Billy D Todd

List of Publications by Year
in descending order

132 papers	4,472 citations	126907 33 h-index	128289 60 g-index
138 all docs	138 docs citations	138 times ranked	2829 citing authors

#	Article	IF	Citations
1	Pressure tensor for inhomogeneous fluids. Physical Review E, 1995, 52, 1627-1638.	2.1	351
2	Departure from Navier-Stokes hydrodynamics in confined liquids. Physical Review E, 1997, 55, 4288-4295.	2.1	293
3	How fast does water flow in carbon nanotubes?. Journal of Chemical Physics, 2013, 138, 094701.	3.0	240
4	Slip length of water on graphene: Limitations of non-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 024705.	3.0	166
5	Surface and bulk properties of metals modelled with Sutton-Chen potentials. Surface Science, 1993, 281, 191-206.	1.9	145
6	Thermostating highly confined fluids. Journal of Chemical Physics, 2010, 132, 244706.	3.0	129
7	Homogeneous non-equilibrium molecular dynamics simulations of viscous flow: techniques and applications. Molecular Simulation, 2007, 33, 189-229.	2.0	110
8	Slip flow in graphene nanochannels. Journal of Chemical Physics, 2011, 135, 144701.	3.0	104
9	A simple, direct derivation and proof of the validity of the SLLOD equations of motion for generalized homogeneous flows. Journal of Chemical Physics, 2006, 124, 194103.	3.0	97
10	Nonequilibrium Molecular Dynamics Simulations of Planar Elongational Flow with Spatially and Temporally Periodic Boundary Conditions. Physical Review Letters, 1998, 81, 1118-1121.	7.8	86
11	Prediction of fluid velocity slip at solid surfaces. Physical Review E, 2011, 84, 016313.	2.1	86
12	Heat flux vector in highly inhomogeneous nonequilibrium fluids. Physical Review E, 1995, 51, 4362-4368.	2.1	83
13	Nonlinear shear and elongational rheology of model polymer melts by non-equilibrium molecular dynamics. Journal of Non-Newtonian Fluid Mechanics, 2003, 111, 1-18.	2.4	72
14	Temperature profile for Poiseuille flow. Physical Review E, 1997, 55, 2800-2807.	2.1	71
15	A study of viscosity inhomogeneity in porous media. Journal of Chemical Physics, 1997, 106, 4684-4695.	3.0	69
16	The heat flux vector for highly inhomogeneous nonequilibrium fluids in very narrow pores. Journal of Chemical Physics, 1995, 103, 9804-9809.	3.0	62
17	Nonlocal Shear Stress for Homogeneous Fluids. Physical Review Letters, 2008, 100, 195901.	7.8	61
18	A new algorithm for unrestricted duration nonequilibrium molecular dynamics simulations of planar elongational flow. Computer Physics Communications, 1999, 117, 191-199.	7.5	57

