David J Keffer

List of Publications by Year in descending order

137 papers	2,942 citations	172386 29 h-index	223716 46 g-index
139 all docs	139 docs citations	139 times ranked	2832 citing authors

#	Article	IF	Citations
1	A Molecular Dynamics Study of a Nafion Polyelectrolyte Membrane and the Aqueous Phase Structure for Proton Transport. Journal of Physical Chemistry B, 2007, 111, 2208-2218.	1.2	207
2	Comparison of the Hydration and Diffusion of Protons in Perfluorosulfonic Acid Membranes with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 13273-13284.	1.2	119
3	On the Relationship between Polymer Electrolyte Structure and Hydrated Morphology of Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry C, 2010, 114, 11279-11292.	1.5	99
4	The effect of nanopore shape on the structure and isotherms of adsorbed fluids. Adsorption, 1996, 2, 9-21.	1.4	68
5	Conversion of Lignin Precursors to Carbon Fibers with Nanoscale Graphitic Domains. ACS Sustainable Chemistry and Engineering, 2014, 2, 2002-2010.	3.2	68
6	Competitive adsorption of CO2/CH4 mixture on dry and wet coal from subcritical to supercritical conditions. Chemical Engineering Journal, 2013, 230, 93-101.	6.6	67
7	A proper approach for nonequilibrium molecular dynamics simulations of planar elongational flow. Journal of Chemical Physics, 2005, 122, 114103.	1.2	65
8	Rotating Phenyl Rings as a Guest-Dependent Switch in Two-Dimensional Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 671-678.	6.6	65
9	Structure of the Ionomer Film in Catalyst Layers of Proton Exchange Membrane Fuel Cells. Journal of Physical Chemistry C, 2013, 117, 25305-25316.	1.5	59
10	The composition dependence of self and transport diffusivities from molecular dynamics simulations. Chemical Engineering Journal, 2004, 100, 51-69.	6.6	57
11	Diffusion and Percolation on Zeolite Sorption Lattices. The Journal of Physical Chemistry, 1996, 100, 967-973.	2.9	52
12	Rheological and structural studies of liquid decane, hexadecane, and tetracosane under planar elongational flow using nonequilibrium molecular-dynamics simulations. Journal of Chemical Physics, 2005, 122, 184906.	1.2	52
13	Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 084902.	1.2	51
14	Rheological and entanglement characteristics of linear-chain polyethylene liquids in planar Couette and planar elongational flows. Journal of Non-Newtonian Fluid Mechanics, 2008, 152, 168-183.	1.0	51
15	Molecular Dynamics Simulation of Poly(ethylene terephthalate) Oligomers. Journal of Physical Chemistry B, 2010, 114, 786-795.	1.2	46
16	Computational chemistry for molecular electronics. Computational Materials Science, 2003, 28, 321-341.	1.4	41
17	A validation of the p-SLLOD equations of motion for homogeneous steady-state flows. Journal of Chemical Physics, 2006, 124, 194104.	1.2	41
18	Effect of Loading and Nanopore Shape on Binary Adsorption Selectivity. The Journal of Physical Chemistry, 1996, 100, 638-645.	2.9	40

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19	Molecular-Level Modeling of the Structure and Wetting of Electrode/Electrolyte Interfaces in Hydrogen Fuel Cells. Journal of Physical Chemistry C, 2008, 112, 1985-1993.	1.5	39
20	Molecular Dynamics Study of Structure and Transport of Water and Hydronium Ions at the Membrane/Vapor Interface of Nafion. Journal of Physical Chemistry C, 2008, 112, 1975-1984.	1.5	39
21	Dynamics of individual molecules of linear polyethylene liquids under shear: Atomistic simulation and comparison with a free-draining bead-rod chain. Journal of Rheology, 2010, 54, 283-310.	1.3	39
