Michael L Klein

List of Publications by Year
in descending order

197 papers	59,070 citations	16451 64 h-index	2571 195 g-index
199 all docs	199 docs citations	199 times ranked	46489 citing authors

#	Article	IF	Citations
1	Dissolving salt is not equivalent to applying a pressure on water. Nature Communications, 2022, 13, 822.	12.8	41
2	SPICA Force Field for Proteins and Peptides. Journal of Chemical Theory and Computation, 2022, 18, 3204-3217.	5.3	21
3	Potential Pro-Inflammatory Effect of Vitamin E Analogs through Mitigation of Tetrahydrocannabinol (THC) Binding to the Cannabinoid 2 Receptor. International Journal of Molecular Sciences, 2022, 23, 4291.	4.1	2
4	Effect of water frustration on water oxidation catalysis in the nanoconfined interlayers of layered manganese oxides birnessite and buserite. Journal of Materials Chemistry A, 2021, 9, 6924-6932.	10.3	15
5	Importance of nuclear quantum effects on the hydration of chloride ion. Physical Review Materials, 2021, 5, .	2.4	11
6	Chain-End Modification: A Starting Point for Controlling Polymer Crystal Nucleation. Macromolecules, 2021, 54, 1599-1610.	4.8	8
7	Targeting SARS-CoV-2 M3CLpro by HCV NS3/4a Inhibitors: In Silico Modeling and In Vitro Screening. Journal of Chemical Information and Modeling, 2021, 61, 1020-1032.	5.4	25
8	Investigations of water/oxide interfaces by molecular dynamics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1537.	14.6	21
9	Discovery of Novel Small-Molecule Inhibitors of SARS-CoV-2 Main Protease as Potential Leads for COVID-19 Treatment. Journal of Chemical Information and Modeling, 2021, 61, 4745-4757.	5.4	12
10	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	2.6	40
11	First-Principles Calculation of Water pK_a Using the Newly Developed SCAN Functional. Journal of Physical Chemistry Letters, 2020, 11, 54-59.	4.6	19
12	Property Decoupling across the Embryonic Nucleusâ€“Melt Interface during Polymer Crystal Nucleation. Journal of Physical Chemistry B, 2020, 124, 4793-4804.	2.6	12
13	A new perspective on lone pair dynamics in halide perovskites. APL Materials, 2020, 8, .	5.1	16
14	Monodisperse Polymer Melts Crystallize via Structurally Polydisperse Nanoscale Clusters: Insights from Polyethylene. Polymers, 2020, 12, 447.	4.5	6
15	Lone Pair Rotational Dynamics in Solids. Physical Review Letters, 2020, 124, 066001.	7.8	12
16	Molecular Simulation of Covalent Bond Dynamics in Liquid Silicon. Journal of Physical Chemistry B, 2020, 124, 3180-3185.	2.6	5
17	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq1 1 0.784314 rgBT /Overl	2.4	7
18	Defect-enriched tunability of electronic and charge-carrier transport characteristics of 2D borocarbonitride (BCN) monolayers from ab initio calculations. Nanoscale, 2019, 11, 19398-19407.	5.6	18