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19	Viscoelastic properties of dendrimers in the melt from nonequlibrium molecular dynamics. Journal of Chemical Physics, 2004, 121, 12050-12059.	3.0	54
20	Viscosity of confined inhomogeneous nonequilibrium fluids. Journal of Chemical Physics, 2004, 121, 10778-10786.	3.0	51
21	Parameterization of the nonlocal viscosity kernel for an atomic fluid. Physical Review E, 2007, 76, 041121.	2.1	51
22	Comparison of planar shear flow and planar elongational flow for systems of small molecules. Journal of Chemical Physics, 2000, 113, 9122-9131.	3.0	45
23	Internal structure of dendrimers in the melt under shear: A molecular dynamics study. Journal of Chemical Physics, 2004, 121, 1091-1096.	3.0	45
24	Electropumping of water with rotating electric fields. Journal of Chemical Physics, 2013, 138, 154712.	3.0	43
25	Molecular simulation of dendrimers and their mixtures under shear: Comparison of isothermal-isobaric (NpT) and isothermal-isochoric (NVT) ensemble systems. Journal of Chemical Physics, 2005, 123, 034905.	3.0	42
26	Nonlocal viscous transport and the effect on fluid stress. Physical Review E, 2008, 78, 051202.	2.1	41
27	The stability of nonequilibrium molecular dynamics simulations of elongational flows. Journal of Chemical Physics, 2000, 112, 40-46.	3.0	40
28	A molecular dynamics study of nitric oxide in water: Diffusion and structure. Journal of Chemical Physics, 2005, 123, 054505.	3.0	40
29	Effects of Confinement on the Dielectric Response of Water Extends up to Mesoscale Dimensions. Langmuir, 2016, 32, 4765-4773.	3.5	38
30	Slip of Alkanes Confined between Surfactant Monolayers Adsorbed on Solid Surfaces. Langmuir, 2018, 34, 3864-3873.	3.5	37
31	Analytic dependence of the pressure and energy of an atomic fluid under shear. Physical Review E, 2001, 63, 021204.	2.1	36
32	Interfacial slip friction at a fluid-solid cylindrical boundary. Journal of Chemical Physics, 2012, 136, 244704.	3.0	35
33	Modeling slip and flow enhancement of water in carbon nanotubes. MRS Bulletin, 2017, 42, 283-288.	3.5	35
34	Continuum Nanofluidics. Langmuir, 2015, 31, 13275-13289.	3.5	33
35	Application of transient-time correlation functions to nonequilibrium molecular-dynamics simulations of elongational flow. Physical Review E, 1997, 56, 6723-6728.	2.1	31
36	Nonlinear shear and elongational rheology of model polymer melts at low strain rates. Journal of Non-Newtonian Fluid Mechanics, 2007, 147, 35-44.	2.4	30

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37	Diffusion of linear polymer melts in shear and extensional flows. Journal of Chemical Physics, 2009, 131, 054904.	3.0	30
38	Molecular Dynamics Study of Nanoconfined Water Flow Driven by Rotating Electric Fields under Realistic Experimental Conditions. Langmuir, 2014, 30, 3095-3109.	3.5	30
39	A technique for the calculation of mass, energy, and momentum densities at planes in molecular dynamics simulations. Journal of Chemical Physics, 1996, 104, 9651-9653.	3.0	29
40	Computer simulation of simple and complex atomistic fluids by nonequilibrium molecular dynamics techniques. Computer Physics Communications, 2001, 142, 14-21.	7.5	28
41	Analysis of the shape of dendrimers under shear. Journal of Chemical Physics, 2006, 124, 044910.	3.0	28
42	Nanoflow hydrodynamics. Physical Review E, 2011, 84, 036311.	2.1	28
43	Equilibrium and nonequilibrium molecular dynamics methods for determining solidâ€“liquid phase coexistence at equilibrium. Journal of Chemical Physics, 2003, 119, 11017-11023.	3.0	26
44	Electropumping of Water in Functionalized Carbon Nanotubes Using Rotating Electric Fields. Journal of Physical Chemistry C, 2017, 121, 28158-28165.	3.1	26
45	Elongational viscosities from nonequilibrium molecular dynamics simulations of oscillatory elongational flow. Journal of Chemical Physics, 1997, 107, 1617-1624.	3.0	25
46	Cell neighbor list method for planar elongational flow: rheology of a diatomic fluid. Computer Physics Communications, 2003, 151, 35-46.	7.5	25
47	Kinetics and chemomechanical properties of the F1-ATPase molecular motor. Journal of Chemical Physics, 2003, 118, 9890-9898.	3.0	25
48	Molecular spin in nano-confined fluidic flows. Microfluidics and Nanofluidics, 2009, 6, 785-795.	2.2	25
49	Rotational and spin viscosities of water: Application to nanofluidics. Journal of Chemical Physics, 2010, 133, 144906.	3.0	25
50	Density dependence of the stress relaxation function of a simple fluid. Physical Review E, 2013, 87, .	2.1	25
51	On the relationship between two-body and three-body interactions from nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 2001, 115, 9410-9413.	3.0	24
52	Scaling behavior for the pressure and energy of shearing fluids. Physical Review E, 2003, 67, 061201.	2.1	23
53	Structural properties of hyperbranched polymers in the melt under shear via nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 2009, 130, 074901.	3.0	23
54	Structural and dynamical properties for confined polymers undergoing planar Poiseuille flow. Journal of Chemical Physics, 2007, 126, 144907.	3.0	22

