

Peter T Cummings

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#	Paper	IF	Citations
460	Tumor morphology and phenotypic evolution driven by selective pressure from the microenvironment. <i>Cell</i> , 2006 , 127, 905-15	56.2	573
459	Three-dimensional tracking of motile bacteria near a solid planar surface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1995 , 92, 6195-9	11.5	280
458	Supercapacitor Capacitance Exhibits Oscillatory Behavior as a Function of Nanopore Size. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2859-2864	6.4	263
457	Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab Initio Potentials. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 12049-12060	3.4	245
456	Water in carbon nanotubes: adsorption isotherms and thermodynamic properties from molecular simulation. <i>Journal of Chemical Physics</i> , 2005 , 122, 234712	3.9	210
455	From dimer to condensed phases at extreme conditions: accurate predictions of the properties of water by a Gaussian charge polarizable model. <i>Journal of Chemical Physics</i> , 2005 , 122, 244511	3.9	190
454	Improvement of Quality in Publication of Experimental Thermophysical Property Data: Challenges, Assessment Tools, Global Implementation, and Online Support. <i>Journal of Chemical & Engineering Data</i> , 2013 , 58, 2699-2716	2.8	187
453	Water Adsorption in Carbon-Slit Nanopores. <i>Langmuir</i> , 2003 , 19, 8583-8591	4	181
452	Characterization of titanium dioxide nanoparticles using molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 15243-9	3.4	179
451	Simulation of supercritical water and of supercritical aqueous solutions. <i>Journal of Chemical Physics</i> , 1991 , 94, 5606-5621	3.9	169
450	Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. <i>Molecular Physics</i> , 1997 , 92, 973-996	1.7	162
449	Oscillatory Behavior of Double-Walled Nanotubes under Extension: A Simple Nanoscale Damped Spring. <i>Nano Letters</i> , 2003 , 3, 1001-1005	11.5	160
448	Fluidity of hydration layers nanoconfined between mica surfaces. <i>Physical Review Letters</i> , 2005 , 94, 026101	10.1	156
447	Solute-induced effects on the structure and thermodynamics of infinitely dilute mixtures. <i>AICHE Journal</i> , 1994 , 40, 1558-1573	3.6	151
446	Simulations of the Quartz(101 1)/Water Interface: A Comparison of Classical Force Fields, Ab Initio Molecular Dynamics, and X-ray Reflectivity Experiments. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 20762-2088	3.8	145
445	Molecular simulation of water along the liquid-vapor coexistence curve from 25 °C to the critical point. <i>Journal of Chemical Physics</i> , 1990 , 93, 7355-7359	3.9	145
444	Engineering a simple polarizable model for the molecular simulation of water applicable over wide ranges of state conditions. <i>Journal of Chemical Physics</i> , 1996 , 105, 8274-8281	3.9	143