#	Article	IF	Citations
19	Halogen Bond Structure and Dynamics from Molecular Simulations. Journal of Physical Chemistry B, 2019, 123, 6266-6273.	2.6	10
20	Suppression of Zika Virus Infection in the Brain by the Antiretroviral Drug Rilpivirine. Molecular Therapy, 2019, 27, 2067-2079.	8.2	20
21	Exponential Scaling of Water Exchange Rates with Ion Interaction Strength from the Perspective of Dynamic Facilitation Theory. Journal of Physical Chemistry A, 2019, 123, 1077-1084.	2.5	5
22	A coarse-grain model for entangled polyethylene melts and polyethylene crystallization. Journal of Chemical Physics, 2019, 150, 244901.	3.0	23
23	Effect of Interlayer Co²⁺ on Structure and Charge Transfer in NiFe Layered Double Hydroxides. Journal of Physical Chemistry C, 2019, 123, 13593-13599.	3.1	11
24	Polymer nucleation under high-driving force, long-chain conditions: Heat release and the separation of time scales. Journal of Chemical Physics, 2019, 150, 114901.	3.0	13
25	TRPA1 modulation by piperidine carboxamides suggests an evolutionarily conserved binding site and gating mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26008-26019.	7.1	18
26	Divining the shape of nascent polymer crystal nuclei. Journal of Chemical Physics, 2019, 151, 144901.	3.0	11
27	Light-induced dilation in nanosheets of charge-transfer complexes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3776-3781.	7.1	20
28	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
29	Effect of Intercalated Metals on the Electrocatalytic Activity of 1T-MoS₂ for the Hydrogen Evolution Reaction. ACS Energy Letters, 2018, 3, 7-13.	17.4	211
30	Bioactive products from singlet oxygen photooxygenation of cannabinoids. European Journal of Medicinal Chemistry, 2018, 143, 983-996.	5.5	7
31	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	7.8	35
32	Bonding in the metallic molecular solid Î±-Gallium. Molecular Physics, 2018, 116, 3372-3379.	1.7	7
33	Effect of Interlayer Spacing on the Activity of Layered Manganese Oxide Bilayer Catalysts for the Oxygen Evolution Reaction. Journal of the American Chemical Society, 2017, 139, 1863-1870.	13.7	144
34	Small molecule modulation of voltage gated sodium channels. Current Opinion in Structural Biology, 2017, 43, 156-162.	5.7	10
35	A Freeâ€Standing Molecular Spinâ€“Charge Converter for Ubiquitous Magneticâ€Energy Harvesting and Sensing. Advanced Materials, 2017, 29, 1605150.	21.0	26
36	Thermal Ripples in Model Molybdenum Disulfide Monolayers. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 152-154.	1.2	2

#	Article	IF	Citations
37	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
38	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	3.2	11
39	Does Proton Conduction in the Voltage-Gated H⁺ Channel hHv1 Involve Grotthuss-Like Hopping via Acidic Residues?. Journal of Physical Chemistry B, 2017, 121, 3340-3351.	2.6	34
40	Nickel Confined in the Interlayer Region of Birnessite: an Active Electrocatalyst for Water Oxidation. Angewandte Chemie, 2016, 128, 10537-10541.	2.0	28
41	Nickel Confined in the Interlayer Region of Birnessite: an Active Electrocatalyst for Water Oxidation. Angewandte Chemie - International Edition, 2016, 55, 10381-10385.	13.8	112
42	On the role of water density fluctuations in the inhibition of a proton channel. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8359-E8368.	7.1	33
43	Isolation of Acacetin from Calea urticifolia with Inhibitory Properties against Human Monoamine Oxidase-A and -B. Journal of Natural Products, 2016, 79, 2538-2544.	3.0	32
44	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	13.6	698
45	Understanding TRPV1 activation by ligands: Insights from the binding modes of capsaicin and resiniferatoxin. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E137-45.	7.1	127
46	Flavonoids from Perovskia atriplicifolia and Their in Vitro Displacement of the Respective Radioligands for Human Opioid and Cannabinoid Receptors. Journal of Natural Products, 2015, 78, 1461-1465.	3.0	21
47	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	1.7	47
48	Frustrated Solvation Structures Can Enhance Electron Transfer Rates. Journal of Physical Chemistry Letters, 2015, 6, 4804-4808.	4.6	67
49	Structure, Dynamics, and Spectral Diffusion of Water from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2014, 118, 29401-29411.	3.1	139
50	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	1.7	37
51	TCR Triggering by pMHC Ligands Tethered on Surfaces via Poly(Ethylene Glycol) Depends on Polymer Length. PLoS ONE, 2014, 9, e112292.	2.5	46
52	Using collective variables to drive molecular dynamics simulations. Molecular Physics, 2013, 111, 3345-3362.	1.7	750
53	Probing the structure of PEGylated-lipid assemblies by coarse-grained molecular dynamics. Soft Matter, 2013, 9, 11549.	2.7	27
54	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. Soft Matter, 2012, 8, 2385-2397.	2.7	125

