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	Anisotropic strength behavior of single-crystal TATB. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 014004.	2.0	10
2	Chemistry-mediated Ostwald ripening in carbon-rich C/O systems at extreme conditions. Nature Communications, 2022, 13, 1424.	12.8	4
3	High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set. Journal of Physical Chemistry Letters, 2022, 13, 2934-2942.	4.6	12
4	Machineâ€Learning a Solution for Reactive Atomistic Simulations of Energetic Materials. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	4
5	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
6	Submicrosecond Aggregation during Detonation Synthesis of Nanodiamond. Journal of Physical Chemistry Letters, 2021, 12, 5286-5293.	4.6	21
7	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
8	Active learning for robust, high-complexity reactive atomistic simulations. Journal of Chemical Physics, 2020, 153, 134117.	3.0	21
9	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
10	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
11	Calculation of the detonation state of HN3 with quantum accuracy. Journal of Chemical Physics, 2020, 153, 224102.	3.0	14
12	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
13	Ultrafast shock synthesis of nanocarbon from a liquid precursor. Nature Communications, 2020, 11, 353.	12.8	33
14	Observation of Variations in Condensed Carbon Morphology Dependent on Composition B Detonation Conditions. Propellants, Explosives, Pyrotechnics, 2020, 45, 347-355.	1.6	11
15	High Explosive Ignition through Chemically Activated Nanoscale Shear Bands. Physical Review Letters, 2020, 124, 206002.	7.8	70
16	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
17	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
18	Detonation synthesis of carbon nano-onions via liquid carbon condensation. Nature Communications, 2019, 10, 3819.	12.8	50

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19	Pressure-induced phase transition in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Applied Physics Letters, 2019, 114, .	3.3	34
20	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
21	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
22	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
23	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
24	Reactive flow modeling of the polymer bonded explosive LX-17 double shock experiments. Journal of Applied Physics, 2018, 124, .	2.5	3
25	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
26	Ultrafast dynamic response of single crystal Î²-HMX. AIP Conference Proceedings, 2017, , .	0.4	2
27	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
28	Grain-Scale Simulation of Shock Initiation in Composite High Explosives. Challenges and Advances in Computational Chemistry and Physics, 2017, , 243-270.	0.6	5
29	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
30	Determination of enthalpies of formation of energetic molecules with composite quantum chemical methods. Chemical Physics Letters, 2016, 648, 31-35.	2.6	15
31	Direct numerical simulation of shear localization and decomposition reactions in shock-loaded HMX crystal. Journal of Applied Physics, 2015, 117, .	2.5	152
32	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
33	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
34	Modeling pore collapse and chemical reactions in shock-loaded HMX crystals. Journal of Physics: Conference Series, 2014, 500, 052002.	0.4	33
35	The Reactivity of Energetic Materials Under High Pressure and Temperature. Advances in Quantum Chemistry, 2014, , 221-252.	0.8	17
36	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

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37	Quantum molecular dynamics simulations of liquid benzene using orbital optimization. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	2
38	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
39	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
40	Science at LLNL with IBM Blue Gene/Q. IBM Journal of Research and Development, 2013, 57, 11:1-11:18.	3.1	5
41	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
42	Understanding the anisotropic initiation sensitivity of shocked pentaerythritol tetranitrate single crystals. Applied Physics Letters, 2013, 103, 131912.	3.3	7
43	Detonation theory for condensed phase explosives with anisotropic properties. , 2012, , .		0
44	Computational study of 3-D hot-spot initiation in shocked insensitive high-explosive. , 2012, , .		12
45	Chemistry resolved kinetic flow modeling of TATB based explosives. , 2012, , .		1
46	Ultrafast Detonation of Hydrazoic Acid (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 392 Td (xmlns:mml="http://www.w3.org/199 Physical Review Letters, 2012, 109, 038301.	7.8	40
47	Tailored ramp-loading via shock release of stepped-density reservoirs. Physics of Plasmas, 2012, 19, .	1.9	23
48	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
49	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
50	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. Journal of Physical Chemistry C, 2012, 116, 2198-2204.	3.1	29
51	Chemical Equilibrium Detonation. , 2012, , 1-31.		32
52	The role of viscosity in TATB hot spot ignition. , 2012, , .		7
53	Synthesis of glycine-containing complexes in impacts of comets on early Earth. Nature Chemistry, 2010, 2, 949-954.	13.6	120
54	Anomalous sound propagation and slow kinetics in dynamically compressed amorphous carbon. Physical Review E, 2010, 81, 016607.	2.1	28