443	Process optimization via simulated annealing: Application to network design. <i>AIChE Journal</i> , 1989 , 35, 725-736	3.6	140
442	Nanoscale perturbations of room temperature ionic liquid structure at charged and uncharged interfaces. <i>ACS Nano</i> , 2012 , 6, 9818-27	16.7	137
441	Statistical mechanical models of chemical reactions. <i>Molecular Physics</i> , 1984 , 51, 253-287	1.7	136
440	Na ⁺ /Cl ⁻ ion pair association in supercritical water. <i>Journal of Chemical Physics</i> , 1995 , 103, 9379-9387	3.9	131
439	Molecular simulation of the transition from liquidlike to solidlike behavior in complex fluids confined to nanoscale gaps. <i>Journal of Chemical Physics</i> , 2001 , 114, 7189-7195	3.9	127
438	Comparison of shear flow of hexadecane in a confined geometry and in bulk. <i>Journal of Chemical Physics</i> , 1997 , 106, 7303-7314	3.9	126
437	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. <i>Advanced Science</i> , 2017 , 4, 1700059	13.6	122
436	Molecular dynamics simulation of titanium dioxide nanoparticle sintering. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 24280-7	3.4	122
435	Molecular simulations of liquid-liquid interfacial properties: water-n-alkane and water-methanol-n-alkane systems. <i>Physical Review E</i> , 2003 , 67, 011603	2.4	122
434	C60 binds to and deforms nucleotides. <i>Biophysical Journal</i> , 2005 , 89, 3856-62	2.9	120
433	Microstructure of Ambient and Supercritical Water. Direct Comparison between Simulation and Neutron Scattering Experiments. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 1309-1316		119
432	Electric Double Layer at the Rutile (110) Surface. 2. Adsorption of Ions from Molecular Dynamics and X-ray Experiments. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 12061-12072	3.4	118
431	Bias-dependent molecular-level structure of electrical double layer in ionic liquid on graphite. <i>Nano Letters</i> , 2013 , 13, 5954-60	11.5	117
430	Dynamics and Structure of Hydration Water on Rutile and Cassiterite Nanopowders Studied by Quasielastic Neutron Scattering and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 4328-4341	3.8	117
429	Molecular Insights into Carbon Supercapacitors Based on Room-Temperature Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3367-3376	6.4	112
428	Alkyl Chain Length and Temperature Effects on Structural Properties of Pyrrolidinium-Based Ionic Liquids: A Combined Atomistic Simulation and Small-Angle X-ray Scattering Study. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 125-130	6.4	112
427	Molecular dynamics simulations of the rheology of normal decane, hexadecane, and tetracosane. <i>Journal of Chemical Physics</i> , 1996 , 105, 1214-1220	3.9	111
426	Comparison of nonequilibrium molecular dynamics with experimental measurements in the nonlinear shear-thinning regime. <i>Physical Review Letters</i> , 2002 , 88, 058302	7.4	110

425	Hydrogen bonding in supercritical water. <i>Journal of Chemical Physics</i> , 1994 , 101, 4466-4469	3.9	109
424	Interaction site models for molecular fluids. <i>Molecular Physics</i> , 1982 , 46, 383-426	1.7	105
423	Curvature Effect on the Capacitance of Electric Double Layers at Ionic Liquid/Onion-Like Carbon Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1058-63	6.4	104
422	Nonequilibrium molecular dynamics approaches to transport properties and non-Newtonian fluid rheology. <i>Industrial & Engineering Chemistry Research</i> , 1992 , 31, 1237-1252	3.9	100
421	The oscillatory damped behaviour of incommensurate double-walled carbon nanotubes. <i>Nanotechnology</i> , 2005 , 16, 186-98	3.4	99
420	Hydration structure of water confined between mica surfaces. <i>Journal of Chemical Physics</i> , 2006 , 124, 74711	3.9	97
419	Structural Origins of Potential Dependent Hysteresis at the Electrified Graphene/Ionic Liquid Interface. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 569-574	3.8	96
418	Supercritical fluid behavior at nanoscale interfaces: Implications for CO ₂ sequestration in geologic formations. <i>Philosophical Magazine</i> , 2010 , 90, 2339-2363	1.6	96
417	Generation of percolation cluster perimeters by a random walk. <i>Journal of Physics A</i> , 1984 , 17, 3009-3017		96
416	Molecular Dynamics Study of the Structure and Thermophysical Properties of Model si Clathrate Hydrates. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 442-451	3.4	94
415	Multiple time step nonequilibrium molecular dynamics simulation of the rheological properties of liquid n-decane. <i>Journal of Chemical Physics</i> , 1996 , 104, 255-262	3.9	94
414	Molecular Simulation of a Dichain Surfactant/Water/Carbon Dioxide System. 1. Structural Properties of Aggregates. <i>Langmuir</i> , 2001 , 17, 1773-1783	4	93
413	Simulated water adsorption isotherms in carbon nanopores. <i>Molecular Physics</i> , 2004 , 102, 243-251	1.7	86
412	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 4668-74	3.6	84
411	Intermolecular potentials and vapor-liquid phase equilibria of perfluorinated alkanes. <i>Fluid Phase Equilibria</i> , 1998 , 146, 51-61	2.5	84
410	Surface protonation at the rutile (110) interface: explicit incorporation of solvation structure within the refined MUSIC model framework. <i>Langmuir</i> , 2008 , 24, 12331-9	4	84
409	Self-Assembly of Reverse Micelles in Water/Surfactant/Carbon Dioxide Systems by Molecular Simulation. <i>Langmuir</i> , 1999 , 15, 5188-5192	4	82
408	Phase transformations during sintering of titania nanoparticles. <i>ACS Nano</i> , 2008 , 2, 1620-4	16.7	81