#	Article	IF	Citations
55	Raft registration across bilayers in a molecularly detailed model. Soft Matter, 2011, 7, 8182.	2.7	51
56	Coarse-grained force field for ionic surfactants. Soft Matter, 2011, 7, 6178.	2.7	69
57	Micellization Studied by GPU-Accelerated Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 4135-4145.	5.3	63
58	Exploring the utility of coarse-grained water models for computational studies of interfacial systems. Molecular Physics, 2010, 108, 2007-2020.	1.7	48
59	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	5.3	366
60	Zwitterionic Lipid Assemblies: Molecular Dynamics Studies of Monolayers, Bilayers, and Vesicles Using a New Coarse Grain Force Field. Journal of Physical Chemistry B, 2010, 114, 6836-6849.	2.6	234
61	Quantum Mechanical and Quantum Mechanical/Molecular Mechanical Studies of the Ironâ^'Dioxygen Intermediates and Proton Transfer in Superoxide Reductase. Journal of Chemical Theory and Computation, 2010, 6, 2896-2909.	5.3	19
62	Formation of Interconnected Aggregates in Aqueous Dicationic Ionic Liquid Solutions. Journal of Chemical Theory and Computation, 2010, 6, 873-879.	5.3	47
63	Coarse-Grained Potential Models for Phenyl-Based Molecules: I. Parametrization Using Experimental Data. Journal of Physical Chemistry B, 2010, 114, 6386-6393.	2.6	59
64	Formation of micelles in aqueous solutions of a room temperature ionic liquid: a study using coarse grained molecular dynamics. Molecular Physics, 2009, 107, 393-401.	1.7	47
65	Transferable Coarse Grain Nonbonded Interaction Model for Amino Acids. Journal of Chemical Theory and Computation, 2009, 5, 2115-2124.	5.3	119
66	Evaluation of Electronic Coupling in Transition-Metal Systems Using DFT: Application to the Hexa-Aquo Ferricâ^'Ferrous Redox Couple. Journal of Chemical Theory and Computation, 2009, 5, 307-323.	5.3	41
67	Unraveling the Catalytic Pathway of Metalloenzyme Farnesyltransferase through QM/MM Computation. Journal of Chemical Theory and Computation, 2009, 5, 1657-1666.	5.3	35
68	Aqueous solutions of imidazolium ionic liquids: molecular dynamics studies. Soft Matter, 2009, 5, 3475.	2.7	58
69	Large-Scale Molecular Dynamics Simulations of Self-Assembling Systems. Science, 2008, 321, 798-800.	12.6	385
70	Coarse-grained molecular modeling of non-ionic surfactant self-assembly. Soft Matter, 2008, 4, 2454.	2.7	226
71	Nonequilibrium Molecular Dynamics. Reviews in Computational Chemistry, 2007, , 291-397.	1.5	19
72	Peptide Hydrolysis in Thermolysin:â€‰Ab Initio QM/MM Investigation of the Glu143-Assisted Water Addition Mechanism. Journal of Chemical Theory and Computation, 2007, 3, 1837-1850.	5.3	60

#	Article	IF	Citations
73	Energy Conservation in Adaptive Hybrid Atomistic/Coarse-Grain Molecular Dynamics. Journal of Chemical Theory and Computation, 2007, 3, 1100-1105.	5.3	151
74	Nanoscale organization in room temperature ionic liquids: a coarse grained molecular dynamics simulation study. Soft Matter, 2007, 3, 1395.	2.7	194
75	Emerging applications of polymersomes in delivery: From molecular dynamics to shrinkage of tumors. Progress in Polymer Science, 2007, 32, 838-857.	24.7	351
76	Computer simulation of aqueous block copolymer assemblies: Length scales and methods. Journal of Polymer Science, Part B: Polymer Physics, 2006, 44, 1907-1918.	2.1	32
77	Structure and dynamics of the aluminum chlorohydrate polymer Al13O4(OH)24(H2O)12Cl7. Physical Chemistry Chemical Physics, 2004, 6, 919.	2.8	32
78	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	2.6	327
79	A coarse grain model for n-alkanes parameterized from surface tension data. Journal of Chemical Physics, 2003, 119, 7043-7049.	3.0	121
80	Molecular Dynamics Investigations of Lipid Langmuir Monolayers Using a Coarse-Grain Model. Journal of Physical Chemistry B, 2003, 107, 13911-13917.	2.6	56
81	Proton tunneling in fatty acid/soap crystals?. Journal of Chemical Physics, 2003, 118, 1-3.	3.0	18
82	Electrostatic interactions in a neutral model phospholipid bilayer by molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 3052-3057.	3.0	88
83	Structure of the strongly associated liquid antimony pentafluoride: An ab initio molecular dynamics study. Journal of Chemical Physics, 2002, 116, 7087-7093.	3.0	11
84	Hydrocarbon Reactivity in the Superacid SbF5/HF:Â an ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2002, 106, 11596-11605.	2.6	18
85	Simulating vaporâ€“liquid nucleation of n-alkanes. Journal of Chemical Physics, 2002, 116, 4317-4329.	3.0	65
86	Influence of a knot on the stretching-induced crystallization of a polymer. Journal of Chemical Physics, 2002, 116, 5333-5336.	3.0	9
87	Simulations of Phospholipids Using a Coarse Grain Model. Journal of Physical Chemistry B, 2001, 105, 9785-9792.	2.6	183
88	Dynamics of Water Molecules in the Br-Solvation Shell:Â An ab Initio Molecular Dynamics Study. Journal of the American Chemical Society, 2001, 123, 9484-9485.	13.7	59
89	First-Principles Molecular Dynamics Study of the Rupture Processes of a Bulklike Polyethylene Knot. Journal of Physical Chemistry B, 2001, 105, 6495-6499.	2.6	26
90	Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium. Journal of Chemical Physics, 2001, 115, 10903-10913.	3.0	116