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55	Quantum mechanical corrections to simulated shock Hugoniot temperatures. Journal of Chemical Physics, 2009, 131, 204103.	3.0	40
56	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	3.0	91
57	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
58	Catalytic behaviour of dense hot water. Nature Chemistry, 2009, 1, 57-62.	13.6	95
59	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
60	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
61	GRAIN-SCALE SIMULATIONS OF HOT-SPOT INITIATION FOR SHOCKED TATB. , 2009, , .		4
62	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
63	Dissociative melting of ice VII at high pressure. Journal of Chemical Physics, 2009, 130, 124514.	3.0	45
64	Nitrogen-Rich Heterocycles as Reactivity Retardants in Shocked Insensitive Explosives. Journal of the American Chemical Society, 2009, 131, 5483-5487.	13.7	189
65	NUCLEAR QUANTUM VIBRATIONAL EFFECTS IN SHOCK HUGONIOT TEMPERATURES. , 2009, , .		0
66	Improved woodâ€“kirkwood detonation chemical kinetics. Theoretical Chemistry Accounts, 2008, 120, 37-43.	1.4	4
67	A transient semimetallic layer in detonating nitromethane. Nature Physics, 2008, 4, 72-76.	16.7	139
68	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
69	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
70	Solvent screening for a hard-to-dissolve molecular crystal. Physical Chemistry Chemical Physics, 2008, 10, 5050.	2.8	25
71	Heterogeneous directional mobility in the early stages of polymer crystallization. Journal of Chemical Physics, 2008, 128, 014903.	3.0	40
72	Exp6-polar thermodynamics of dense supercritical water. Journal of Chemical Physics, 2008, 128, 174502.	3.0	24

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73	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
74	AB INITIO MOLECULAR DYNAMICS SIMULATIONS OF WATER UNDER STATIC AND SHOCK COMPRESSED CONDITIONS. AIP Conference Proceedings, 2008, , .	0.4	2
75	A TRANSIENT SEMI-METALLIC LAYER IN DETONATING NITROMETHANE. , 2008, , .		1
76	Phase separation in H2O:N2 mixture: Molecular dynamics simulations using atomistic force fields. Journal of Chemical Physics, 2007, 126, 044510.	3.0	12
77	Simulation of Nonlinear Electronic Spectroscopy in the Condensed Phase. Advances in Chemical Physics, 2007, , 435-516.	0.3	45
78	Mesoscale modeling of irreversible volume growth in powders of anisotropic crystals. Applied Physics Letters, 2007, 90, 254105.	3.3	28
79	New phases of hydrogen-bonded systems at extreme conditions. Phase Transitions, 2007, 80, 1073-1084.	1.3	9
80	X-ray scattering intensities of water at extreme pressure and temperature. Journal of Chemical Physics, 2007, 126, 134505.	3.0	12
81	Molecular Dynamics Investigation of Adhesion between TATB Surfaces and Amorphous Fluoropolymers. Macromolecules, 2007, 40, 3422-3428.	4.8	45
82	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
83	Analysis of simulation technique for steady shock waves in materials with analytical equations of state. Physical Review E, 2006, 74, 056706.	2.1	52
84	Tight Binding Molecular Dynamic Simulation of PETN Decomposition at An Extreme Condition. Materials Research Society Symposia Proceedings, 2006, 987, 1.	0.1	2
85	Atomistic simulations of spinodal phase separation preceding polymer crystallization. Nature Materials, 2006, 5, 39-43.	27.5	161
86	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
87	Chemistry of H2O and HF under Extreme Conditions. AIP Conference Proceedings, 2006, , .	0.4	0
88	Recent Advances in Modeling Hugoniots with Cheetah. AIP Conference Proceedings, 2006, , .	0.4	8
89	A Multi-Scale Approach to Molecular Dynamics Simulations of Shock Waves. , 2005, , 297-326.		25
90	The Equation of State and Chemistry at Extreme Conditions. , 2005, , 399-429.		0

