Laurence E Fried

List of Publications by Year
in descending order

150	6,256	66343	76900
papers	citations	42 h-index	74 g-index

163	163	163	3604
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Design and Synthesis of Energetic Materials. Annual Review of Materials Research, 2001, 31, 291-321.	9.3	402
2	Dynamic Ionization of Water under Extreme Conditions. Physical Review Letters, 2005, 94, 125508.	7.8	212
3	A Method for Tractable Dynamical Studies of Single and Double Shock Compression. Physical Review Letters, 2003, 90, 235503.	7.8	209
4	Nitrogen-Rich Heterocycles as Reactivity Retardants in Shocked Insensitive Explosives. Journal of the American Chemical Society, 2009, 131, 5483-5487.	13.7	189
5	Simulation of the intermolecular vibrational spectra of liquid water and water clusters. Journal of Chemical Physics, 1993, 98, 4413-4421.	3.0	165
6	Atomistic simulations of spinodal phase separation preceding polymer crystallization. Nature Materials, 2006, 5, 39-43.	27.5	161
7	Direct numerical simulation of shear localization and decomposition reactions in shock-loaded HMX crystal. Journal of Applied Physics, 2015, 117, .	2.5	152
8	Explicit Gibbs free energy equation of state applied to the carbon phase diagram. Physical Review B, 2000, 61, 8734-8743.	3.2	146
9	Decomposition of HMX at Extreme Conditions:Â A Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2002, 106, 9024-9029.	2.5	145
10	Generation of methane in the Earth's mantle: In situ high pressure-temperature measurements of carbonate reduction. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 14023-14026.	7.1	143
11	A transient semimetallic layer in detonating nitromethane. Nature Physics, 2008, 4, 72-76.	16.7	139
12	Semiclassical quantization using classical perturbation theory: Algebraic quantization of multidimensional systems. Journal of Chemical Physics, 1987, 86, 6270-6282.	3.0	134
13	Ultrafast pump-probe spectroscopy: femtosecond dynamics in Liouville space. The Journal of Physical Chemistry, 1989, 93, 8149-8162.	2.9	134
14	Energy Transfer Rates in Primary, Secondary, and Insensitive Explosives. The Journal of Physical Chemistry, 1994, 98, 9786-9791.	2.9	122
15	Synthesis of glycine-containing complexes in impacts of comets on early Earth. Nature Chemistry, 2010, 2, 949-954.	13.6	120
16	Ab Initio Study of RDX Decomposition Mechanisms. Journal of Physical Chemistry A, 1997, 101, 8675-8679.	2.5	109
17	Electronic excitations in shocked nitromethane. Physical Review B, 2000, 62, 16500-16509.	3.2	105
18	Early chemistry in hot and dense nitromethane: Molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 10146-10153.	3.0	103