#	Article	IF	Citations
91	Two possible conducting states of the influenza A virus M2 ion channel. FEBS Letters, 2000, 473, 195-198.	2.8	38
92	Molecular dynamics simulation of four-Î±-helix bundles that bind the anesthetic halothane. FEBS Letters, 2000, 478, 61-66.	2.8	10
93	Ab Initio Molecular Dynamics Study of the Superacid System SbF5/HF Solution. Journal of Physical Chemistry B, 2000, 104, 10074-10079.	2.6	26
94	First-Principles Study of Bond Rupture of Entangled Polymer Chains. Journal of Physical Chemistry B, 2000, 104, 2197-2200.	2.6	25
95	Conformational and orientational order and disorder in solid polytetrafluoroethylene. Molecular Physics, 1999, 97, 355-373.	1.7	37
96	Polyethylene under tensil load: Strain energy storage and breaking of linear and knotted alkanes probed by first-principles molecular dynamics calculations. Journal of Chemical Physics, 1999, 111, 9434-9440.	3.0	46
97	Influence of a knot on the strength of a polymer strand. Nature, 1999, 399, 46-48.	27.8	206
98	Molecular Dynamics Study of a Lipidâ˜'DNA Complex. Journal of Physical Chemistry B, 1999, 103, 10075-10080.	2.6	97
99	Molecular dynamics simulation of a synthetic four-Î±-helix bundle that binds the anesthetic halothane. FEBS Letters, 1999, 455, 332-338.	2.8	10
100	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	21.0	429
101	Molecular dynamics study of the LS3 voltage-gated ion channel. FEBS Letters, 1998, 427, 267-270.	2.8	43
102	Simulation of the HIV-1 Vpu transmembrane domain as a pentameric bundle. FEBS Letters, 1998, 431, 143-148.	2.8	66
103	The M2 channel of influenza A virus: a molecular dynamics study. FEBS Letters, 1998, 434, 265-271.	2.8	81
104	Constant pressure and temperature molecular-dynamics simulation of the hydrated diphytanolphosphatidylcholine lipid bilayer. Journal of Chemical Physics, 1998, 109, 2826-2832.	3.0	54
105	Trimethylaluminum:Â A Computer Study of the Condensed Phases and the Gas Dimer. Journal of Physical Chemistry B, 1998, 102, 10136-10141.	2.6	12
106	Response to â€œComment on â€˜Modified nonequilibrium molecular dynamics for fluid flows with energy conservationâ€™â€‰â€•[J. Chem. Phys. 108, 4351 (1998)]. Journal of Chemical Physics, 1998, 108, 4353-4354.	3.0	12
107	Ion channels: a challenge for computer simulations. , 1998, , .		1
108	Centroid path integral molecular-dynamics studies of a para-hydrogen slab containing a lithium impurity. Journal of Chemical Physics, 1998, 109, 610-617.	3.0	38

