R Benny Gerber

List of Publications by Citations

334 papers	12,785 citations	58 h-index	95 g-index
346 ext. papers	13,483 ext. citations	5 avg, IF	6.45 L-index

#	Paper	IF	Citations
334	Experiments and simulations of ion-enhanced interfacial chemistry on aqueous NaCl aerosols. *Science*, **2000**, 288, 301-6	33.3	566
333	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	3.9	401
332	Vibrational wave functions and spectroscopy of (H2O)n, n=2,3,4,5: Vibrational self-consistent field with correlation corrections. *Journal of Chemical Physics*, **1996**, 105, 10332-10348	3.9	354
331	Time-dependent self-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	3.9	350
330	Noble-gas hydrides: new chemistry at low temperatures. *Accounts of Chemical Research*, **2009**, 42, 183-91	24.3	219
329	Mo/llerPlesset perturbation theory applied to vibrational problems. *Journal of Chemical Physics*, **1996**, 105, 11261-11267	3.9	214
328	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. *Advances in Chemical Physics*, **2007**, 97-132		168
327	Anharmonic Vibrational Spectroscopy of Hydrogen-Bonded Systems Directly Computed from ab Initio Potential Surfaces: (H2O)n, n = 2, 3; Cl-(H2O)n, n = 1, 2; H+(H2O)n, n = 1, 2; H2OCH3OH. *Journal of Physical Chemistry A*, **2000**, 104, 2772-2779	2.8	167
326	Formation of novel rare-gas molecules in low-temperature matrices. *Annual Review of Physical Chemistry*, **2004**, 55, 55-78	15.7	162
325	Molecular scattering from surfaces: theoretical methods and results. *Chemical Reviews*, **1987**, 87, 29-79	68.1	158
324	Excited vibrational states of polyatomic molecules: the semiclassical self-consistent field approach. *The Journal of Physical Chemistry*, **1986**, 90, 20-30		150
323	Calculation of vibrational transition frequencies and intensities in water dimer: comparison of different vibrational approaches. *Journal of Physical Chemistry A*, **2008**, 112, 4324-35	2.8	149
322	A gate to organokrypton chemistry: HKrCCH. *Journal of the American Chemical Society*, **2003**, 125, 6876-7	16.4	147
321	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. *Physical Chemistry Chemical Physics*, **2013**, 15, 9468-92	3.6	143
320	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, 18719-24	11.5	131
319	Degenerate perturbation theory corrections for the vibrational self-consistent field approximation: Method and applications. *Journal of Chemical Physics*, **2002**, 117, 3541-3547	3.9	131
318	HKrF in solid krypton. *Journal of Chemical Physics*, **2002**, 116, 2508-2515	3.9	125

317	Calculations predict a stable molecular crystal of N8. *Nature Chemistry*, **2014**, 6, 52-6	17.6	107
316	Vibrational deactivation of diatomic molecules by collisions with solid surfaces. *Journal of Chemical Physics*, **1981**, 74, 4709-4725	3.9	107
315	Anharmonic wave functions of proteins: quantum self-consistent field calculations of BPTI. *Science*, **1995**, 268, 1319-22	33.3	106
314	Validity of time-dependent self-consistent-field (TDSCF) approximations for unimolecular dynamics: A test for photodissociation of the XeHI cluster. *Journal of Chemical Physics*, **1990**, 93, 6484-6490	3.9	104
313	New experimental and theoretical approach to the heterogeneous hydrolysis of NO2: key role of molecular nitric acid and its complexes. *Journal of Physical Chemistry A*, **2006**, 110, 6886-97	2.8	103
312	Quantum Chemical Calculations on Novel Molecules from Xenon Insertion into Hydrocarbons. *Journal of Physical Chemistry A*, **2002**, 106, 11950-11955	2.8	101
311	Rotationally inelastic molecule-surface scattering in the sudden approximation. *Journal of Chemical Physics*, **1980**, 73, 4397-4412	3.9	101
310	Ab Initio and Improved Empirical Potentials for the Calculation of the Anharmonic Vibrational States and Intramolecular Mode Coupling of N-Methylacetamide. *Journal of Physical Chemistry A*, **2002**, 106, 8696-8707	2.8	98
309	A small neutral molecule with two noble-gas atoms: HXeOXeH. *Journal of the American Chemical Society*, **2008**, 130, 6114-8	16.4	97
308	Combined ab initio and anharmonic vibrational spectroscopy calculations for rare gas containing fluorohydrides, HRgF. *Chemical Physics Letters*, **2000**, 331, 308-316	2.5	97
307	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, 13647-54	11.5	96
306	Exact time-dependent quantum mechanical dissociation dynamics of I2He: Comparison of exact time-dependent quantum calculation with the quantum time-dependent self-consistent field (TDSCF) approximation. *Journal of Chemical Physics*, **1987**, 87, 2760-2765	3.9	92
305	Anharmonic Vibrational Spectroscopy of Glycine: Testing of ab Initio and Empirical Potentials. *Journal of Physical Chemistry A*, **2000**, 104, 10035-10044	2.8	91
304	Vibrational spectroscopy of the G...C base pair: experiment, harmonic and anharmonic calculations, and the nature of the anharmonic couplings. *Journal of Physical Chemistry A*, **2005**, 109, 6974-84	2.8	90
303	Transition from Hydrogen Bonding to Ionization in (HCl)n(NH3)n and (HCl)n(H2O)n Clusters: Consequences for Anharmonic Vibrational Spectroscopy. *Journal of Physical Chemistry A*, **2001**, 105, 8323-8332	2.8	90
302	Ab initio vibrational calculations for H2SO4 and H2SO4 x H2O: spectroscopy and the nature of the anharmonic couplings. *Journal of Physical Chemistry A*, **2005**, 109, 6565-74	2.8	89
301	Spectroscopically-tested, improved, semi-empirical potentials for biological molecules: Calculations for glycine, alanine and proline. *Physical Chemistry Chemical Physics*, **2004**, 6, 2543	3.6	88
300	Photochemical Reactions in Weakly Bound Clusters. *Annual Review of Physical Chemistry*, **1994**, 45, 275-314	15.7	87

