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	Comparison of simple potential functions for simulating liquid water. Journal of Chemical Physics, 1983, 79, 926-935.	3.0	34,333
2	Constant pressure molecular dynamics algorithms. Journal of Chemical Physics, 1994, 101, 4177-4189.	3.0	4,379
3	NosÃ©â€“Hoover chains: The canonical ensemble via continuous dynamics. Journal of Chemical Physics, 1992, 97, 2635-2643.	3.0	4,240
4	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	1,508
5	Using collective variables to drive molecular dynamics simulations. Molecular Physics, 2013, 111, 3345-3362.	1.7	750
6	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	13.6	698
7	A polarizable model for water using distributed charge sites. Journal of Chemical Physics, 1988, 89, 7556-7560.	3.0	471
8	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	21.0	429
9	Efficient molecular dynamics and hybrid Monte Carlo algorithms for path integrals. Journal of Chemical Physics, 1993, 99, 2796-2808.	3.0	414
10	Simulation of a monolayer of alkyl thiol chains. Journal of Chemical Physics, 1989, 91, 4994-5001.	3.0	387
11	Large-Scale Molecular Dynamics Simulations of Self-Assembling Systems. Science, 2008, 321, 798-800.	12.6	385
12	Molecularâ€dynamics simulation of aqueous mixtures: Methanol, acetone, and ammonia. Journal of Chemical Physics, 1990, 93, 5156-5166.	3.0	378
13	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
14	Emerging applications of polymersomes in delivery: From molecular dynamics to shrinkage of tumors. Progress in Polymer Science, 2007, 32, 838-857.	24.7	351
15	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
16	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	2.6	327
17	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
18	Coarse-grained molecular modeling of non-ionic surfactant self-assembly. Soft Matter, 2008, 4, 2454.	2.7	226

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19	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
20	Influence of a knot on the strength of a polymer strand. Nature, 1999, 399, 46-48.	27.8	206
21	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
22	Ab InitioMolecular Dynamics Simulations. The Journal of Physical Chemistry, 1996, 100, 12878-12887.	2.9	198
23	Nanoscale organization in room temperature ionic liquids: a coarse grained molecular dynamics simulation study. Soft Matter, 2007, 3, 1395.	2.7	194
24	Simulations of Phospholipids Using a Coarse Grain Model. Journal of Physical Chemistry B, 2001, 105, 9785-9792.	2.6	183
25	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
26	An Ewald summation method for planar surfaces and interfaces. Molecular Physics, 1992, 75, 379-395.	1.7	176
27	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
28	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
29	Energy Conservation in Adaptive Hybrid Atomistic/Coarse-Grain Molecular Dynamics. Journal of Chemical Theory and Computation, 2007, 3, 1100-1105.	5.3	151
30	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	148
31	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
32	Structure, Dynamics, and Spectral Diffusion of Water from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2014, 118, 29401-29411.	3.1	139
33	Modified nonequilibrium molecular dynamics for fluid flows with energy conservation. Journal of Chemical Physics, 1997, 106, 5615-5621.	3.0	130
34	Molecular dynamics calculations for the liquid and cubic plastic crystal phases of carbon tetrachloride. Molecular Physics, 1982, 45, 521-542.	1.7	128
35	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
36	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. Soft Matter, 2012, 8, 2385-2397.	2.7	125

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37	Disorder in the pseudohexagonal rotator phase ofn-alkanes: molecular-dynamics calculations for tricosane. Molecular Physics, 1989, 67, 957-979.	1.7	123
38	A coarse grain model for n-alkanes parameterized from surface tension data. Journal of Chemical Physics, 2003, 119, 7043-7049.	3.0	121
39	Transferable Coarse Grain Nonbonded Interaction Model for Amino Acids. Journal of Chemical Theory and Computation, 2009, 5, 2115-2124.	5.3	119
40	Computer simulation of muonium in water. Journal of Chemical Physics, 1984, 80, 5719-5724.	3.0	118
41	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
42	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
43	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
44	Molecular Dynamics Study of a Lipidâ^'DNA Complex. Journal of Physical Chemistry B, 1999, 103, 10075-10080.	2.6	97
45	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
46	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
47	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
48	Molecular Dynamics Simulations of a Calcium Carbonate/Calcium Sulfonate Reverse Micelleâ€. The Journal of Physical Chemistry, 1996, 100, 6637-6648.	2.9	94
49	Electrostatic interactions in a neutral model phospholipid bilayer by molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 3052-3057.	3.0	88
50	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
51	Simulation of a sodium dodecylsulfate micelle in aqueous solution. International Journal of Quantum Chemistry, 1990, 38, 103-117.	2.0	84
52	The M2 channel of influenza A virus: a molecular dynamics study. FEBS Letters, 1998, 434, 265-271.	2.8	81
53	A molecular dynamics study of methanol near the liquidâ€“glass transition. Journal of Chemical Physics, 1992, 96, 4681-4692.	3.0	76
54	Shear viscosity of polar fluids: Molecular dynamics calculations of water. Journal of Chemical Physics, 1996, 105, 11190-11195.	3.0	75