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91	Quantitative molecular thermochemistry based on path integrals. Journal of Chemical Physics, 2005, 123, 034103.	3.0	12
92	Polymerization of Formic Acid under High Pressure. Physical Review Letters, 2005, 94, 065505.	7.8	62
93	Dynamic Ionization of Water under Extreme Conditions. Physical Review Letters, 2005, 94, 125508.	7.8	212
94	Bonding in the Superionic Phase of Water. Physical Review Letters, 2005, 94, 217801.	7.8	99
95	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
96	Simulations of Fluid Nitromethane under Extreme Conditions. AIP Conference Proceedings, 2004, , .	0.4	1
97	Ab initio based force field and molecular dynamics simulations of crystalline TATB. Journal of Chemical Physics, 2004, 120, 7059-7066.	3.0	90
98	Early chemistry in hot and dense nitromethane: Molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 10146-10153.	3.0	103
99	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
100	Sparse Partial Equilibrium Tables in Chemically Resolved Reactive Flow. AIP Conference Proceedings, 2004, , .	0.4	0
101	Explosive chemistry: Simulating the chemistry of energetic materials at extreme conditions. Journal of Computer-Aided Materials Design, 2003, 10, 75-97.	0.7	40
102	Molecular interactions of TATB clusters. Chemical Physics Letters, 2003, 374, 286-296.	2.6	33
103	A Method for Tractable Dynamical Studies of Single and Double Shock Compression. Physical Review Letters, 2003, 90, 235503.	7.8	209
104	MEASURED SOUND VELOCITIES OF H2O AND CH3OH. High Pressure Research, 2003, 23, 229-233.	1.2	9
105	Ultrafast crystallization of polar polymer melts. Journal of Chemical Physics, 2003, 118, 3827-3834.	3.0	31
106	A path integral approach to molecular thermochemistry. Journal of Chemical Physics, 2003, 118, 1596-1603.	3.0	23
107	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
108	The equation of state and chemistry of detonation products. Theoretical and Computational Chemistry, 2003, , 193-224.	0.4	6

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109	An improved thermodynamic energy estimator for path integral simulations. Journal of Chemical Physics, 2002, 116, 5951-5955.	3.0	31
110	Hugoniot Constraint Molecular Dynamics Study of a Transformation to a Metastable Phase in Shocked Silicon. AIP Conference Proceedings, 2002, , .	0.4	2
111	Calculation of Chemical Detonation Waves with Hydrodynamics and a Thermochemical Equation of State. AIP Conference Proceedings, 2002, , .	0.4	1
112	Detonation Product EOS Studies: Using ISLS to Refine Cheetah. AIP Conference Proceedings, 2002, , .	0.4	0
113	Decomposition of HMX at Extreme Conditions:Â A Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2002, 106, 9024-9029.	2.5	145
114	Improved heat capacity estimator for path integral simulations. Journal of Chemical Physics, 2002, 117, 3020-3026.	3.0	31
115	Electronic Excitations, Vibrational Spectra, and Chemistry in Nitromethane and HMX. AIP Conference Proceedings, 2002, , .	0.4	5
116	Towards unraveling the photochemistry of TATB. Thermochimica Acta, 2002, 384, 85-90.	2.7	20
117	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
118	Structure of Chlorotrifluoroethylene/Vinylidene Fluoride Random Copolymers and Homopolymers by Molecular Dynamics Simulations. Macromolecules, 2001, 34, 3050-3059.	4.8	30
119	Design and Synthesis of Energetic Materials. Annual Review of Materials Research, 2001, 31, 291-321.	9.3	402
120	Detonation Energies from the Cylinder Test and CHEETAH V3.0. Propellants, Explosives, Pyrotechnics, 2001, 26, 180.	1.6	26
121	Internal Rotation in Energetic Systems:Â TATB. Journal of Physical Chemistry A, 2001, 105, 6765-6768.	2.5	25
122	The equation of state of HF under shock compression. AIP Conference Proceedings, 2000, , .	0.4	0
123	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
124	Electronic excitations in shocked nitromethane. Physical Review B, 2000, 62, 16500-16509.	3.2	105
125	Explicit Gibbs free energy equation of state applied to the carbon phase diagram. Physical Review B, 2000, 61, 8734-8743.	3.2	146
126	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