22	Evaluation of functionalized isoreticular metal organic frameworks (IRMOFs) as smart nanoporous preconcentrators of RDX. Sensors and Actuators B: Chemical, 2010, 148, 459-468.	4.0	38
23	A coarse-grained model for polyethylene glycol polymer. Journal of Chemical Physics, 2011, 135, 214903.	1.2	36
24	An examination of the validity of nonequilibrium molecular-dynamics simulation algorithms for arbitrary steady-state flows. Journal of Chemical Physics, 2005, 123, 114106.	1.2	34
25	Structure Formation under Steady-State Isothermal Planar Elongational Flow ofn-Eicosane: A Comparison between Simulation and Experiment. Physical Review Letters, 2006, 96, 037802.	2.9	34
26	Applications of a general random-walk theory for confined diffusion. Physical Review E, 2011, 83, 011120.	0.8	32
27	Molecular Dynamics Simulations of Hydration Effects on Solvation, Diffusivity, and Permeability in Chitosan/Chitin Films. Journal of Physical Chemistry B, 2016, 120, 8997-9010.	1.2	32
28	Coarse-Grained Molecular Dynamics Simulation of Polyethylene Terephthalate (PET). Macromolecules, 2010, 43, 10722-10734.	2.2	31
29	Insights into the structure of mixed CO₂/CH₄in gas hydrates. American Mineralogist, 2015, 100, 1203-1208.	0.9	31
30	Vaporâ˜Liquid Equilibrium of Ethanol by Molecular Dynamics Simulation and Voronoi Tessellation. Journal of Physical Chemistry B, 2007, 111, 13278-13286.	1.2	30
31	A molecular dynamics study of the stressâ€“optical behavior of a linear short-chain polyethylene melt under shear. Rheologica Acta, 2007, 46, 1171-1186.	1.1	30
32	A compendium of potential energy maps of zeolites and molecular sieves. Journal of Molecular Graphics, 1996, 14, 108-116.	1.7	29
33	Single-chain dynamics of linear polyethylene liquids under shear flow. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 769-772.	0.9	29
34	A Reactive Molecular Dynamics Algorithm for Proton Transport in Aqueous Systems. Journal of Physical Chemistry C, 2010, 114, 11965-11976.	1.5	29
35	Modeling shear thickening in dilute polymer solutions: Temperature, concentration, and molecular weight dependencies. Journal of Applied Polymer Science, 2003, 90, 2997-3011.	1.3	28
36	Molecular simulations of adsorption and diffusion of RDX in IRMOF-1. Molecular Simulation, 2009, 35, 910-919.	0.9	28

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37	Effective potentials between nanoparticles in suspension. Journal of Chemical Physics, 2011, 134, 144902.	1.2	28
38	Evidence of Single-File Diffusion in Zeolites. Science, 1996, 274, 164-164.	6.0	27
39	Structure and Dynamics of a Benzenedithiol Monolayer on a Au(111) Surface. Journal of Physical Chemistry B, 2003, 107, 11940-11950.	1.2	27
40	Measuring Coexisting Densities from a Two-Phase Molecular Dynamics Simulation by Voronoi Tessellations. Journal of Physical Chemistry B, 2007, 111, 3469-3475.	1.2	27
41	Effect of Charge Distribution on RDX Adsorption in IRMOF-10. Langmuir, 2010, 26, 5942-5950.	1.6	27
42	Processingâ€“Structureâ€“Property Relationships for Ligninâ€Based Carbonaceous Materials Used in Energyâ€Storage Applications. Energy Technology, 2017, 5, 1311-1321.	1.8	27
43	Determination of statistically reliable transport diffusivities from molecular dynamics simulation. Journal of Non-Newtonian Fluid Mechanics, 2004, 120, 41-53.	1.0	25
44	Molecular Dynamic Simulations of the Effect on the Hydration of Nafion in the Presence of a Platinum Nanoparticle. Journal of Physical Chemistry C, 2012, 116, 12890-12899.	1.5	25
45	Kinetics of Methane Hydrate Decomposition Studied via in Situ Low Temperature X-ray Powder Diffraction. Journal of Physical Chemistry A, 2013, 117, 3593-3598.	1.1	25