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55	Structure and dynamics of carbon dioxide clusters: A molecular dynamics study. Journal of Chemical Physics, 1989, 90, 4441-4449.	3.0	73
56	Pathâ€integral Monte Carlo studies ofparaâ€hydrogen clusters. Journal of Chemical Physics, 1992, 97, 3590-3599.	3.0	73
57	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
58	Centroid path integral molecular dynamics simulation of lithium para-hydrogen clusters. Journal of Chemical Physics, 1997, 106, 1154-1169.	3.0	69
59	Coarse-grained force field for ionic surfactants. Soft Matter, 2011, 7, 6178.	2.7	69
60	Frustrated Solvation Structures Can Enhance Electron Transfer Rates. Journal of Physical Chemistry Letters, 2015, 6, 4804-4808.	4.6	67
61	Simulation of the HIV-1 Vpu transmembrane domain as a pentameric bundle. FEBS Letters, 1998, 431, 143-148.	2.8	66
62	Simulating vaporâ€“liquid nucleation of n-alkanes. Journal of Chemical Physics, 2002, 116, 4317-4329.	3.0	65
63	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
64	An ab initio molecular orbital study of NaCN and KCN. Journal of Chemical Physics, 1981, 75, 3909-3915.	3.0	64
65	Simulation of an excess electron in a hard sphere fluid. Journal of Chemical Physics, 1985, 83, 3042-3049.	3.0	63
66	Micellization Studied by GPU-Accelerated Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 4135-4145.	5.3	63
67	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
68	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
69	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
70	Aqueous solutions of imidazolium ionic liquids: molecular dynamics studies. Soft Matter, 2009, 5, 3475.	2.7	58
71	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
72	Quantum simulation studies of singlet and triplet bipolarons in liquid ammonia. Journal of Chemical Physics, 1993, 98, 555-563.	3.0	56

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73	Molecular Dynamics Investigations of Lipid Langmuir Monolayers Using a Coarse-Grain Model. Journal of Physical Chemistry B, 2003, 107, 13911-13917.	2.6	56
74	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
75	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
76	Constant pressure and temperature molecular-dynamics simulation of the hydrated diphytanolphosphatidylcholine lipid bilayer. Journal of Chemical Physics, 1998, 109, 2826-2832.	3.0	54
77	Molecular dynamics simulation of the plastic phase of solid methane. Journal of Chemical Physics, 1980, 72, 5348-5356.	3.0	53
78	Raft registration across bilayers in a molecularly detailed model. Soft Matter, 2011, 7, 8182.	2.7	51
79	Exploring the utility of coarse-grained water models for computational studies of interfacial systems. Molecular Physics, 2010, 108, 2007-2020.	1.7	48
80	Quantum simulation studies of metalâ€“ammonia solutions. Journal of Chemical Physics, 1994, 100, 7590-7601.	3.0	47
81	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
82	Formation of Interconnected Aggregates in Aqueous Dicationic Ionic Liquid Solutions. Journal of Chemical Theory and Computation, 2010, 6, 873-879.	5.3	47
83	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
84	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
85	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
86	TCR Triggering by pMHC Ligands Tethered on Surfaces via Poly(Ethylene Glycol) Depends on Polymer Length. PLoS ONE, 2014, 9, e112292.	2.5	46
87	Lattice vibrations and infrared absorption of ice Ih. Journal of Chemical Physics, 1986, 85, 2414-2418.	3.0	45
88	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
89	Molecular dynamics study of the LS3 voltage-gated ion channel. FEBS Letters, 1998, 427, 267-270.	2.8	43
90	Anion ordering in alkali cyanide crystals. Journal of Chemical Physics, 1986, 84, 3975-3985.	3.0	42

