J Paul Devlin

List of Publications by Year
in descending order

82 papers	3,838 citations	159358 30 h-index	123241 61 g-index
82 all docs	82 docs citations	82 times ranked	2377 citing authors

#	Article	IF	Citations
1	Water surface is acidic. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7342-7347.	3.3	332
2	Solid water clusters in the size range of tensâ€"thousands of H2O: a combined computational/spectroscopic outlook. International Reviews in Physical Chemistry, 2004, 23, 375-433.	0.9	210
3	Surface of ice as viewed from combined spectroscopic and computer modeling studies. The Journal of Physical Chemistry, 1995, 99, 16534-16548.	2.9	172
4	Probing icy surfaces with the danglingâ€OHâ€mode absorption: Large ice clusters and microporous amorphous ice. Journal of Chemical Physics, 1991, 95, 1378-1384.	1.2	167
5	Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic?. Physical Chemistry Chemical Physics, 2007, 9, 4736.	1.3	151
6	Clathrate hydrates with hydrogen-bonding guests. Physical Chemistry Chemical Physics, 2009, 11, 10245.	1.3	149
7	Infrared Spectra of Large H2O Clusters:â€‰ New Understanding of the Elusive Bending Mode of Ice. Journal of Physical Chemistry A, 2001, 105, 974-983.	1.1	146
8	Carbon dioxide clathrate hydrate epitaxial growth: spectroscopic evidence for formation of the simple type-II carbon dioxide hydrate. The Journal of Physical Chemistry, 1991, 95, 3811-3815.	2.9	144
9	The vibrational and electronic spectra of the monoâ€, diâ€, and trianon salts of TCNQ. Journal of Chemical Physics, 1979, 70, 1851-1859.	1.2	141
10	Defect Activity in Amorphous Ice From Isotopic Exchange Data: Insight into the Glass Transition. The Journal of Physical Chemistry, 1995, 99, 11584-11590.	2.9	141
11	Spectra of dangling OH groups at ice cluster surfaces and within pores of amorphous ice. Journal of Chemical Physics, 1991, 94, 812-813.	1.2	138
12	Infrared spectra of hydrogen chloride complexed/ionized in amorphous hydrates and at ice surfaces in the 15-90 K range. The Journal of Physical Chemistry, 1993, 97, 10312-10318.	2.9	134
13	Solvation and Ionization Stages of HCl on Ice Nanocrystals. Journal of Physical Chemistry A, 2002, 106, 9374-9389.	1.1	127
14	Proton trapping and defect energetics in ice from FTâ€IR monitoring of photoinduced isotopic exchange of isolated D2O. Journal of Chemical Physics, 1988, 88, 3086-3091.	1.2	95
15	Spectroscopically evaluated rates and energies for proton transfer and Bjerrum defect migration in cubic ice. The Journal of Physical Chemistry, 1984, 88, 363-368.	2.9	89
16	Vibrational spectra and point defect activities of icy solids and gas phase clusters. International Reviews in Physical Chemistry, 1990, 9, 29-65.	0.9	78
17	FTâ€IR spectra of vacuum deposited clathrate hydrates of oxirane H2S, THF, and ethane. Journal of Chemical Physics, 1985, 83, 4387-4394.	1.2	71
18	FT-IR spectra of 90 K films of simple, mixed, and double clathrate hydrates of trimethylene oxide, methyl chloride, carbon dioxide, tetrahydrofuran, and ethylene oxide containing decoupled water-d2. The Journal of Physical Chemistry, 1988, 92, 631-635.	2.9	71