46	Nanoparticle adhesion in proton exchange membrane fuel cell electrodes. Journal of Power Sources, 2013, 241, 634-646.	4.0	25
47	Behavior of Oil Droplets on an Electrified Solid Metal Surface Immersed in Ionic Surfactant Solutions. Langmuir, 2005, 21, 1758-1765.	1.6	23
48	Toward a Predictive Understanding of Water and Charge Transport in Proton Exchange Membranes. Journal of Physical Chemistry B, 2011, 115, 3052-3061.	1.2	23
49	An examination of the shear-thickening behavior of high molecular weight polymers dissolved in low-viscosity Newtonian solvents. Journal of Applied Polymer Science, 2002, 85, 1714-1735.	1.3	22
50	A comparison of simple rheological models and simulation data of n-hexadecane under shear and elongational flows. Journal of Rheology, 2006, 50, 625-640.	1.3	22
51	On the Relationship between Fickian Diffusivities at the Continuum and Molecular Levels. Journal of Physical Chemistry B, 2005, 109, 5279-5288.	1.2	21
52	Energetic and entropic elasticity of nonisothermal flowing polymers: Experiment, theory, and simulation. Journal of Rheology, 2008, 52, 105-140.	1.3	21
53	Atomistic and Coarse-Grained Molecular Dynamics Simulation of a Cross-Linked Sulfonated Poly(1,3-cyclohexadiene)-Based Proton Exchange Membrane. Macromolecules, 2012, 45, 6669-6685.	2.2	21
54	Guestâ€“Host Interactions in Mixed CH₄â€“CO₂ Hydrates: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 19575-19583.	1.5	20

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55	Hierarchical Lignin-Based Carbon Matrix and Carbon Dot Composite Electrodes for High-Performance Supercapacitors. ACS Omega, 2021, 6, 7851-7861.	1.6	20
56	Lithium and Sodium Ion Binding Mechanisms and Diffusion Rates in Lignin-Based Hard Carbon Models. ACS Omega, 2021, 6, 19883-19892.	1.6	20
57	Unidirectional and single-file diffusion in AlPO4-5: molecular dynamics investigations. Molecular Physics, 1996, 87, 367-388.	0.8	20
58	Thermodynamic method for prediction of surfactant-modified oil droplet contact angle. Journal of Colloid and Interface Science, 2004, 270, 229-241.	5.0	19
59	Proton transport in water confined in carbon nanotubes: a reactive molecular dynamics study. Molecular Simulation, 2010, 36, 568-578.	0.9	19
60	Reactive Molecular Dynamics Study of Proton Transport in Polymer Electrolyte Membranes. Journal of Physical Chemistry C, 2011, 115, 18835-18846.	1.5	19
61	Absorbing boundary conditions for molecular dynamics and multiscale modeling. Physical Review B, 2007, 76, .	1.1	18
62	A Grand Canonical Monte Carlo Study of the Adsorption of Methane, Ethane, and Their Mixtures in One-Dimensional Nanoporous Materials. Langmuir, 2002, 18, 10455-10461.	1.6	16
63	Visualization of conformational changes of linear short-chain polyethylenes under shear and elongational flows. Journal of Molecular Graphics and Modelling, 2008, 26, 1046-1056.	1.3	16
64	Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes. Journal of Rheology, 2008, 52, 567-589.	1.3	16
65	Multi-scale models for cross-linked sulfonated poly (1, 3-cyclohexadiene) polymer. Polymer, 2012, 53, 1517-1528.	1.8	16
66	A Reactive Molecular Dynamics Study of the Thermal Decomposition of Perfluorodimethyl Ether. Journal of Physical Chemistry B, 2009, 113, 13670-13677.	1.2	15
67	Use of the Ornstein-Zernike Percus-Yevick equation to extract interaction potentials from pair correlation functions. Physical Review E, 2010, 81, 061204.	0.8	15
68	Structural analysis of lignin-derived carbon composite anodes. Journal of Applied Crystallography, 2014, 47, 1577-1584.	1.9	15
69	Direct Formation and Structural Characterization of Electride C12A7. Materials, 2019, 12, 84.	1.3	15