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55	Nonlocal viscosity of polymer melts approaching their glassy state. Journal of Chemical Physics, 2010, 133, 144907.	3.0	22
56	Non-Newtonian behavior and molecular structure of Cooee bitumen under shear flow: A non-equilibrium molecular dynamics study. Journal of Chemical Physics, 2015, 142, 244501.	3.0	22
57	Prediction of Kapitza resistance at fluid-solid interfaces. Journal of Chemical Physics, 2019, 151, 194502.	3.0	21
58	A non-local hydrodynamic model for the shear viscosity of confined fluids: analysis of a homogeneous kernel. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 035501.	2.1	20
59	A new algorithm for extended nonequilibrium molecular dynamics simulations of mixed flow. Journal of Chemical Physics, 2010, 133, 154116.	3.0	20
60	Flow of water through carbon nanotubes predicted by different atomistic water models. Journal of Chemical Physics, 2019, 150, 194501.	3.0	20
61	Kapitza resistance at waterâ€“graphene interfaces. Journal of Chemical Physics, 2020, 152, 224703.	3.0	20
62	On the Arnold cat map and periodic boundary conditions for planar elongational flow. Molecular Physics, 2003, 101, 3445-3454.	1.7	19
63	Rheology of hyperbranched polymer melts undergoing planar Couette flow. Journal of Chemical Physics, 2009, 131, 044902.	3.0	19
64	Computation of thermodynamic and transport properties to predict thermophoretic effects in an argon-krypton mixture. Journal of Chemical Physics, 2013, 139, 144504.	3.0	19
65	A new and effective method for thermostatting confined fluids. Journal of Chemical Physics, 2014, 140, 054502.	3.0	19
66	Transient-time correlation function applied to mixed shear and elongational flows. Journal of Chemical Physics, 2012, 136, 064105.	3.0	18
67	Nonequilibrium molecular dynamics simulation of dendrimers and hyperbranched polymer melts undergoing planar elongational flow. Journal of Rheology, 2014, 58, 281-305.	2.6	18
68	Analytical Diffusion Mechanism (ADiM) model combining specular, Knudsen and surface diffusion. Journal of Membrane Science, 2015, 485, 1-9.	8.2	18
69	Brownian dynamics simulations of planar mixed flows of polymer solutions at finite concentrations. Chemical Engineering Science, 2015, 121, 245-257.	3.8	18
70	Fast transport of water in carbon nanotubes: a review of current accomplishments and challenges. Molecular Simulation, 2021, 47, 905-924.	2.0	18
71	Nanoconfinement Effects on the Kapitza Resistance at Waterâ€“CNT Interfaces. Langmuir, 2021, 37, 2355-2361.	3.5	18
72	Porous Aromatic Frameworks Impregnated with Lithiated Fullerenes for Natural Gas Purification. Journal of Physical Chemistry C, 2015, 119, 9347-9354.	3.1	17

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73	Energy and pressure of shearing fluids at different state points. Physical Review E, 2001, 64, 021201.	2.1	16
74	Pressure tensor and heat flux vector for inhomogeneous nonequilibrium fluids under the influence of three-body forces. Physical Review E, 2004, 69, 031111.	2.1	16
75	Challenges in Nanofluidicsâ€"Beyond Navierâ€"Stokes at the Molecular Scale. Processes, 2018, 6, 144.	2.8	16
76	Efficiency of Electropumping in Nanochannels. Nano Letters, 2020, 20, 3396-3402.	9.1	16
77	Viscous properties of isotropic fluids composed of linear molecules: Departure from the classical Navier-Stokes theory in nano-confined geometries. Physical Review E, 2009, 80, 046322.	2.1	15
78	Shear rheology and structural properties of chemically identical dendrimer-linear polymer blends through molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 194905.	3.0	15
79	Molecular simulation of the shear viscosity and the self-diffusion coefficient of mercury along the vapor-liquid coexistence curve. Journal of Chemical Physics, 2005, 123, 034511.	3.0	14
80	Local linear viscoelasticity of confined fluids. Journal of Chemical Physics, 2007, 126, 144706.	3.0	13
81	Linear and nonlinear density response functions for a simple atomic fluid. Journal of Chemical Physics, 2013, 139, 044510.	3.0	13
82	Nonlocal response functions for predicting shear flow of strongly inhomogeneous fluids. I. Sinusoidally driven shear and sinusoidally driven inhomogeneity. Physical Review E, 2015, 91, 062132.	2.1	13
83	Viscoelasticity of liquid water investigated using molecular dynamics simulations. Physical Review Fluids, 2019, 4, .	2.5	13
84	Nonlinear response theory for time-periodic elongational flows. Physical Review E, 1998, 58, 4587-4593.	2.1	12
85	Power-law exponents for the shear viscosity of non-Newtonian simple fluids. Physical Review E, 2005, 72, 041204.	2.1	12
86	Allosteric Conformational Transition in Adenylate Kinase: Dynamic Correlations and Implication for Allostery. Australian Journal of Chemistry, 2010, 63, 405.	0.9	12
87	Viscosity kernel of molecular fluids: Butane and polymer melts. Physical Review E, 2010, 82, 011801.	2.1	12
88	Porous Aromatic Frameworks Impregnated with Fullerenes for Enhanced Methanol/Water Separation. Langmuir, 2014, 30, 14621-14630.	3.5	12
89	Nonlocal response functions for predicting shear flow of strongly inhomogeneous fluids. II. Sinusoidally driven shear and multisinusoidal inhomogeneity. Physical Review E, 2015, 92, 012108.	2.1	12
90	Measuring heat flux beyond Fourierâ€™s law. Journal of Chemical Physics, 2019, 150, 064103.	3.0	12

