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	Hydrodynamic slip of alkali chloride solutions in uncharged graphene nanochannels. Journal of Chemical Physics, 2022, 156, 014704.	3.0	4
2	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
3	Effects of Electrostatic Interactions on Kapitza Resistance in Hexagonal Boron Nitrideâ€“Water Interfaces. Langmuir, 2022, 38, 8783-8793.	3.5	8
4	Fast transport of water in carbon nanotubes: a review of current accomplishments and challenges. Molecular Simulation, 2021, 47, 905-924.	2.0	18
5	Nanoconfinement Effects on the Kapitza Resistance at Waterâ€“CNT Interfaces. Langmuir, 2021, 37, 2355-2361.	3.5	18
6	The phase space distribution of confined fluids under shear is not fractal. Journal of Chemical Physics, 2021, 154, 094116.	3.0	0
7	Improved methodology to compute the intrinsic friction coefficient at solidâ€“liquid interfaces. Journal of Chemical Physics, 2021, 154, 184707.	3.0	7
8	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
9	Generalized hydrodynamics of the Lennard-Jones liquid in view of hidden scale invariance. Physical Review E, 2021, 104, 054126.	2.1	3
10	Kapitza resistance at waterâ€“graphene interfaces. Journal of Chemical Physics, 2020, 152, 224703.	3.0	20
11	Efficiency of Electropumping in Nanochannels. Nano Letters, 2020, 20, 3396-3402.	9.1	16
12	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
13	Inducing a Net Positive Flow of Water in Functionalized Concentric Carbon Nanotubes Using Rotating Electric Fields. Langmuir, 2019, 35, 14742-14749.	3.5	8
14	Flow of water through carbon nanotubes predicted by different atomistic water models. Journal of Chemical Physics, 2019, 150, 194501.	3.0	20
15	Measuring heat flux beyond Fourierâ€™s law. Journal of Chemical Physics, 2019, 150, 064103.	3.0	12
16	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
17	Prediction of Kapitza resistance at fluid-solid interfaces. Journal of Chemical Physics, 2019, 151, 194502.	3.0	21
18	Viscoelasticity of liquid water investigated using molecular dynamics simulations. Physical Review Fluids, 2019, 4, .	2.5	13

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19	Slip of Alkanes Confined between Surfactant Monolayers Adsorbed on Solid Surfaces. Langmuir, 2018, 34, 3864-3873.	3.5	37
20	Challenges in Nanofluidicsâ€"Beyond Navierâ€"Stokes at the Molecular Scale. Processes, 2018, 6, 144.	2.8	16
21	Modeling slip and flow enhancement of water in carbon nanotubes. MRS Bulletin, 2017, 42, 283-288.	3.5	35
22	Electropumping of Water in Functionalized Carbon Nanotubes Using Rotating Electric Fields. Journal of Physical Chemistry C, 2017, 121, 28158-28165.	3.1	26
23	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
24	Effects of Confinement on the Dielectric Response of Water Extends up to Mesoscale Dimensions. Langmuir, 2016, 32, 4765-4773.	3.5	38
25	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
26	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
27	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
28	Porous Aromatic Frameworks Impregnated with Lithiated Fullerenes for Natural Gas Purification. Journal of Physical Chemistry C, 2015, 119, 9347-9354.	3.1	17
29	Analytical Diffusion Mechanism (ADiM) model combining specular, Knudsen and surface diffusion. Journal of Membrane Science, 2015, 485, 1-9.	8.2	18
30	Continuum Nanofluidics. Langmuir, 2015, 31, 13275-13289.	3.5	33
31	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
32	Brownian dynamics simulations of planar mixed flows of polymer solutions at finite concentrations. Chemical Engineering Science, 2015, 121, 245-257.	3.8	18
33	A new and effective method for thermostatting confined fluids. Journal of Chemical Physics, 2014, 140, 054502.	3.0	19
34	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
35	Nonequilibrium molecular dynamics simulation of dendrimers and hyperbranched polymer melts undergoing planar elongational flow. Journal of Rheology, 2014, 58, 281-305.	2.6	18
36	Porous Aromatic Frameworks Impregnated with Fullerenes for Enhanced Methanol/Water Separation. Langmuir, 2014, 30, 14621-14630.	3.5	12