#	Article	IF	Citations
109	An ab initio path integral molecular dynamics study of double proton transfer in the formic acid dimer. Journal of Chemical Physics, 1998, 109, 5290-5299.	3.0	107
110	Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution. Molecular Physics, 1998, 95, 377-384.	1.7	20
111	From Molecules to Materials: Current Trends and Future Directions. , 1998, 10, 1297.		1
112	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	21.0	9
113	Ab initio molecular dynamics study of polyfluoride anions. Journal of Chemical Physics, 1997, 107, 8012-8019.	3.0	32
114	Centroid path integral molecular dynamics simulation of lithium para-hydrogen clusters. Journal of Chemical Physics, 1997, 106, 1154-1169.	3.0	69
115	A Phenomenological Model of the LS2 Ion Channel. Materials Research Society Symposia Proceedings, 1997, 489, 131.	0.1	0
116	Structure of Solid Poly(tetrafluoroethylene):â€‰ A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. Journal of Physical Chemistry B, 1997, 101, 2745-2749.	2.6	40
117	The effects of pressure on structural and dynamical properties of associated liquids: Molecular dynamics calculations for the extended simple point charge model of water. Journal of Chemical Physics, 1997, 107, 8561-8567.	3.0	95
118	Modified nonequilibrium molecular dynamics for fluid flows with energy conservation. Journal of Chemical Physics, 1997, 106, 5615-5621.	3.0	130
119	Determination of the Pressureâ^'Viscosity Coefficient of Decane by Molecular Simulation. The Journal of Physical Chemistry, 1996, 100, 16779-16781.	2.9	20
120	Profile unbiased thermostat with dynamical streaming velocities. Journal of Chemical Physics, 1996, 105, 11183-11189.	3.0	23
121	Shear viscosity of polar fluids: Molecular dynamics calculations of water. Journal of Chemical Physics, 1996, 105, 11190-11195.	3.0	75
122	Ab InitioMolecular Dynamics Simulations. The Journal of Physical Chemistry, 1996, 100, 12878-12887.	2.9	198
123	Molecular Dynamics Simulations of a Calcium Carbonate/Calcium Sulfonate Reverse Micelleâ€. The Journal of Physical Chemistry, 1996, 100, 6637-6648.	2.9	94
124	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	1,508
125	Molecular Dynamics Investigation of the Lamellar Liquid-Crystal D-Phase in the Octylammonium Chloride/Water System. Molecular Simulation, 1996, 16, 219-228.	2.0	3
126	Hydrodynamic boundary conditions for confined fluids via a nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 1996, 105, 3211-3214.	3.0	16

#	Article	IF	Citations
127	Simulation Studies of Ultrathin Films of Linear and Branched Alkanes on a Metal Substrate. The Journal of Physical Chemistry, 1996, 100, 11960-11963.	2.9	32
128	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	148
129	Ab Initio Molecular Dynamics Simulations of Molecular Crystals. Materials Research Society Symposia Proceedings, 1995, 408, 477.	0.1	2
130	Structure of CAl12. Journal of Chemical Physics, 1995, 103, 8075-8080.	3.0	30
131	Decane under shear: A molecular dynamics study using reversible NVTâ€SLLOD and NPTâ€SLLOD algorithms. Journal of Chemical Physics, 1995, 103, 10192-10200.	3.0	57
132	Calculation of the shear viscosity of decane using a reversible multiple timeâ€step algorithm. Journal of Chemical Physics, 1995, 102, 3376-3380.	3.0	94
133	Cation transport in lithium sulphate based crystals. Molecular Physics, 1995, 86, 923-938.	1.7	25
134	Quantum simulation studies of metalâ€“ammonia solutions. Journal of Chemical Physics, 1994, 100, 7590-7601.	3.0	47
135	Constant pressure molecular dynamics algorithms. Journal of Chemical Physics, 1994, 101, 4177-4189.	3.0	4,379
136	Computer simulations and the interpretation of incoherent neutron scattering experiments on the solid rotator phases of long-chain alkanes. Molecular Physics, 1994, 83, 439-458.	1.7	45
137	Efficient molecular dynamics and hybrid Monte Carlo algorithms for path integrals. Journal of Chemical Physics, 1993, 99, 2796-2808.	3.0	414
138	Nature of lithium trapping sites in the quantum solids paraâ€hydrogen and orthoâ€deuterium. Journal of Chemical Physics, 1993, 99, 9013-9020.	3.0	46
139	Quantum simulation studies of singlet and triplet bipolarons in liquid ammonia. Journal of Chemical Physics, 1993, 98, 555-563.	3.0	56
140	Pathâ€integral Monte Carlo study of a lithium impurity in paraâ€hydrogen: Clusters and the bulk liquid. Journal of Chemical Physics, 1993, 99, 8997-9012.	3.0	55
141	The electronic states of lithium atoms in ammonia clusters and solution. Journal of Chemical Physics, 1992, 96, 7662-7671.	3.0	26
142	Pathâ€integral Monte Carlo studies ofparaâ€hydrogen clusters. Journal of Chemical Physics, 1992, 97, 3590-3599.	3.0	73
143	An Ewald summation method for planar surfaces and interfaces. Molecular Physics, 1992, 75, 379-395.	1.7	176
144	A molecular dynamics study of methanol near the liquidâ€“glass transition. Journal of Chemical Physics, 1992, 96, 4681-4692.	3.0	76