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91	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
92	Electronic states and dynamical behavior of LiXen and CsXen clusters. Journal of Chemical Physics, 1991, 95, 1318-1336.	3.0	41
93	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
94	Dissolving salt is not equivalent to applying a pressure on water. Nature Communications, 2022, 13, 822.	12.8	41
95	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
96	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
97	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
98	Is hydrogen chloride an associated liquid?. Molecular Physics, 1981, 42, 243-247.	1.7	39
99	Adiabatic dynamics of the solvated electron in liquid ammonia. Journal of Chemical Physics, 1989, 91, 5665-5671.	3.0	39
100	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
101	Two possible conducting states of the influenza A virus M2 ion channel. FEBS Letters, 2000, 473, 195-198.	2.8	38
102	Pressure induced amorphization of ice Ih. Journal of Chemical Physics, 1990, 92, 3992-3994.	3.0	37
103	Conformational and orientational order and disorder in solid polytetrafluoroethylene. Molecular Physics, 1999, 97, 355-373.	1.7	37
104	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	1.7	37
105	Unraveling the Catalytic Pathway of Metalloenzyme Farnesyltransferase through QM/MM Computation. Journal of Chemical Theory and Computation, 2009, 5, 1657-1666.	5.3	35
106	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
107	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
108	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

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109	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
110	Ab initio molecular dynamics study of polyfluoride anions. Journal of Chemical Physics, 1997, 107, 8012-8019.	3.0	32
111	Structure and dynamics of the aluminum chlorohydrate polymer Al13O4(OH)24(H2O)12Cl7. Physical Chemistry Chemical Physics, 2004, 6, 919.	2.8	32
112	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
113	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
114	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
115	Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. Journal of Chemical Physics, 1988, 89, 4918-4923.	3.0	30
116	Structure of CAl12. Journal of Chemical Physics, 1995, 103, 8075-8080.	3.0	30
117	Nickel Confined in the Interlayer Region of Birnessite: an Active Electrocatalyst for Water Oxidation. Angewandte Chemie, 2016, 128, 10537-10541.	2.0	28
118	Simulation of the cubic to orthorhombic phase transition in potassium cyanide. Journal of Chemical Physics, 1985, 83, 3638-3644.	3.0	27
119	Probing the structure of PEGylated-lipid assemblies by coarse-grained molecular dynamics. Soft Matter, 2013, 9, 11549.	2.7	27
120	The electronic states of lithium atoms in ammonia clusters and solution. Journal of Chemical Physics, 1992, 96, 7662-7671.	3.0	26
121	Ab Initio Molecular Dynamics Study of the Superacid System SbF5/HF Solution. Journal of Physical Chemistry B, 2000, 104, 10074-10079.	2.6	26
122	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
123	A Freeâ€Standing Molecular Spinâ€“Charge Converter for Ubiquitous Magneticâ€Energy Harvesting and Sensing. Advanced Materials, 2017, 29, 1605150.	21.0	26
124	Cation transport in lithium sulphate based crystals. Molecular Physics, 1995, 86, 923-938.	1.7	25
125	First-Principles Study of Bond Rupture of Entangled Polymer Chains. Journal of Physical Chemistry B, 2000, 104, 2197-2200.	2.6	25
126	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

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127	Effective pair potentials and the structure of ices VIII and IX. Journal of Chemical Physics, 1984, 81, 6406-6407.	3.0	24
128	Lattice dynamics of solid ammonia. Journal of Chemical Physics, 1978, 68, 5553-5557.	3.0	23
129	Molecular properties of CNâ^ions in alkali cyanide crystals. Journal of Chemical Physics, 1986, 85, 3913-3916.	3.0	23
130	Profile unbiased thermostat with dynamical streaming velocities. Journal of Chemical Physics, 1996, 105, 11183-11189.	3.0	23
131	A coarse-grain model for entangled polyethylene melts and polyethylene crystallization. Journal of Chemical Physics, 2019, 150, 244901.	3.0	23
132	Polymorphic phase transitions in alkali cyanide crystals. Molecular Physics, 1983, 50, 243-246.	1.7	22
133	Molecular dynamics calculations for solid bicyclo (2.2.2) octane. Molecular Physics, 1984, 52, 269-279.	1.7	22
134	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
135	Investigations of water/oxide interfaces by molecular dynamics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1537.	14.6	21
136	SPICA Force Field for Proteins and Peptides. Journal of Chemical Theory and Computation, 2022, 18, 3204-3217.	5.3	21
137	Determination of the Pressureâ^Viscosity Coefficient of Decane by Molecular Simulation. The Journal of Physical Chemistry, 1996, 100, 16779-16781.	2.9	20
138	Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution. Molecular Physics, 1998, 95, 377-384.	1.7	20
139	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
140	Suppression of Zika Virus Infection in the Brain by the Antiretroviral Drug Rilpivirine. Molecular Therapy, 2019, 27, 2067-2079.	8.2	20
141	Nonequilibrium Molecular Dynamics. Reviews in Computational Chemistry, 2007, , 291-397.	1.5	19
142	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
143	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
144	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