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19	Solvation structure and the timeâ€resolved Stokes shift in nonâ€Debye solvents. Journal of Chemical Physics, 1990, 93, 932-946.	3.0	99
20	Bonding in the Superionic Phase of Water. Physical Review Letters, 2005, 94, 217801.	7.8	99
21	Catalytic behaviour of dense hot water. Nature Chemistry, 2009, 1, 57-62.	13.6	95
22	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	3.0	91
23	Ab initio based force field and molecular dynamics simulations of crystalline TATB. Journal of Chemical Physics, 2004, 120, 7059-7066.	3.0	90
24	Ring Closure Mediated by Intramolecular Hydrogen Transfer in the Decomposition of a Pushâ^'Pull Nitroaromatic:Â TATB. Journal of Physical Chemistry A, 2000, 104, 6447-6452.	2.5	87
25	Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression. Journal of Chemical Physics, 2008, 128, 184701.	3.0	84
26	An accurate equation of state for the exponential-6 fluid applied to dense supercritical nitrogen. Journal of Chemical Physics, 1998, 109, 7338-7348.	3.0	79
27	Electronic structure of solid 1,3,5-triamino-2,4,6-trinitrobenzene under uniaxial compression: Possible role of pressure-induced metallization in energetic materials. Physical Review B, 2003, 67, .	3.2	77
28	Semiclassical quantization of polyatomic molecules: some recent developments. The Journal of Physical Chemistry, 1987, 91, 3721-3730.	2.9	71
29	High Explosive Ignition through Chemically Activated Nanoscale Shear Bands. Physical Review Letters, 2020, 124, 206002.	7.8	70
30	Structure, dynamics, and the electronic absorption of benzeneâ€“argon clusters. Journal of Chemical Physics, 1992, 96, 116-135.	3.0	68
31	Polymerization of Formic Acid under High Pressure. Physical Review Letters, 2005, 94, 065505.	7.8	62
32	ChIMES: A Force Matched Potential with Explicit Three-Body Interactions for Molten Carbon. Journal of Chemical Theory and Computation, 2017, 13, 6222-6229.	5.3	54
33	BKWC: An Empirical BKW Parametrization Based on Cylinder Test data. Propellants, Explosives, Pyrotechnics, 1996, 21, 215-223.	1.6	53
34	Analysis of simulation technique for steady shock waves in materials with analytical equations of state. Physical Review E, 2006, 74, 056706.	2.1	52
35	Simulation of the femtosecond optical response of a solute in water. Physical Review Letters, 1992, 68, 1842-1845.	7.8	50
36	Detonation synthesis of carbon nano-onions via liquid carbon condensation. Nature Communications, 2019, 10, 3819.	12.8	50

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37	DFT and ab Initio Study of the Unimolecular Decomposition of the Lowest Singlet and Triplet States of Nitromethane. Journal of Physical Chemistry A, 1998, 102, 9884-9889.	2.5	49
38	A classical theory of pumpâ€“probe photodissociation for arbitrary pulse durations. Journal of Chemical Physics, 1990, 93, 3063-3071.	3.0	46
39	Nearly Equivalent Inter- and Intramolecular Hydrogen Bonding in 1,3,5-Triamino-2,4,6-trinitrobenzene at High Pressure. Journal of Physical Chemistry C, 2012, 116, 2116-2122.	3.1	46
40	Simulation of Nonlinear Electronic Spectroscopy in the Condensed Phase. Advances in Chemical Physics, 2007, , 435-516.	0.3	45
41	Molecular Dynamics Investigation of Adhesion between TATB Surfaces and Amorphous Fluoropolymers. Macromolecules, 2007, 40, 3422-3428.	4.8	45
42	Dissociative melting of ice VII at high pressure. Journal of Chemical Physics, 2009, 130, 124514.	3.0	45
43	Intersystem Crossings in Model Energetic Materials. Journal of Physical Chemistry A, 1999, 103, 9349-9354.	2.5	43
44	Explosive chemistry: Simulating the chemistry of energetic materials at extreme conditions. Journal of Computer-Aided Materials Design, 2003, 10, 75-97.	0.7	40
45	Heterogeneous directional mobility in the early stages of polymer crystallization. Journal of Chemical Physics, 2008, 128, 014903.	3.0	40
46	Quantum mechanical corrections to simulated shock Hugoniot temperatures. Journal of Chemical Physics, 2009, 131, 204103.	3.0	40
47	Ultrafast Detonation of Hydrazoic Acid (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 352 Td (xmlns:mml="http://www.v3 Physical Review Letters, 2012, 109, 038301.	7.8	40
48	PERTURB: A program for calculating vibrational energies by generalized algebraic quantization. Computer Physics Communications, 1988, 51, 103-114.	7.5	39
49	Melting and the electronic absorption of benzene-argon clusters. Physical Review Letters, 1991, 66, 2340-2343.	7.8	38
50	Monte Carlo simulations of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB): Pressure and temperature effects for the solid phase and vapor-liquid phase equilibria. Journal of Chemical Physics, 2008, 129, 194510.	3.0	37
51	The Microstructure of TATBâ€Based Explosive Formulations During Temperature Cycling Using Ultraâ€Smallâ€Angle Xâ€Ray Scattering. Propellants, Explosives, Pyrotechnics, 2009, 34, 406-414.	1.6	36
52	The solubility and recrystallization of 1,3,5-triamino-2,4,6-trinitrobenzene in a 3-ethyl-1-methylimidazolium acetateâ€“DMSO co-solvent system. New Journal of Chemistry, 2009, 33, 50-56.	2.8	36
53	First-principles high-pressure unreacted equation of state and heat of formation of crystal 2,6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105). Journal of Chemical Physics, 2014, 141, 064702.	3.0	36
54	Pressure-induced phase transition in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Applied Physics Letters, 2019, 114, .	3.3	34