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37	Molecular Dynamics Study of Nanoconfined Water Flow Driven by Rotating Electric Fields under Realistic Experimental Conditions. Langmuir, 2014, 30, 3095-3109.	3.5	30
38	Generalized extended Navier-Stokes theory: Correlations in molecular fluids with intrinsic angular momentum. Journal of Chemical Physics, 2013, 138, 034503.	3.0	10
39	How fast does water flow in carbon nanotubes?. Journal of Chemical Physics, 2013, 138, 094701.	3.0	240
40	Strategies toward Enhanced Low-Pressure Volumetric Hydrogen Storage in Nanoporous Cryoadsorbents. Langmuir, 2013, 29, 15689-15697.	3.5	11
41	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
42	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
43	Linear and nonlinear density response functions for a simple atomic fluid. Journal of Chemical Physics, 2013, 139, 044510.	3.0	13
44	Density dependence of the stress relaxation function of a simple fluid. Physical Review E, 2013, 87, .	2.1	25
45	Electropumping of water with rotating electric fields. Journal of Chemical Physics, 2013, 138, 154712.	3.0	43
46	Effects of nanoscale density inhomogeneities on shearing fluids. Physical Review E, 2013, 88, 052143.	2.1	10
47	Nonlocal viscosity kernel of mixtures. Physical Review E, 2012, 85, 022201.	2.1	1
48	Interfacial slip friction at a fluid-solid cylindrical boundary. Journal of Chemical Physics, 2012, 136, 244704.	3.0	35
49	Slip length of water on graphene: Limitations of non-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 024705.	3.0	166
50	Transient-time correlation function applied to mixed shear and elongational flows. Journal of Chemical Physics, 2012, 136, 064105.	3.0	18
51	Ergodicity of a Single Particle Confined in a Nanopore. Journal of Statistical Physics, 2012, 148, 1156-1169.	1.2	1
52	Nanoflow hydrodynamics. Physical Review E, 2011, 84, 036311.	2.1	28
53	Prediction of fluid velocity slip at solid surfaces. Physical Review E, 2011, 84, 016313.	2.1	86
54	Planar mixed flow and chaos: Lyapunov exponents and the conjugate-pairing rule. Journal of Chemical Physics, 2011, 134, 114112.	3.0	0

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55	Slip flow in graphene nanochannels. Journal of Chemical Physics, 2011, 135, 144701.	3.0	104
56	Thermostating highly confined fluids. Journal of Chemical Physics, 2010, 132, 244706.	3.0	129
57	Rotational and spin viscosities of water: Application to nanofluidics. Journal of Chemical Physics, 2010, 133, 144906.	3.0	25
58	A new algorithm for extended nonequilibrium molecular dynamics simulations of mixed flow. Journal of Chemical Physics, 2010, 133, 154116.	3.0	20
59	Lyapunov spectra and conjugate-pairing rule for confined atomic fluids. Journal of Chemical Physics, 2010, 132, 244508.	3.0	8
60	Nonlocal viscosity of polymer melts approaching their glassy state. Journal of Chemical Physics, 2010, 133, 144907.	3.0	22
61	An extended analysis of the viscosity kernel for monatomic and diatomic fluids. Journal of Physics Condensed Matter, 2010, 22, 195105.	1.8	8
62	Allosteric Conformational Transition in Adenylate Kinase: Dynamic Correlations and Implication for Allostery. Australian Journal of Chemistry, 2010, 63, 405.	0.9	12
63	Viscosity kernel of molecular fluids: Butane and polymer melts. Physical Review E, 2010, 82, 011801.	2.1	12
64	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
65	Rheology of hyperbranched polymer melts undergoing planar Couette flow. Journal of Chemical Physics, 2009, 131, 044902.	3.0	19
66	Diffusion of linear polymer melts in shear and extensional flows. Journal of Chemical Physics, 2009, 131, 054904.	3.0	30
67	The effect of interbranch spacing on structural and rheological properties of hyperbranched polymer melts. Journal of Chemical Physics, 2009, 131, 164901.	3.0	9
68	Propagation speed of a chemical wave front: effect of confinement. Molecular Simulation, 2009, 35, 186-192.	2.0	0
69	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
70	Molecular spin in nano-confined fluidic flows. Microfluidics and Nanofluidics, 2009, 6, 785-795.	2.2	25
71	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
72	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

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73	Rheology and Structural Properties of Hyperbranched Polymers: a Non-Equilibrium Molecular Dynamics Study. AIP Conference Proceedings, 2008, , .	0.4	0
74	Rotational viscosity of fluids composed of linear molecules: An equilibrium molecular dynamics study. Journal of Chemical Physics, 2008, 128, 224507.	3.0	7
75	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
76	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
77	Chaotic properties of isokinetic-isobaric atomic systems under planar shear and elongational flows. Physical Review E, 2008, 77, 056217.	2.1	4
78	Nonlocal viscous transport and the effect on fluid stress. Physical Review E, 2008, 78, 051202.	2.1	41
79	Nonlocal Shear Stress for Homogeneous Fluids. Physical Review Letters, 2008, 100, 195901.	7.8	61
80	Structural and dynamical properties for confined polymers undergoing planar Poiseuille flow. Journal of Chemical Physics, 2007, 126, 144907.	3.0	22
81	Parameterization of the nonlocal viscosity kernel for an atomic fluid. Physical Review E, 2007, 76, 041121.	2.1	51
82	Boundary condition independence of molecular dynamics simulations of planar elongational flow. Physical Review E, 2007, 75, 066702.	2.1	5
83	Local linear viscoelasticity of confined fluids. Journal of Chemical Physics, 2007, 126, 144706.	3.0	13
84	Molecular dynamics simulation of planar elongational flow at constant pressure and constant temperature. Journal of Chemical Physics, 2007, 126, 044506.	3.0	11
85	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
86	Homogeneous non-equilibrium molecular dynamics simulations of viscous flow: techniques and applications. Molecular Simulation, 2007, 33, 189-229.	2.0	110
87	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
88	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
89	Analysis of the shape of dendrimers under shear. Journal of Chemical Physics, 2006, 124, 044910.	3.0	28
90	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