299	Reactions of Methanesulfonic Acid with Amines and Ammonia as a Source of New Particles in Air. *Journal of Physical Chemistry B*, **2016**, 120, 1526-36	3.4	86
298	Solvation effects on chemical reaction dynamics in clusters: Photodissociation of HI in XeNHI. *Physical Review Letters*, **1990**, 64, 1453-1456	7.4	86
297	Dynamics of molecular reactions in solids: Photodissociation of F2 in crystalline Ar. *Journal of Chemical Physics*, **1990**, 92, 3551-3558	3.9	86
296	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	3.4	84
295	Dynamics of molecular reactions in solids: Photodissociation of HI in crystalline Xe. *Journal of Chemical Physics*, **1988**, 89, 174-183	3.9	82
294	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	3.9	81
293	Mixed quantum wave packet/classical trajectory treatment of the photodissociation process ArHCl-ÿAr+H+Cl. *Journal of Chemical Physics*, **1992**, 97, 7242-7250	3.9	77
292	Vibrational spectroscopy and matrix-site geometries of HArF, HKrF, HXeCl, and HXeI in rare-gas solids. *Journal of Chemical Physics*, **2002**, 116, 5521-5529	3.9	73
291	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	3.9	70
290	Dynamics of vibrational overtone excitations of H2SO4, H2SO4-H2O: hydrogen-hopping and photodissociation processes. *Journal of the American Chemical Society*, **2006**, 128, 9594-5	16.4	69
289	First compounds with argon□arbon and argon□ilicon chemical bonds. *Journal of Chemical Physics*, **2003**, 119, 6415-6417	3.9	69
288	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	24.3	68
287	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	3.9	68
286	New particle formation and growth from methanesulfonic acid, trimethylamine and water. *Physical Chemistry Chemical Physics*, **2015**, 17, 13699-709	3.6	67
285	Ionization of N2O4 in contact with water: mechanism, time scales and atmospheric implications. *Journal of the American Chemical Society*, **2009**, 131, 12180-5	16.4	67
284	Theoretical study of decomposition pathways for HArF and HKrF. *Chemical Physics Letters*, **2002**, 364, 628-633	2.5	67
283	Anharmonic vibrational spectroscopy of the glycine□water complex: Calculations for ab initio, empirical, and hybrid quantum mechanics/molecular mechanics potentials. *Journal of Chemical Physics*, **2001**, 115, 1340-1348	3.9	64
282	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		64