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55	Molecular interactions of TATB clusters. Chemical Physics Letters, 2003, 374, 286-296.	2.6	33
56	New theoretical insight into the interactions and properties of formic acid: Development of a quantum-based pair potential for formic acid. Journal of Chemical Physics, 2005, 123, 144702.	3.0	33
57	Modeling pore collapse and chemical reactions in shock-loaded HMX crystals. Journal of Physics: Conference Series, 2014, 500, 052002.	0.4	33
58	Ultrafast dynamic response of single-crystal Î²-HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine). Journal of Applied Physics, 2018, 123, .	2.5	33
59	Ultrafast shock synthesis of nanocarbon from a liquid precursor. Nature Communications, 2020, 11, 353.	12.8	33
60	Chemical Equilibrium Detonation. , 2012, , 1-31.		32
61	An improved thermodynamic energy estimator for path integral simulations. Journal of Chemical Physics, 2002, 116, 5951-5955.	3.0	31
62	Improved heat capacity estimator for path integral simulations. Journal of Chemical Physics, 2002, 117, 3020-3026.	3.0	31
63	Ultrafast crystallization of polar polymer melts. Journal of Chemical Physics, 2003, 118, 3827-3834.	3.0	31
64	Structure of Chlorotrifluoroethylene/Vinylidene Fluoride Random Copolymers and Homopolymers by Molecular Dynamics Simulations. Macromolecules, 2001, 34, 3050-3059.	4.8	30
65	Internal Rotation of Amino and Nitro Groups in TATB:Â MP2 Versus DFT (B3LYP). Journal of Physical Chemistry A, 2002, 106, 8806-8810.	2.5	30
66	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. Journal of Physical Chemistry C, 2012, 116, 2198-2204.	3.1	29
67	Mesoscale modeling of irreversible volume growth in powders of anisotropic crystals. Applied Physics Letters, 2007, 90, 254105.	3.3	28
68	Anomalous sound propagation and slow kinetics in dynamically compressed amorphous carbon. Physical Review E, 2010, 81, 016607.	2.1	28
69	Determination of a Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Carbon Under Extreme Pressures and Temperatures. Journal of Physical Chemistry C, 2013, 117, 7885-7894.	3.1	28
70	Using Force-Matched Potentials To Improve the Accuracy of Density Functional Tight Binding for Reactive Conditions. Journal of Chemical Theory and Computation, 2015, 11, 4530-4535.	5.3	28
71	Development of a Multicenter Density Functional Tight Binding Model for Plutonium Surface Hydriding. Journal of Chemical Theory and Computation, 2018, 14, 2652-2660.	5.3	27
72	Generalized algebraic quantization: corrections to arbitrary order in Planck's constant. The Journal of Physical Chemistry, 1988, 92, 3144-3154.	2.9	26