#	Article	IF	Citations
145	NosÃ©â€“Hoover chains: The canonical ensemble via continuous dynamics. Journal of Chemical Physics, 1992, 97, 2635-2643.	3.0	4,240
146	Electronic states and dynamical behavior of LiXen and CsXen clusters. Journal of Chemical Physics, 1991, 95, 1318-1336.	3.0	41
147	Molecular Dynamics Simulation of A Langmuir Monolayer. Materials Research Society Symposia Proceedings, 1991, 237, 271.	0.1	4
148	Simulation of a sodium dodecylsulfate micelle in aqueous solution. International Journal of Quantum Chemistry, 1990, 38, 103-117.	2.0	84
149	Pressure induced amorphization of ice Ih. Journal of Chemical Physics, 1990, 92, 3992-3994.	3.0	37
150	Shortâ€rrange structure of liquid pyrrole. Journal of Chemical Physics, 1990, 92, 6973-6974.	3.0	9
151	Structural relaxation and dynamical correlations in a molten state near the liquidâ€“glass transition: A molecular dynamics study. Journal of Chemical Physics, 1990, 92, 1294-1303.	3.0	160
152	Molecular dynamics simulation of the effects of temperature on a dense monolayer of longâ€chain molecules. Journal of Chemical Physics, 1990, 93, 7483-7492.	3.0	182
153	Molecularâ€dynamics simulation of aqueous mixtures: Methanol, acetone, and ammonia. Journal of Chemical Physics, 1990, 93, 5156-5166.	3.0	378
154	A Computer Simulation Study of Supercooled Liquid and Amorphous-Solid Methanol. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1989, 44, 585-590.	1.5	7
155	Isotopic shift in the melting curve of helium: A path integral Monte Carlo study. Journal of Chemical Physics, 1989, 90, 5644-5650.	3.0	42
156	Adiabatic dynamics of the solvated electron in liquid ammonia. Journal of Chemical Physics, 1989, 91, 5665-5671.	3.0	39
157	Disorder in the pseudohexagonal rotator phase ofn-alkanes: molecular-dynamics calculations for tricosane. Molecular Physics, 1989, 67, 957-979.	1.7	123
158	A molecular dynamics study of the low temperature structure and dynamics of ethane monolayers physisorbed on the graphite basal plane. Journal of Chemical Physics, 1989, 90, 1960-1967.	3.0	31
159	Structure and dynamics of the fluorperovskite, RbCaF3. Journal of Chemical Physics, 1989, 90, 5005-5010.	3.0	11
160	Structure and dynamics of carbon dioxide clusters: A molecular dynamics study. Journal of Chemical Physics, 1989, 90, 4441-4449.	3.0	73
161	Simulation of a monolayer of alkyl thiol chains. Journal of Chemical Physics, 1989, 91, 4994-5001.	3.0	387
162	A polarizable model for water using distributed charge sites. Journal of Chemical Physics, 1988, 89, 7556-7560.	3.0	471