70	Efficient parallel algorithms for molecular dynamics simulations using variable charge transfer electrostatic potentials. International Journal of Quantum Chemistry, 2000, 80, 733-742.	1.0	14
71	Interfacial Li-ion localization in hierarchical carbon anodes. Carbon, 2017, 111, 828-834.	5.4	14
72	A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the isobaricâ€“isothermal ensemble. Molecular Simulation, 2006, 32, 345-356.	0.9	13

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73	Structure and Diffusion in Cross-Linked and Sulfonated Poly(1,3-cyclohexadiene)/Polyethylene Glycol-Based Proton Exchange Membranes. Journal of Physical Chemistry C, 2013, 117, 4901-4912.	1.5	13
74	Exploiting Single-File Motion in One-Dimensional Nanoporous Materials for Hydrocarbon Separation. Separation Science and Technology, 2003, 38, 977-998.	1.3	12
75	Agreement between Analytical Theory and Molecular Dynamics Simulation for Adsorption and Diffusion in Crystalline Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 376-386.	1.2	12
76	On the relationship between the structure of metalâ€“organic frameworks and the adsorption and diffusion of hydrogen. Molecular Simulation, 2011, 37, 621-639.	0.9	12
77	Impact of oxidation on nanoparticle adhesion to carbon substrates. RSC Advances, 2013, 3, 15792.	1.7	12
78	The temperature dependence of single-file separation mechanisms in one-dimensional nanoporous materials. Chemical Engineering Journal, 1999, 74, 33-42.	6.6	10
79	Entropy-driven structure and dynamics in carbon nanocrystallites. Journal of Nanoparticle Research, 2014, 16, 1.	0.8	10
80	Hydrogen adsorption and diffusion in amorphous, metal-decorated nanoporous silica. International Journal of Hydrogen Energy, 2014, 39, 9241-9253.	3.8	10
81	Elucidating nano and meso-structures of lignin carbon composites: A comprehensive study of feedstock and temperature dependence. Carbon, 2020, 161, 856-869.	5.4	10
82	Estimation and analysis of the rheological properties of a perfluoropolyether through molecular dynamics simulation. Journal of Fluorine Chemistry, 2006, 127, 787-795.	0.9	9
83	High temperature proton exchange membranes with enhanced proton conductivities at low humidity and high temperature based on polymer blends and block copolymers of poly(1,3-cyclohexadiene) and poly(ethylene glycol). Polymer, 2015, 77, 208-217.	1.8	9
84	Molecular Rotational Dynamics in Mixed CH₄â€“CO₂ Hydrates: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 26251-26262.	1.5	9
85	A generalized analytical theory for adsorption of fluids in nanoporous materials. Molecular Physics, 2002, 100, 2689-2701.	0.8	8
86	Thermodynamic Model for the Prediction of Contact Angles of Oil Droplets on Solid Surfaces in SDS Solutions. Separation Science and Technology, 2003, 38, 2815-2835.	1.3	8
87	Surfactant and Electric Field Strength Effects on Surface Tension at Liquid/Liquid/Solid Interfaces. Langmuir, 2006, 22, 5358-5365.	1.6	8
88	Theoretical Calculation of Thermodynamic Properties of Naphthalene, Methylnaphthalenes, and Dimethylnaphthalenes. Journal of Chemical & Engineering Data, 2007, 52, 1843-1850.	1.0	8
89	A comparison between entropies of aromatic compounds from quantum mechanical calculations and experiment. Computational and Theoretical Chemistry, 2007, 802, 23-34.	1.5	8
90	A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the canonical ensemble. Journal of Non-Newtonian Fluid Mechanics, 2008, 152, 129-139.	1.0	8

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91	Effects of ultramicroelectrode dimensions on the electropolymerization of polypyrrole. Journal of Applied Physics, 2009, 105, 124312.	1.1	8