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73	Detonation Energies from the Cylinder Test and CHEETAH V3.0. Propellants, Explosives, Pyrotechnics, 2001, 26, 180.	1.6	26
74	Avoided crossings and resummation of nearly resonant molecular vibrations: Reconstruction of an effective secular equation. Journal of Chemical Physics, 1989, 90, 6378-6390.	3.0	25
75	Internal Rotation in Energetic Systems:Â TATB. Journal of Physical Chemistry A, 2001, 105, 6765-6768.	2.5	25
76	A Multi-Scale Approach to Molecular Dynamics Simulations of Shock Waves. , 2005, , 297-326.		25
77	Solvent screening for a hard-to-dissolve molecular crystal. Physical Chemistry Chemical Physics, 2008, 10, 5050.	2.8	25
78	Nanosecond Time-Resolved and Steady-State Infrared Studies of Photoinduced Decomposition of TATB at Ambient and Elevated Pressure. Journal of Physical Chemistry A, 2009, 113, 5881-5887.	2.5	25
79	Exp6-polar thermodynamics of dense supercritical water. Journal of Chemical Physics, 2008, 128, 174502.	3.0	24
80	Using Force Matching To Determine Reactive Force Fields for Water under Extreme Thermodynamic Conditions. Journal of Chemical Theory and Computation, 2017, 13, 135-146.	5.3	24
81	A path integral approach to molecular thermochemistry. Journal of Chemical Physics, 2003, 118, 1596-1603.	3.0	23
82	Tailored ramp-loading via shock release of stepped-density reservoirs. Physics of Plasmas, 2012, 19, .	1.9	23
83	Application of the ChIMES Force Field to Nonreactive Molecular Systems: Water at Ambient Conditions. Journal of Chemical Theory and Computation, 2019, 15, 436-447.	5.3	23
84	Active learning for robust, high-complexity reactive atomistic simulations. Journal of Chemical Physics, 2020, 153, 134117.	3.0	21
85	Submicrosecond Aggregation during Detonation Synthesis of Nanodiamond. Journal of Physical Chemistry Letters, 2021, 12, 5286-5293.	4.6	21
86	Towards unraveling the photochemistry of TATB. Thermochimica Acta, 2002, 384, 85-90.	2.7	20
87	Irreversible volume growth in polymer-bonded powder systems: Effects of crystalline anisotropy, particle size distribution, and binder strength. Journal of Applied Physics, 2008, 103, 053504.	2.5	18
88	Resolving Detonation Nanodiamond Size Evolution and Morphology at Sub-Microsecond Timescales during High-Explosive Detonations. Journal of Physical Chemistry C, 2019, 123, 19153-19164.	3.1	18
89	The Reactivity of Energetic Materials Under High Pressure and Temperature. Advances in Quantum Chemistry, 2014, , 221-252.	0.8	17
90	Many-body reactive force field development for carbon condensation in C/O systems under extreme conditions. Journal of Chemical Physics, 2020, 153, 054103.	3.0	17