#	Article	IF	Citations
163	Structure of Physisorbed Overlayers of Dipolar Molecules: A Combined Study by Atomic-Beam Scattering and Molecular Dynamics. Physical Review Letters, 1988, 61, 710-713.	7.8	54
164	Optimization of a distributed Gaussian basis set using simulated annealing: Application to the adiabatic dynamics of the solvated electron. Journal of Chemical Physics, 1988, 89, 1592-1607.	3.0	84
165	Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. Journal of Chemical Physics, 1988, 89, 4918-4923.	3.0	30
166	Molecular Dynamics Study of A Model Langmuir-Blodgett Film. Materials Research Society Symposia Proceedings, 1988, 141, 411.	0.1	3
167	Lattice vibrations and infrared absorption of ice Ih. Journal of Chemical Physics, 1986, 85, 2414-2418.	3.0	45
168	Translational and rotational disorder in solid nâ€alkanes: Constant temperatureâ€“constant pressure molecular dynamics calculations using infinitely long flexible chains. Journal of Chemical Physics, 1986, 85, 1613-1620.	3.0	96
169	Anion ordering in alkali cyanide crystals. Journal of Chemical Physics, 1986, 84, 3975-3985.	3.0	42
170	Molecular properties of CNâ¯ions in alkali cyanide crystals. Journal of Chemical Physics, 1986, 85, 3913-3916.	3.0	23
171	Simulation of an excess electron in a hard sphere fluid. Journal of Chemical Physics, 1985, 83, 3042-3049.	3.0	63
172	Simulation of the cubic to orthorhombic phase transition in potassium cyanide. Journal of Chemical Physics, 1985, 83, 3638-3644.	3.0	27
173	Elastic constants of solid ammonia. Journal of Chemical Physics, 1985, 83, 5346-5347.	3.0	2
174	Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations. Journal of Chemical Physics, 1985, 83, 5802-5809.	3.0	72
175	Structure of solid tâ€butyl cyanide: Interpretation of experimental data by means of molecular dynamics simulation. Journal of Chemical Physics, 1985, 83, 4726-4733.	3.0	7
176	Molecular dynamics calculations for solid bicyclo (2.2.2) octane. Molecular Physics, 1984, 52, 269-279.	1.7	22
177	Computer simulation of muonium in water. Journal of Chemical Physics, 1984, 80, 5719-5724.	3.0	118
178	Orientational ordering in solid parahydrogen and orthodeuterium. Journal of Chemical Physics, 1984, 81, 6207-6213.	3.0	13
179	Effective pair potentials and the structure of ices VIII and IX. Journal of Chemical Physics, 1984, 81, 6406-6407.	3.0	24
180	Comparison of simple potential functions for simulating liquid water. Journal of Chemical Physics, 1983, 79, 926-935.	3.0	34,333

#	Article	IF	Citations
181	A study of solid and liquid carbon tetrafluoride using the constant pressure molecular dynamics technique. Journal of Chemical Physics, 1983, 78, 6928-6939.	3.0	205
182	Polymorphic phase transitions in alkali cyanide crystals. Molecular Physics, 1983, 50, 243-246.	1.7	22
183	Ab Initio Interatomic Potential Curves for NaNO2and the Simulation of the Molten Salt. Journal of the Physical Society of Japan, 1983, 52, 1168-1172.	1.6	5
184	Molecular dynamics calculations for HCl in a matrix of solid Ar. Molecular Physics, 1982, 46, 1063-1071.	1.7	12
185	Molecular dynamics calculations for the liquid and cubic plastic crystal phases of carbon tetrachloride. Molecular Physics, 1982, 45, 521-542.	1.7	128
186	An ab initio molecular orbital study of NaCN and KCN. Journal of Chemical Physics, 1981, 75, 3909-3915.	3.0	64
187	Phonon spectra of methane physisorbed on graphite. Journal of Chemical Physics, 1981, 74, 1488-1494.	3.0	15
188	Is hydrogen chloride an associated liquid?. Molecular Physics, 1981, 42, 243-247.	1.7	39
189	Structure and dynamics of associated molecular systems. III. Computer simulation of liquid hydrogen chloride. Journal of Chemical Physics, 1980, 72, 5710-5717.	3.0	64
190	Structure and dynamics of associated molecular systems. IV. The orientationally disordered phase I of solid DCl. Journal of Chemical Physics, 1980, 73, 532-537.	3.0	10
191	Molecular dynamics simulation of the plastic phase of solid methane. Journal of Chemical Physics, 1980, 72, 5348-5356.	3.0	53
192	Orientational phases of classical octopoles on a triangular lattice and the adsorption of methane on graphite. Journal of Chemical Physics, 1979, 71, 2399-2403.	3.0	39
193	Lattice dynamics of solid ammonia. Journal of Chemical Physics, 1978, 68, 5553-5557.	3.0	23
194	Lattice dynamics of solid Ne. Journal of Low Temperature Physics, 1976, 22, 501-506.	1.4	8
195	Selfâ€consistent phonon calculation of the elastic constants of the Î² phase of solid N2. Journal of Chemical Physics, 1976, 64, 5121-5125.	3.0	11
196	Interatomic potentials and phonon spectra of dilute rareâ€gas mixtures. Journal of Chemical Physics, 1974, 61, 3210-3216.	3.0	15
197	Coarse Grained-to-Atomistic Mapping Algorithm: A Tool for Multiscale Simulations. , 0, , 73-88.		1