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91	The strain rate dependence of shear viscosity, pressure and energy from two-body and three-body interactions. Fluid Phase Equilibria, 2001, 183-184, 371-379.	2.5	11
92	Cats, maps and nanoflows: some recent developments in nonequilibrium nanofluidics. Molecular Simulation, 2005, 31, 411-428.	2.0	11
93	Chaotic properties of planar elongational flow and planar shear flow: Lyapunov exponents, conjugate-pairing rule, and phase space contraction. Physical Review E, 2006, 73, 046206.	2.1	11
94	Molecular dynamics simulation of planar elongational flow at constant pressure and constant temperature. Journal of Chemical Physics, 2007, 126, 044506.	3.0	11
95	Coarseâ€grained dynamics of the receiver domain of NtrC: Fluctuations, correlations and implications for allosteric cooperativity. Proteins: Structure, Function and Bioinformatics, 2008, 73, 218-227.	2.6	11
96	Dynamical properties of a confined diatomic fluid undergoing zero mean oscillatory flow: Effect of molecular rotation. Physical Review E, 2008, 77, 066707.	2.1	11
97	A comparison of model linear chain molecules with constrained and flexible bond lengths under planar Couette and extensional flows. Molecular Simulation, 2009, 35, 1153-1167.	2.0	11
98	Strategies toward Enhanced Low-Pressure Volumetric Hydrogen Storage in Nanoporous Cryoadsorbents. Langmuir, 2013, 29, 15689-15697.	3.5	11
99	A constitutive framework for the non-Newtonian pressure tensor of a simple fluid under planar flows. Journal of Chemical Physics, 2013, 138, 244508.	3.0	11
100	A molecular dynamics investigation of the planar elongational rheology of chemically identical dendrimer-linear polymer blends. Journal of Chemical Physics, 2015, 142, 174911.	3.0	11
101	Dynamic and coordinating domain motions in the active subunits of the F1-ATPase molecular motor. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1553-1560.	2.3	10
102	Generalized extended Navier-Stokes theory: Correlations in molecular fluids with intrinsic angular momentum. Journal of Chemical Physics, 2013, 138, 034503.	3.0	10
103	Effects of nanoscale density inhomogeneities on shearing fluids. Physical Review E, 2013, 88, 052143.	2.1	10
104	Frequency-Dependent Elongational Viscosity by Nonequilibrium Molecular Dynamics. International Journal of Thermophysics, 1998, 19, 1063-1072.	2.1	9
105	Complex cooperativity of ATP hydrolysis in the F1-ATPase molecular motor. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2004, 1698, 197-202.	2.3	9
106	Cooperativity in the motor activities of the ATP-fueled molecular motors. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1752, 111-123.	2.3	9
107	The effect of interbranch spacing on structural and rheological properties of hyperbranched polymer melts. Journal of Chemical Physics, 2009, 131, 164901.	3.0	9
108	Comment on â€œMolecular simulation and continuum mechanics study of simple fluids in nonisothermal planar Couette flowsâ€•[J. Chem. Phys. 107, 2589 (1997)]. Journal of Chemical Physics, 1999, 111, 10730-10731.	3.0	8