92	Hierarchical Model for the Analysis of Scattering Data of Complex Materials. Jom, 2016, 68, 1583-1588.	0.9	8
93	Li-Ion Localization and Energetics as a Function of Anode Structure. ACS Applied Materials & Interfaces, 2017, 9, 6988-7002.	4.0	8
94	Lithium and sodium ion binding in nanostructured carbon composites. Molecular Simulation, 2021, 47, 878-887.	0.9	8
95	Local structure and distortions of mixed methane-carbon dioxide hydrates. Communications Chemistry, 2021, 4, .	2.0	8
96	Single-file motion of polyatomic molecules in one-dimensional nanoporous materials. Molecular Physics, 2002, 100, 2727-2733.	0.8	7
97	Molecularâ€Level Investigation of Critical Gap Size between Catalyst Particles and Electrolyte in Hydrogen Proton Exchange Membrane Fuel Cells. Fuel Cells, 2008, 8, 422-428.	1.5	7
98	A multiscale modeling demonstration based on the pair correlation function. Journal of Non-Newtonian Fluid Mechanics, 2008, 152, 140-147.	1.0	7
99	Effect of Low Concentration Salt on Organic Contact Angle in Ionic Surfactant Solutions: Insight from Theory and Experiment. Separation Science and Technology, 2008, 43, 310-330.	1.3	7
100	Structure and proton transport in proton exchange membranes based on cross-linked sulfonated poly (1, 3-cyclohexadiene) with varying local acid environment. Polymer, 2013, 54, 2299-2307.	1.8	7
101	Intrinsic relationships between proton conductivity and nanopore size and functionalization. Microporous and Mesoporous Materials, 2013, 177, 17-24.	2.2	7
102	The effect of process parameters on the amorphous citrate sol-gel synthesis of Cu-doped Ca12Al14O33. Materialia, 2018, 4, 466-477.	1.3	7
103	Entropy Pair Functional Theory: Direct Entropy Evaluation Spanning Phase Transitions. Entropy, 2021, 23, 234.	1.1	7
104	An analytical theory for diffusion of fluids in crystalline nanoporous materials. Molecular Physics, 2003, 101, 1399-1412.	0.8	6
105	Comparison of rheological properties of short-chain perfluoropolyethers through simulation and experiment. Molecular Simulation, 2007, 33, 871-878.	0.9	6
106	Methane and carbon dioxide adsorption and diffusion in amorphous, metal-decorated nanoporous silica. Molecular Simulation, 2014, 40, 618-633.	0.9	6
107	Materials Fingerprinting Classification. Computer Physics Communications, 2021, 266, 108019.	3.0	6
108	Development of Nanocrystalline Graphite from Lignin Sources. ACS Sustainable Chemistry and Engineering, 2022, 10, 1786-1794.	3.2	6

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109	Obtaining transport diffusion coefficients from self-diffusion coefficients in nanoporous adsorption systems. Molecular Physics, 2004, 102, 471-483.	0.8	5
110	Shear Thickening in Dilute Polymer Solutions: Transient Analysis. Chemical Engineering Communications, 2005, 192, 89-107.	1.5	5
111	Lithium diffusion at Si-C interfaces in silicon-graphene composites. Applied Physics Letters, 2014, 105, .	1.5	5
112	Electron beam induced radiation damage in the catalyst layer of a proton exchange membrane fuel cell. Scanning, 2014, 36, 338-346.	0.7	5
113	The Adsorption Properties of Amorphous, Metal-Decorated Microporous Silsesquioxanes for Mixtures of Carbon Dioxide, Methane and Hydrogen. Journal of Physical Chemistry C, 2014, 118, 13008-13017.	1.5	5
114	Ab Initio Molecular Dynamics Simulations of an Excess Proton in a Triethylene Glycolâ€“Water Solution: Solvation Structure, Mechanism, and Kinetics. Journal of Physical Chemistry B, 2016, 120, 5223-5242.	1.2	5