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127	Intersystem Crossings in Model Energetic Materials. Journal of Physical Chemistry A, 1999, 103, 9349-9354.	2.5	43
128	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
129	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
130	Kinetic calculations of explosives with slow-burning constituents. , 1998, , .		0
131	Ab Initio Study of RDX Decomposition Mechanisms. Journal of Physical Chemistry A, 1997, 101, 8675-8679.	2.5	109
132	BKWC: An Empirical BKW Parametrization Based on Cylinder Test data. Propellants, Explosives, Pyrotechnics, 1996, 21, 215-223.	1.6	53
133	Energy Transfer Rates in Primary, Secondary, and Insensitive Explosives. The Journal of Physical Chemistry, 1994, 98, 9786-9791.	2.9	122
134	Nonlinear optical properties of confined excitons in clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 126-130.	1.0	1
135	Simulation of the intermolecular vibrational spectra of liquid water and water clusters. Journal of Chemical Physics, 1993, 98, 4413-4421.	3.0	165
136	Simulation of the femtosecond optical response of a solute in water. Physical Review Letters, 1992, 68, 1842-1845.	7.8	50
137	Structure, dynamics, and the electronic absorption of benzeneâ€“argon clusters. Journal of Chemical Physics, 1992, 96, 116-135.	3.0	68
138	Energy Transfer Dynamics and Impact Sensitivity. Materials Research Society Symposia Proceedings, 1992, 296, 35.	0.1	4
139	Simulation of the Ultrafast Optical Response of Water. Springer Proceedings in Physics, 1992, , 295-298.	0.2	0
140	Melting and the electronic absorption of benzene-argon clusters. Physical Review Letters, 1991, 66, 2340-2343.	7.8	38
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	Solvation structure and the timeâ€resolved Stokes shift in nonâ€Debye solvents. Journal of Chemical Physics, 1990, 93, 932-946.	3.0	99
143	A classical theory of pumpâ€“probe photodissociation for arbitrary pulse durations. Journal of Chemical Physics, 1990, 93, 3063-3071.	3.0	46
144	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

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145	Ultrafast pump-probe spectroscopy: femtosecond dynamics in Liouville space. The Journal of Physical Chemistry, 1989, 93, 8149-8162.	2.9	134
146	PERTURB: A program for calculating vibrational energies by generalized algebraic quantization. Computer Physics Communications, 1988, 51, 103-114.	7.5	39
147	Generalized algebraic quantization: corrections to arbitrary order in Planck's constant. The Journal of Physical Chemistry, 1988, 92, 3144-3154.	2.9	26
148	Semiclassical quantization of polyatomic molecules: some recent developments. The Journal of Physical Chemistry, 1987, 91, 3721-3730.	2.9	71
149	Semiclassical quantization using classical perturbation theory: Algebraic quantization of multidimensional systems. Journal of Chemical Physics, 1987, 86, 6270-6282.	3.0	134
150	PERTURB: A special-purpose algebraic manipulation program for classical perturbation theory. Journal of Computational Chemistry, 1987, 8, 397-411.	3.3	9