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19	Ice Surface Reactions with Acids and Bases. Journal of Physical Chemistry B, 1997, 101, 2327-2332.	1.2	70
20	Vibronic interactions, resonance Raman spectra and bond strengths for the radical anion salts of tetracyanoethylene. Journal of Chemical Physics, 1973, 58, 4750-4756.	1.2	68
21	Vibrational Spectra and Structures of Ionic Liquids. II. The Pure Alkali Metal Nitrates. Journal of Chemical Physics, 1968, 48, 3891-3896.	1.2	52
22	Mobile Bjerrum defects: A criterion for iceâ€like crystal growth. Journal of Chemical Physics, 1987, 87, 4126-4131.	1.2	47
23	Hydrogen Bond Surface Chemistry:Â Interaction of NH3with an Ice Particle. Journal of Physical Chemistry B, 2000, 104, 9203-9209.	1.2	44
24	Classical to Nonclassical Transition of Etherâ^'HCN Clathrate Hydrates at Low Temperature. Journal of Physical Chemistry Letters, 2010, 1, 290-294.	2.1	40
25	Rate Study of Ice Particle Conversion to Ammonia Hemihydrate:â€‰ Hydrate Crust Nucleation and NH3 Diffusion. Journal of Physical Chemistry A, 2000, 104, 5770-5777.	1.1	39
26	Protonic and Bjerrum defect activity near the surface of ice at T<145 K. Journal of Chemical Physics, 2001, 115, 9835-9842.	1.2	39
27	Response to Comment on Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic? by J. K. Beattie, Phys. Chem. Chem. Phys., 2007,9, DOI: 10.1039/b713702h. Physical Chemistry Chemical Physics, 2008, 10, 332-333.	1.3	37
28	Molecular bending mode frequencies of the surface and interior of crystalline ice. Journal of Chemical Physics, 1998, 108, 4525-4529.	1.2	35
29	Evidence for the surface origin of point defects in ice: Control of interior proton activity by adsorbates. Journal of Chemical Physics, 2007, 127, 091101.	1.2	33
30	Decoupled isotopomer vibrational frequencies in cubic ice: A simple unified view of the Fermi diads of decoupled H2O, HOD, and D2O. Journal of Chemical Physics, 1986, 84, 6095-6100.	1.2	32
31	Rates and Mechanisms of Conversion of Ice Nanocrystals to Ether Clathrate Hydrates:â€‰ Guest-Molecule Catalytic Effects at â^¼120 K. Journal of Physical Chemistry A, 2006, 110, 1901-1906.	1.1	30
32	Infrared Spectrum of Molten Silver Nitrate. Journal of Chemical Physics, 1966, 44, 2203-2204.	1.2	29
33	Polarized Raman spectra for the full range of isotopic dilution for ice Ic and amorphous ice: Mixtures of intact H2O and D2O. Journal of Chemical Physics, 1989, 90, 1322-1329.	1.2	29
34	Coated Ice Nanocrystals from Waterâ^'Adsorbate Vapor Mixtures:â€‰ Formation of Etherâ^'CO2 Clathrate Hydrate Nanocrystals at 120 K. Journal of Physical Chemistry B, 1998, 102, 4526-4535.	1.2	29
35	Clathrateâ€"hydrate ultrafast nucleation and crystallization from supercooled aqueous nanodroplets. Chemical Physics Letters, 2010, 492, 1-8.	1.2	27
36	Glassy water Raman spectrum from a trapped laser beam. Journal of Chemical Physics, 1973, 59, 547-548.	1.2	26