115	Evaluation of nano- and mesoscale structural features in composite materials through hierarchical decomposition of the radial distribution function. Journal of Applied Crystallography, 2018, 51, 76-86.	1.9	5
116	A test case for predicting the rheological properties of polymeric liquids: the multiple coupled Maxwell modes model. Journal of Non-Newtonian Fluid Mechanics, 2004, 120, 11-32.	1.0	4
117	Using multiple-mode models for fitting and predicting rheological properties of polymeric melts. Journal of Applied Polymer Science, 2006, 99, 405-423.	1.3	4
118	A Quantum Mechanical Study of the Decomposition of CF3OCF3 and CF3CF2OCF2CF3 in the Presence of AlF3. Journal of Physical Chemistry A, 2008, 112, 2604-2609.	1.1	4
119	Comparison of perfluoropolyethers andn-alkanes under shear via nonequilibrium molecular dynamics simulation. Molecular Simulation, 2008, 34, 231-242.	0.9	4
120	Molecular simulations of H2 adsorption in metal-porphyrin frameworks: A potential new material evaluation. Journal of Renewable and Sustainable Energy, 2011, 3, 053105.	0.8	4
121	Influence of Aqueous/Solid Interactions on Organic Droplet Shape in Liquid/Liquid/Solid Systems. Separation Science and Technology, 2006, 41, 2515-2531.	1.3	2
122	Structure of oxidised silver (1â€‰1â€‰1) and (1â€‰1â€‰0) surfaces. Molecular Simulation, 2017, 43, 355-369.	0.9	2
123	Local structure analysis of low-temperature neutron pair distribution function coupled with molecular dynamics simulations of CH4 and CO2 hydrates from 2 to 210ÂK. Fuel, 2021, 299, 120908.	3.4	2
124	Scaling point set registration in 3D across thread counts on multicore and hardware accelerator platforms through autotuning for large scale analysis of scientific point clouds. , 2017, , .		1
125	Reactive molecular dynamics simulations of an excess proton in polyethylene glycol-water solutions. Molecular Simulation, 2019, 45, 381-393.	0.9	1
126	Bayesian Point Set Registration. MATRIX Book Series, 2019, , 99-120.	0.2	1

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127	Assessment of Local Observation of Atomic Ordering in Alloys via the Radial Distribution Function: A Computational and Experimental Approach. Frontiers in Materials, 2021, 8, .	1.2	1
128	Board 130: NSF S-STEM: Transfer Success Co-Design for Engineering Disciplines (TranSCEnD). , 0, , .		1
129	Exploration of Entropy Pair Functional Theory. Entropy, 2022, 24, 603.	1.1	1
130	In situ inelastic neutron scattering of mixed CH4â€“CO2 hydrates. Fuel, 2022, 327, 125197.	3.4	1
131	Atomic-Scale Simulations of Structural Properties of Ceramics. Materials Research Society Symposia Proceedings, 1996, 453, 209.	0.1	0
132	Using multiple-mode models for fitting and predicting the rheological properties of polymeric melts. II. Single and double step-strain flows. Journal of Applied Polymer Science, 2007, 105, 2884-2892.	1.3	0
133	Self-Consistent Multiscale Modeling in the Presence of Inhomogeneous Fields. Multiscale Modeling and Simulation, 2009, 8, 193-203.	0.6	0
134	Nano-Particle Adhesion in PEM Fuel Cell Electrodes. ECS Meeting Abstracts, 2012, , .	0.0	0
135	Molecular-Level Modeling of the Structure and Proton Transport within the Membrane Electrode Assembly of Hydrogen Proton Exchange Membrane Fuel Cells. Modern Aspects of Electrochemistry, 2010, , 133-202.	0.2	0
136	In situ characterization of the synthesis of Ca12Al14O33 under non-ambient atmospheres. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a349-a349.	0.0	0
137	Local Structure Analysis and Modelling of Ligninâ€Based Carbon Composites through the Hierarchical Decomposition of the Radial Distribution Function. ChemistryOpen, 2022, 11, e202100220.	0.9	0