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91	Shock Hugoniot measurements of single-crystal 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) compressed to 83â€‰GPa. Journal of Applied Physics, 2020, 127, .	2.5	17
92	The equation of state of supercritical HF, HCl, and reactive supercritical mixtures containing the elements H, C, F, and Cl. Journal of Chemical Physics, 1999, 110, 12023-12032.	3.0	16
93	Semi-Automated Creation of Density Functional Tight Binding Models through Leveraging Chebyshev Polynomial-Based Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 4435-4448.	5.3	16
94	First principles simulation of a superionic phase of hydrogen fluoride (HF) at high pressures and temperatures. Journal of Chemical Physics, 2006, 125, 044501.	3.0	15
95	Determination of enthalpies of formation of energetic molecules with composite quantum chemical methods. Chemical Physics Letters, 2016, 648, 31-35.	2.6	15
96	Understanding the solubility of triamino-trinitrobenzene in hydrous tetramethylammonium fluoride: a first principles molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2012, 14, 4884.	2.8	14
97	Calculation of the detonation state of HN3 with quantum accuracy. Journal of Chemical Physics, 2020, 153, 224102.	3.0	14
98	Quantitative molecular thermochemistry based on path integrals. Journal of Chemical Physics, 2005, 123, 034103.	3.0	12
99	Phase separation in H2O:N2 mixture: Molecular dynamics simulations using atomistic force fields. Journal of Chemical Physics, 2007, 126, 044510.	3.0	12
100	X-ray scattering intensities of water at extreme pressure and temperature. Journal of Chemical Physics, 2007, 126, 134505.	3.0	12
101	Computational study of 3-D hot-spot initiation in shocked insensitive high-explosive. , 2012, , .		12
102	Investigating 3,4-bis(3-nitrofurazan-4-yl)furoxan detonation with a rapidly tuned density functional tight binding model. Journal of Chemical Physics, 2021, 154, 164115.	3.0	12
103	High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set. Journal of Physical Chemistry Letters, 2022, 13, 2934-2942.	4.6	12
104	Observation of Variations in Condensed Carbon Morphology Dependent on Composition B Detonation Conditions. Propellants, Explosives, Pyrotechnics, 2020, 45, 347-355.	1.6	11
105	Anisotropic strength behavior of single-crystal TATB. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 014004.	2.0	10
106	PERTURB: A special-purpose algebraic manipulation program for classical perturbation theory. Journal of Computational Chemistry, 1987, 8, 397-411.	3.3	9
107	MEASURED SOUND VELOCITIES OF H2O AND CH3OH. High Pressure Research, 2003, 23, 229-233.	1.2	9
108	New phases of hydrogen-bonded systems at extreme conditions. Phase Transitions, 2007, 80, 1073-1084.	1.3	9

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109	Recent Advances in Modeling Hugoniots with Cheetah. AIP Conference Proceedings, 2006, , .	0.4	8
110	The role of viscosity in TATB hot spot ignition. , 2012, , .		7
111	Understanding the anisotropic initiation sensitivity of shocked pentaerythritol tetranitrate single crystals. Applied Physics Letters, 2013, 103, 131912.	3.3	7
112	The equation of state and chemistry of detonation products. Theoretical and Computational Chemistry, 2003, , 193-224.	0.4	6
113	Application of the TraPPE Force Field to Predicting Isothermal Pressureâ€“Volume Curves at High Pressures and High Temperatures. International Journal of Thermophysics, 2007, 28, 796-804.	2.1	6
114	Double shock experiments and reactive flow modeling on LX-17 to understand the reacted equation of state. Journal of Physics: Conference Series, 2014, 500, 052047.	0.4	6
115	Electronic Excitations, Vibrational Spectra, and Chemistry in Nitromethane and HMX. AIP Conference Proceedings, 2002, , .	0.4	5
116	Science at LLNL with IBM Blue Gene/Q. IBM Journal of Research and Development, 2013, 57, 11:1-11:18.	3.1	5
117	Grain-Scale Simulation of Shock Initiation in Composite High Explosives. Challenges and Advances in Computational Chemistry and Physics, 2017, , 243-270.	0.6	5
118	Force Matching Approaches to Extend Density Functional Theory to Large Time and Length Scales. Challenges and Advances in Computational Chemistry and Physics, 2019, , 71-93.	0.6	5
119	Energy Transfer Dynamics and Impact Sensitivity. Materials Research Society Symposia Proceedings, 1992, 296, 35.	0.1	4
120	Improved woodâ€“kirkwood detonation chemical kinetics. Theoretical Chemistry Accounts, 2008, 120, 37-43.	1.4	4
121	GRAIN-SCALE SIMULATIONS OF HOT-SPOT INITIATION FOR SHOCKED TATB. , 2009, , .		4
122	High-pressure isothermal equation of state of composite materials: A case study of LX-17 polymer bonded explosive. Applied Physics Letters, 2019, 115, 051902.	3.3	4
123	Simulating transient heat transfer in graphene at finite Knudsen number via the Boltzmann transport equation and molecular dynamics. Physical Review B, 2020, 102, .	3.2	4
124	Chemistry-mediated Ostwald ripening in carbon-rich C/O systems at extreme conditions. Nature Communications, 2022, 13, 1424.	12.8	4
125	Machineâ€Learning a Solution for Reactive Atomistic Simulations of Energetic Materials. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	4
126	Nitrous acid under high temperature and pressure â€“ From atomistic simulations to equation of state for thermochemical modeling. Chemical Physics Letters, 2009, 468, 197-200.	2.6	3