281	Anharmonic Vibrational Spectroscopy of the F-(H2O)nComplexes,n= 1, 2. *Journal of Physical Chemistry A*, **2003**, 107, 4952-4956	2.8	63
280	A remedy for zero-point energy problems in classical trajectories: A combined semiclassical/classical molecular dynamics algorithm. *Journal of Chemical Physics*, **1992**, 96, 2034-2038	3.9	63
279	Quantum Molecular Dynamics of Ultrafast Processes in Large Polyatomic Systems. *Chemical Reviews*, **1999**, 99, 1583-1606	68.1	62
278	Vibrational states and structure of Ar3: The role of three-body forces. *Journal of Chemical Physics*, **1991**, 94, 6728-6736	3.9	61
277	Hybrid quantum/semiclassical wave packet method for molecular dynamics: Application to photolysis of Ar...HCl. *Journal of Chemical Physics*, **1993**, 98, 427-436	3.9	60
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275	Early structural evolution of native cytochrome c after solvent removal. *ChemBioChem*, **2008**, 9, 2417-23	3.8	57
274	Effects of solvation by a single atom on photodissociation: Classical and quantum/classical studies of HCl photolysis in Ar???HCl. *Journal of Chemical Physics*, **1992**, 97, 3297-3306	3.9	57
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272	Photodissociation dynamics of HCl in solid Ar: Cage exit, nonadiabatic transitions, and recombination. *Journal of Chemical Physics*, **1997**, 106, 6574-6587	3.9	56
271	Photooxidation of ammonia on TiO2 as a source of NO and NO2 under atmospheric conditions. *Journal of the American Chemical Society*, **2013**, 135, 8606-15	16.4	54
270	Vibrational spectra of □glucose, ▯glucose, and sucrose: anharmonic calculations and experiment. *Journal of Physical Chemistry A*, **2011**, 115, 5859-72	2.8	54
269	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	3.9	54
268	The dynamics of water evaporation from partially solvated cytochrome c in the gas phase. *Physical Chemistry Chemical Physics*, **2007**, 9, 4690-7	3.6	54
267	Quantum dynamics of large polyatomic systems using a classically based separable potential method. *Journal of Chemical Physics*, **1995**, 102, 6046-6056	3.9	54
266	Dynamics of dissociation and energy transfer in molecular collisions with solid surfaces. *The Journal of Physical Chemistry*, **1986**, 90, 4483-4491		54
265	Theoretical study of anharmonic vibrational spectra of HNO3, HNO3▯H2O, HNO4: Fundamental, overtone and combination excitations. *Chemical Physics*, **2005**, 313, 213-224	2.3	52
264	Ultraviolet spectroscopy of water clusters: Excited electronic states and absorption line shapes of (H2O)n, n=2▯. *Journal of Chemical Physics*, **1998**, 109, 8747-8750	3.9	51

263	A quantitative approximation for the quantum dynamics of hydrogen transfer: Transition state dynamics and decay in ClHCl. *Journal of Chemical Physics*, **1994**, 101, 1975-1987	3.9	51
262	Vibrational spectroscopy of (SO4(2-)).(H2O)n clusters, n=1-5: harmonic and anharmonic calculations and experiment. *Journal of Chemical Physics*, **2007**, 127, 094305	3.9	50
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260	Anharmonic vibrational spectroscopy calculations with electronic structure potentials: comparison of MP2 and DFT for organic molecules. *Theoretical Chemistry Accounts*, **2008**, 120, 273-279	1.9	49
259	Molecular dynamics simulations of reactions in solids: Photodissociation of Cl2 in crystalline Xe. *Journal of Chemical Physics*, **1989**, 91, 1611-1617	3.9	49
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256	Mid-IR spectra of different conformers of phenylalanine in the gas phase. *Physical Chemistry Chemical Physics*, **2008**, 10, 1248-56	3.6	48
255	Photodissociation of ICN in solid and in liquid Ar: Dynamics of the cage effect and of excited-state isomerization. *Journal of Chemical Physics*, **1994**, 100, 4242-4252	3.9	48
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251	Nonadiabatic dynamics and electronic energy relaxation of Cl(2P) atoms in solid Ar. *Journal of Chemical Physics*, **1996**, 105, 4626-4635	3.9	47
250	Atom scattering studies of liquid structure and dynamics: Collisions of Xe with a model of squalane. *Journal of Chemical Physics*, **1994**, 100, 8408-8417	3.9	47
249	Atom scattering from isolated adsorbates on surfaces: Rainbows, diffraction interferences, and trapping resonances. *Journal of Chemical Physics*, **1988**, 88, 7209-7220	3.9	47
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240	Catalytic role for water in the atmospheric production of ClNO. *Journal of Physical Chemistry A*, **2010**, 114, 4609-18	2.8	38
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235	Acceleration of Correlation-corrected Vibrational Self-consistent Field Calculation Times for Large Polyatomic Molecules. *Theoretical Chemistry Accounts*, **2006**, 117, 69-72	1.9	37
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232	Complexes of HNO3 and NO3 - with NO2 and N2O4, and their potential role in atmospheric HONO formation. *Physical Chemistry Chemical Physics*, **2008**, 10, 6019-32	3.6	36
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207	Hygroscopic growth and deliquescence of NaCl nanoparticles mixed with surfactant SDS. *Journal of Physical Chemistry B*, **2010**, 114, 2435-49	3.4	31
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