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37	Infrared spectra of matrix isolated alkali metal perchlorate ion pairs. Journal of Chemical Physics, 1975, 62, 1982-1986.	1.2	26
38	Preferential deuterium bonding at the ice surface: A probe of surface water molecule mobility. Journal of Chemical Physics, 2000, 112, 5527-5529.	1.2	26
39	Covalent and Ionic States of Strong Acids at the Ice Surface. Israel Journal of Chemistry, 1999, 39, 261-272.	1.0	24
40	Controlling Nonclassical Content of Clathrate Hydrates Through the Choice of Molecular Guests and Temperature. Journal of Physical Chemistry A, 2011, 115, 5822-5832.	1.1	24
41	Rates and Mechanisms of Conversion of Ice Nanocrystals to Hydrates of HCl and HBr:Â Acid Diffusion in the Ionic Hydrates. Journal of Physical Chemistry B, 2005, 109, 3392-3401.	1.2	23
42	HCl Solvation at the Surface and within Methanol Clusters/Nanoparticles II:Â Evidence for Molecular Wires. Journal of Physical Chemistry B, 2006, 110, 21751-21763.	1.2	21
43	Catalytic activity of methanol in all-vapor subsecond clathrate-hydrate formation. Journal of Chemical Physics, 2014, 140, 164505.	1.2	21
44	Vibrational Spectra and Structures of Ionic Liquids. IV. Isotopic Dilution of the Alkali Metal and Ammonium Nitrates. Journal of Chemical Physics, 1970, 52, 2267-2273.	1.2	20
45	Infrared spectra of large clusters containing small ether molecules: Liquid, crystalline, and clathrateâ€hydrate cluster spectra. Journal of Chemical Physics, 1990, 92, 36-42.	1.2	20
46	Solvation Stages of HCl and HBr in Crystalline Phases with Methanol and Small Ethers:Â Acidâˆ'Ether Cluster Complexes in Amorphous and Crystal Phases. Journal of Physical Chemistry A, 2004, 108, 2030-2043.	1.1	20
47	Instant Conversion of Air to a Clathrate Hydrate: CO₂ Hydrates Directly from Moist Air and Moist CO₂(g). Journal of Physical Chemistry A, 2010, 114, 13129-13133.	1.1	20
48	Ion pair and partially hydrated Li+NO3âˆ' ion pair structures: Correlation of molecular orbital results with matrix isolation data. Journal of Chemical Physics, 1978, 68, 826-831.	1.2	19
49	FTâ€IR investigation of proton transfer in irradiated ice at 90 K in the absence of mobile bjerrum defects. Journal of Chemical Physics, 1984, 81, 3250-3255.	1.2	19
50	Determination of proton-transfer rates and energetics for the clathrate hydrate of oxirane by FT-IR spectroscopy. The Journal of Physical Chemistry, 1985, 89, 3552-3555.	2.9	19
51	Infrared spectrum of D2O vibrationally decoupled in glassy H2O. Journal of Chemical Physics, 1977, 67, 4779-4780.	1.2	18
52	Vibrational spectra of matrix isolated alkali metal chlorate ion pairs. Journal of Chemical Physics, 1974, 60, 2540-2546.	1.2	16
53	Direct spectroscopic observation of proton exchange and Bjerrum defect migration in cubic ice. Journal of Chemical Physics, 1980, 72, 6807-6808.	1.2	14
54	Dependence of ion pairing and solvation on solution temperature: Evidence from DMSO solution and matrixâ€solvation spectra. Journal of Chemical Physics, 1987, 86, 4391-4395.	1.2	14