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109	Lyapunov spectra and conjugate-pairing rule for confined atomic fluids. Journal of Chemical Physics, 2010, 132, 244508.	3.0	8
110	An extended analysis of the viscosity kernel for monatomic and diatomic fluids. Journal of Physics Condensed Matter, 2010, 22, 195105.	1.8	8
111	Inducing a Net Positive Flow of Water in Functionalized Concentric Carbon Nanotubes Using Rotating Electric Fields. Langmuir, 2019, 35, 14742-14749.	3.5	8
112	Effects of Electrostatic Interactions on Kapitza Resistance in Hexagonal Boron Nitrideâ€“Water Interfaces. Langmuir, 2022, 38, 8783-8793.	3.5	8
113	Mass and Energy Transport Through Slit Pores: Application to Planar Poiseuille Flow. Molecular Simulation, 1996, 17, 317-332.	2.0	7
114	Rotational viscosity of fluids composed of linear molecules: An equilibrium molecular dynamics study. Journal of Chemical Physics, 2008, 128, 224507.	3.0	7
115	Improved methodology to compute the intrinsic friction coefficient at solidâ€“liquid interfaces. Journal of Chemical Physics, 2021, 154, 184707.	3.0	7
116	Equilibrium and nonequilibrium molecular dynamics methods to compute the first normal stress coefficient of a model polymer solution. Physical Review Fluids, 2020, 5, .	2.5	7
117	Boundary condition independence of molecular dynamics simulations of planar elongational flow. Physical Review E, 2007, 75, 066702.	2.1	5
118	Limits to Auger-electron core-loss electron coincidence spectroscopy. Surface Science, 1992, 278, 193-201.	1.9	4
119	Chaotic properties of isokinetic-isobaric atomic systems under planar shear and elongational flows. Physical Review E, 2008, 77, 056217.	2.1	4
120	Hydrodynamic slip of alkali chloride solutions in uncharged graphene nanochannels. Journal of Chemical Physics, 2022, 156, 014704.	3.0	4
121	Slip and stress from low shear rate nonequilibrium molecular dynamics: The transient-time correlation function technique. Journal of Chemical Physics, 2022, 156, 184111.	3.0	4
122	Computation of the equilibrium three-particle entropy for dense atomic fluids by molecular dynamics simulation. Journal of Chemical Physics, 2019, 151, 164102.	3.0	3
123	Beyond Traditional Effective Intermolecular Potentials and Pairwise Interactions in Molecular Simulation. Lecture Notes in Computer Science, 2002, , 932-941.	1.3	3
124	Electropumping of nanofluidic water by linear and angular momentum coupling: theoretical foundations and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 25003-25018.	2.8	3
125	Generalized hydrodynamics of the Lennard-Jones liquid in view of hidden scale invariance. Physical Review E, 2021, 104, 054126.	2.1	3
126	Deviations From Classical Hydrodynamic Theory in Highly Confined Planar Poiseuille Flow of a Polymer Solution. Computational Methods in Science and Technology, 2017, 23, .	0.3	2

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127	Nonlocal viscosity kernel of mixtures. Physical Review E, 2012, 85, 022201.	2.1	1
128	Ergodicity of a Single Particle Confined in a Nanopore. Journal of Statistical Physics, 2012, 148, 1156-1169.	1.2	1
129	Rheology and Structural Properties of Hyperbranched Polymers: a Non-Equilibrium Molecular Dynamics Study. AIP Conference Proceedings, 2008, , .	0.4	0
130	Propagation speed of a chemical wave front: effect of confinement. Molecular Simulation, 2009, 35, 186-192.	2.0	0
131	Planar mixed flow and chaos: Lyapunov exponents and the conjugate-pairing rule. Journal of Chemical Physics, 2011, 134, 114112.	3.0	0
132	The phase space distribution of confined fluids under shear is not fractal. Journal of Chemical Physics, 2021, 154, 094116.	3.0	0