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91	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
92	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
93	Power-law exponents for the shear viscosity of non-Newtonian simple fluids. Physical Review E, 2005, 72, 041204.	2.1	12
94	Cats, maps and nanoflows: some recent developments in nonequilibrium nanofluidics. Molecular Simulation, 2005, 31, 411-428.	2.0	11
95	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
96	A molecular dynamics study of nitric oxide in water: Diffusion and structure. Journal of Chemical Physics, 2005, 123, 054505.	3.0	40
97	Viscoelastic properties of dendrimers in the melt from nonequlibrium molecular dynamics. Journal of Chemical Physics, 2004, 121, 12050-12059.	3.0	54
98	Internal structure of dendrimers in the melt under shear: A molecular dynamics study. Journal of Chemical Physics, 2004, 121, 1091-1096.	3.0	45
99	Viscosity of confined inhomogeneous nonequilibrium fluids. Journal of Chemical Physics, 2004, 121, 10778-10786.	3.0	51
100	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
101	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
102	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
103	Cell neighbor list method for planar elongational flow: rheology of a diatomic fluid. Computer Physics Communications, 2003, 151, 35-46.	7.5	25
104	On the Arnold cat map and periodic boundary conditions for planar elongational flow. Molecular Physics, 2003, 101, 3445-3454.	1.7	19
105	Scaling behavior for the pressure and energy of shearing fluids. Physical Review E, 2003, 67, 061201.	2.1	23
106	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
107	Kinetics and chemomechanical properties of the F1-ATPase molecular motor. Journal of Chemical Physics, 2003, 118, 9890-9898.	3.0	25
108	Beyond Traditional Effective Intermolecular Potentials and Pairwise Interactions in Molecular Simulation. Lecture Notes in Computer Science, 2002, , 932-941.	1.3	3

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109	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
110	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
111	Computer simulation of simple and complex atomistic fluids by nonequilibrium molecular dynamics techniques. Computer Physics Communications, 2001, 142, 14-21.	7.5	28
112	Energy and pressure of shearing fluids at different state points. Physical Review E, 2001, 64, 021201.	2.1	16
113	Analytic dependence of the pressure and energy of an atomic fluid under shear. Physical Review E, 2001, 63, 021204.	2.1	36
114	The stability of nonequilibrium molecular dynamics simulations of elongational flows. Journal of Chemical Physics, 2000, 112, 40-46.	3.0	40
115	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
116	A new algorithm for unrestricted duration nonequilibrium molecular dynamics simulations of planar elongational flow. Computer Physics Communications, 1999, 117, 191-199.	7.5	57
117	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
118	Frequency-Dependent Elongational Viscosity by Nonequilibrium Molecular Dynamics. International Journal of Thermophysics, 1998, 19, 1063-1072.	2.1	9
119	Nonlinear response theory for time-periodic elongational flows. Physical Review E, 1998, 58, 4587-4593.	2.1	12
120	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
121	Application of transient-time correlation functions to nonequilibrium molecular-dynamics simulations of elongational flow. Physical Review E, 1997, 56, 6723-6728.	2.1	31
122	Elongational viscosities from nonequilibrium molecular dynamics simulations of oscillatory elongational flow. Journal of Chemical Physics, 1997, 107, 1617-1624.	3.0	25
123	A study of viscosity inhomogeneity in porous media. Journal of Chemical Physics, 1997, 106, 4684-4695.	3.0	69
124	Temperature profile for Poiseuille flow. Physical Review E, 1997, 55, 2800-2807.	2.1	71
125	Departure from Navier-Stokes hydrodynamics in confined liquids. Physical Review E, 1997, 55, 4288-4295.	2.1	293
126	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

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127	Mass and Energy Transport Through Slit Pores: Application to Planar Poiseuille Flow. Molecular Simulation, 1996, 17, 317-332.	2.0	7
128	Pressure tensor for inhomogeneous fluids. Physical Review E, 1995, 52, 1627-1638.	2.1	351
129	Heat flux vector in highly inhomogeneous nonequilibrium fluids. Physical Review E, 1995, 51, 4362-4368.	2.1	83
130	The heat flux vector for highly inhomogeneous nonequilibrium fluids in very narrow pores. Journal of Chemical Physics, 1995, 103, 9804-9809.	3.0	62
131	Surface and bulk properties of metals modelled with Sutton-Chen potentials. Surface Science, 1993, 281, 191-206.	1.9	145
132	Limits to Auger-electron core-loss electron coincidence spectroscopy. Surface Science, 1992, 278, 193-201.	1.9	4