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55	Ice Nanoparticles and Ice Adsorbate Interactions: FTIR Spectroscopy and Computer Simulations. Springer Series in Cluster Physics, 2003, , 425-462.	0.3	14
56	Infrared Techniques for Fused Salts. Review of Scientific Instruments, 1964, 35, 1206-1207.	0.6	13
57	Comment on â€œHCl adsorption on ice at low temperature: a combined X-ray absorption, photoemission and infrared studyâ€• by P. Parent, J. Lasne, G. Marcotte and C. Laffon, Phys. Chem. Chem. Phys., 2011,13, 7142. Physical Chemistry Chemical Physics, 2012, 14, 1048-1049.	1.3	13
58	Observation of a nonlinear photoacoustic signal with potential application to nanosecond time resolution. Applied Physics Letters, 1977, 31, 24-25.	1.5	12
59	NH3 as unique non-classical content-former within clathrate hydrates. Journal of Chemical Physics, 2017, 146, 234508.	1.2	12
60	Vibrational Spectra and Structures of Ionic Liquids. III. KNO3â€“AgNO3 Mixtures. Journal of Chemical Physics, 1968, 49, 1441-1442.	1.2	11
61	Cooperative effects in the spectra of the internal modes of molten salts. Journal of Chemical Physics, 1973, 58, 817-818.	1.2	11
62	Relating the current science of ion-defect behavior in ice to a plausible mechanism for directional charge transfer during ice particle collisions. Physical Chemistry Chemical Physics, 2011, 13, 19707.	1.3	11
63	Isotopically decoupled vibrational spectra and proton exchange rates for crystalline NH3 and ammonia hydrate. Journal of Chemical Physics, 1981, 75, 5609-5614.	1.2	10
64	Infrared spectra of gasâ€phase water microparticles: Crystalline, amorphous, and clathrateâ€“hydrate clusters of H2O, D2O, and H2O/D2O. Journal of Chemical Physics, 1989, 91, 5850-5851.	1.2	10
65	Communication: Quantitative Fourier-transform infrared data for competitive loading of small cages during all-vapor instantaneous formation of gas-hydrate aerosols. Journal of Chemical Physics, 2011, 135, 141103.	1.2	10
66	Tracking all-vapor instant gas-hydrate formation and guest molecule populations: A possible probe for molecules trapped in water nanodroplets. Journal of Chemical Physics, 2012, 137, 204501.	1.2	10
67	Theoretical study of [Li(H2O)n]+and [K(H2O)n]+(n= 1âˆ’4) complexes. International Journal of Quantum Chemistry, 1995, 53, 49-56.	1.0	9
68	Molecular Modes and Dynamics of HCl and DCl Guests of Gas Clathrate Hydrates. Journal of Physical Chemistry A, 2015, 119, 9018-9026.	1.1	9
69	NH3 as simple clathrate-hydrate catalyst: Experiment and theory. Journal of Chemical Physics, 2018, 148, 234501.	1.2	9
70	Polarized Raman Spectra of Cesium Nitrate in Solid and Molten States: The Nature of the Disordered Phases. Journal of Chemical Physics, 1972, 56, 4688-4694.	1.2	8
71	An alternate interpretation of the conductivity of HClâ€doped ice. Journal of Chemical Physics, 1988, 89, 5967-5968.	1.2	8
72	Communication: Fourier-transform infrared probing of remarkable quantities of gas trapped in cold homogeneously nucleated nanodroplets. Journal of Chemical Physics, 2013, 139, 021107.	1.2	7

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73	Spectroscopic Observation of Surface Distortion in Ionic Crystals. I. Lithium and Sodium Nitrate. Journal of Chemical Physics, 1969, 51, 302-308.	1.2	5
74	Ureyâ€Bradley ``Nonbonded'' Forces. Journal of Chemical Physics, 1963, 39, 2385-2385.	1.2	4
75	CO2 and C2H2 in cold nanodroplets of oxygenated organic molecules and water. Journal of Chemical Physics, 2014, 141, 18C506.	1.2	4
76	ATR Spectra of Crystalline LiNO3 and NaNO3. Journal of Chemical Physics, 1970, 52, 5495-5496.	1.2	3
77	Solvation studies in argon matrices: Details of the stepwise formation of Snâ‹…Li+NO3â^' ion pair solvates where S is H2O, THF, DMF, and glyme. Journal of Chemical Physics, 1985, 82, 1167-1173.	1.2	3
78	A test of the intrinsic nature of the shallow proton traps in ice. Journal of Chemical Physics, 1986, 84, 4111-4112.	1.2	3
79	MClO3 ion pairs in glassy H2O and NH3. Journal of Chemical Physics, 1974, 61, 1596-1597.	1.2	2
80	H-bonding behavior of ethylene oxide within the clathrate hydrates revisited: Experiment and theory. Chemical Physics Letters, 2020, 754, 137728.	1.2	1
81	Discussion of â€œVibrational Spectroscopic Determination of Structure and Ion Pairing in Complexes of Poly(ethylene oxide) with Lithium Saltsâ€•[B. L. Papke, M. A. Ratner, and D. F. Shriver (pp. 1434â€"1438, Vol.) Tj ETQq1 1 0.784314 rgB	1.2	0
82	Can sulfur-containing molecules solvate/ionize HCl? Solid state solvation of HCl on/in methanethiol clusters/nanoparticles. Journal of Chemical Physics, 2019, 151, 194309.	1.2	0