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127	Study of thermal sensitivity and thermal explosion violence of energetic materials in the LLNL ODTX system. Journal of Physics: Conference Series, 2014, 500, 052019.	0.4	3
128	Reactive flow modeling of the polymer bonded explosive LX-17 double shock experiments. Journal of Applied Physics, 2018, 124, .	2.5	3
129	Hugoniot Constraint Molecular Dynamics Study of a Transformation to a Metastable Phase in Shocked Silicon. AIP Conference Proceedings, 2002, , .	0.4	2
130	Tight Binding Molecular Dynamic Simulation of PETN Decomposition at An Extreme Condition. Materials Research Society Symposia Proceedings, 2006, 987, 1.	0.1	2
131	AB INITIO MOLECULAR DYNAMICS SIMULATIONS OF WATER UNDER STATIC AND SHOCK COMPRESSED CONDITIONS. AIP Conference Proceedings, 2008, , .	0.4	2
132	Experimental Measurement of Speeds of Sound in Dense Supercritical Carbon Monoxide and Development of a High-Pressure, High-Temperature Equation of State. Journal of Physical Chemistry B, 2013, 117, 5675-5682.	2.6	2
133	Quantum molecular dynamics simulations of liquid benzene using orbital optimization. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	2
134	Ultrafast dynamic response of single crystal Î²-HMX. AIP Conference Proceedings, 2017, , .	0.4	2
135	Nonlinear optical properties of confined excitons in clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 126-130.	1.0	1
136	Calculation of Chemical Detonation Waves with Hydrodynamics and a Thermochemical Equation of State. AIP Conference Proceedings, 2002, , .	0.4	1
137	Simulations of Fluid Nitromethane under Extreme Conditions. AIP Conference Proceedings, 2004, , .	0.4	1
138	A TRANSIENT SEMI-METALLIC LAYER IN DETONATING NITROMETHANE. , 2008, , .		1
139	Chemistry resolved kinetic flow modeling of TATB based explosives. , 2012, , .		1
140	Double shock experiments performed at -55Â°C on LX-17 with reactive flow modeling to understand the reacted equation of state. AIP Conference Proceedings, 2018, , .	0.4	1
141	Solvation Structure in the Time Resolved Stokes Shift and Adiabatic Electron Transfer. Molecular Crystals and Liquid Crystals, 1991, 194, 263-268.	0.7	0
142	Kinetic calculations of explosives with slow-burning constituents. , 1998, , .		0
143	The equation of state of HF under shock compression. AIP Conference Proceedings, 2000, , .	0.4	0
144	Detonation Product EOS Studies: Using ISLS to Refine Cheetah. AIP Conference Proceedings, 2002, , .	0.4	0

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145	Sparse Partial Equilibrium Tables in Chemically Resolved Reactive Flow. AIP Conference Proceedings, 2004, , .	0.4	0
146	The Equation of State and Chemistry at Extreme Conditions. , 2005, , 399-429.		0
147	Chemistry of H2O and HF under Extreme Conditions. AIP Conference Proceedings, 2006, , .	0.4	0
148	NUCLEAR QUANTUM VIBRATIONAL EFFECTS IN SHOCK HUGONIOT TEMPERATURES. , 2009, , .		0
149	Detonation theory for condensed phase explosives with anisotropic properties. , 2012, , .		0
150	Simulation of the Ultrafast Optical Response of Water. Springer Proceedings in Physics, 1992, , 295-298.	0.2	0