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145	Proton tunneling in fatty acid/soap crystals?. Journal of Chemical Physics, 2003, 118, 1-3.	3.0	18
146	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
147	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
148	Hydrodynamic boundary conditions for confined fluids via a nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 1996, 105, 3211-3214.	3.0	16
149	A new perspective on lone pair dynamics in halide perovskites. APL Materials, 2020, 8, .	5.1	16
150	Interatomic potentials and phonon spectra of dilute rareâ€gas mixtures. Journal of Chemical Physics, 1974, 61, 3210-3216.	3.0	15
151	Phonon spectra of methane physisorbed on graphite. Journal of Chemical Physics, 1981, 74, 1488-1494.	3.0	15
152	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
153	Orientational ordering in solid parahydrogen and orthodeuterium. Journal of Chemical Physics, 1984, 81, 6207-6213.	3.0	13
154	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
155	Molecular dynamics calculations for HCl in a matrix of solid Ar. Molecular Physics, 1982, 46, 1063-1071.	1.7	12
156	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
157	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
158	Property Decoupling across the Embryonic Nucleusâ€“Melt Interface during Polymer Crystal Nucleation. Journal of Physical Chemistry B, 2020, 124, 4793-4804.	2.6	12
159	Lone Pair Rotational Dynamics in Solids. Physical Review Letters, 2020, 124, 066001.	7.8	12
160	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
161	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
162	Structure and dynamics of the fluorperovskite, RbCaF3. Journal of Chemical Physics, 1989, 90, 5005-5010.	3.0	11

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163	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
164	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	3.2	11
165	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
166	Divining the shape of nascent polymer crystal nuclei. Journal of Chemical Physics, 2019, 151, 144901.	3.0	11
167	Importance of nuclear quantum effects on the hydration of chloride ion. Physical Review Materials, 2021, 5, .	2.4	11
168	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
169	Molecular dynamics simulation of a synthetic four-Î±-helix bundle that binds the anesthetic halothane. FEBS Letters, 1999, 455, 332-338.	2.8	10
170	Molecular dynamics simulation of four-Î±-helix bundles that bind the anesthetic halothane. FEBS Letters, 2000, 478, 61-66.	2.8	10
171	Small molecule modulation of voltage gated sodium channels. Current Opinion in Structural Biology, 2017, 43, 156-162.	5.7	10
172	Halogen Bond Structure and Dynamics from Molecular Simulations. Journal of Physical Chemistry B, 2019, 123, 6266-6273.	2.6	10
173	Shortâ€range structure of liquid pyrrole. Journal of Chemical Physics, 1990, 92, 6973-6974.	3.0	9
174	Influence of a knot on the stretching-induced crystallization of a polymer. Journal of Chemical Physics, 2002, 116, 5333-5336.	3.0	9
175	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	21.0	9
176	Lattice dynamics of solid Ne. Journal of Low Temperature Physics, 1976, 22, 501-506.	1.4	8
177	Chain-End Modification: A Starting Point for Controlling Polymer Crystal Nucleation. Macromolecules, 2021, 54, 1599-1610.	4.8	8
178	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
179	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
180	Bioactive products from singlet oxygen photooxygenation of cannabinoids. European Journal of Medicinal Chemistry, 2018, 143, 983-996.	5.5	7

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181	Bonding in the metallic molecular solid Î±-Gallium. Molecular Physics, 2018, 116, 3372-3379.	1.7	7
182	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.4	7
183	Monodisperse Polymer Melts Crystallize via Structurally Polydisperse Nanoscale Clusters: Insights from Polyethylene. Polymers, 2020, 12, 447.	4.5	6
184	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
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