experimentsâ€. Journal of Physical Chemistry A, 2007, 111, 7374-7381.	1.1	30
146	Vibrational spectroscopy of triacetone triperoxide (TATP): Anharmonic fundamentals, overtones and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1438-1445.	2.0	30
147	Direct visualization of the Hâ€“Xe bond in xenon hydrides: Xenon isotopic shift in the IR spectra. Journal of Chemical Physics, 2009, 131, 151101.	1.2	30
148	Quantum theory of the photodissociation of IBr adsorbed on an MgO(001) surface. Journal of Chemical Physics, 1990, 92, 7708-7715.	1.2	29
149	Dynamics of Electronic States and Spinâ^'Flip for Photodissociation of Dihalogens in Matrices:â€‰ Experiment and Semiclassical Surface-Hopping and Quantum Model Simulations for F₂ and ClF in Solid Ar. Journal of Physical Chemistry A, 2007, 111, 9573-9585.	1.1	29
150	Raman and IR spectra of butane: Anharmonic calculations and interpretation of room temperature spectra. Chemical Physics Letters, 2011, 515, 7-12.	1.2	29
151	Theoretical Prediction of Chemically Bound Compounds Made of Argon and Hydrocarbons. Journal of the American Chemical Society, 2006, 128, 7156-7157.	6.6	28
152	Conformational Structures of a Decapeptide Validated by First Principles Calculations and Cold Ion Spectroscopy. ChemPhysChem, 2015, 16, 1374-1378.	1.0	28
153	Absorption spectra of benzoic acid in water at different pH and in the presence of salts: insights from the integration of experimental data and theoretical cluster models. Physical Chemistry Chemical Physics, 2020, 22, 5046-5056.	1.3	28
154	The semiclassical selfâ€consistent field method for polyatomic vibrations: Use of hyperspherical coordinates for H2O and CO2. Journal of Chemical Physics, 1986, 85, 3425-3431.	1.2	27
155	Isotopic Hydration of Cellobiose: Vibrational Spectroscopy and Dynamical Simulations. Journal of Physical Chemistry A, 2011, 115, 9498-9509.	1.1	27
156	Quantum Monte Carlo studies of small B(H2)nclusters. Journal of Chemical Physics, 1994, 101, 2577-2591.	1.2	26
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