407	Determination of the Gibbs Free Energy of Gas Replacement in SI Clathrate Hydrates by Molecular Simulation. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 7982-7987	2.8	81
406	A molecular dynamics study of a short-chain polyethylene melt.. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2000 , 93, 83-99	2.7	81
405	Mathematical modeling of cancer: the future of prognosis and treatment. <i>Clinica Chimica Acta</i> , 2005 , 357, 173-9	6.2	79
404	Molecular Dynamics Study of Water Adsorption on TiO ₂ Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 6920-6926	3.8	78
403	Recent developments in non-Newtonian molecular dynamics. <i>Physics Reports</i> , 1998 , 305, 1-92	27.7	75
402	Precision and accuracy of staged free-energy perturbation methods for computing the chemical potential by molecular simulation. <i>Fluid Phase Equilibria</i> , 1998 , 150-151, 41-49	2.5	75
401	SHARP REGULARITY COEFFICIENT ESTIMATES FOR COMPLEX-VALUED ACOUSTIC AND ELASTIC HELMHOLTZ EQUATIONS. <i>Mathematical Models and Methods in Applied Sciences</i> , 2006 , 16, 139-160	3.5	74
400	Critical behavior of the Yukawa fluid in the mean spherical approximation. <i>Journal of Chemical Physics</i> , 1983 , 78, 1917-1923	3.9	72
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398	Molecular simulation study of solvation structure in supercritical aqueous solutions. <i>Chemical Engineering Science</i> , 1994 , 49, 2735-2748	4.4	70
397	Shear behavior of squalane and tetracosane under extreme confinement. I. Model, simulation method, and interfacial slip. <i>Journal of Chemical Physics</i> , 1997 , 107, 10316-10326	3.9	69
396	Electric Double Layer at the Rutile (110) Surface. 3. Inhomogeneous Viscosity and Diffusivity Measurement by Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 3071-3079	3.8	66
395	Rheology of lubricant basestocks: A molecular dynamics study of C30 isomers. <i>Journal of Chemical Physics</i> , 2000 , 113, 8833-8840	3.9	66
394	Simulated water adsorption in chemically heterogeneous carbon nanotubes. <i>Journal of Chemical Physics</i> , 2006 , 124, 74710	3.9	65
393	Statistical mechanical models of chemical reactions. <i>Molecular Physics</i> , 1985 , 55, 33-48	1.7	65
392	An off-lattice hybrid discrete-continuum model of tumor growth and invasion. <i>Biophysical Journal</i> , 2010 , 98, 37-47	2.9	63
391	Solvation in supercritical water. <i>Fluid Phase Equilibria</i> , 1992 , 71, 1-16	2.5	63
390	On the Yukawa closure of the Ornstein-Zernike equation. <i>Molecular Physics</i> , 1979 , 38, 997-1001	1.7	63

389	Simple transferable intermolecular potential for the molecular simulation of water over wide ranges of state conditions. <i>Fluid Phase Equilibria</i> , 1998 , 150-151, 73-81	2.5	62
388	Electric double layer at metal oxide surfaces: static properties of the cassiterite-water interface. <i>Langmuir</i> , 2007 , 23, 4925-37	4	61
387	Molecular dynamics study of the nano-rheology of n-dodecane confined between planar surfaces. <i>Journal of Chemical Physics</i> , 2003 , 118, 8941-8944	3.9	61
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384	Exact asymptotic form of the site-site direct correlation function for rigid polar molecules. <i>Molecular Physics</i> , 1981 , 44, 529-531	1.7	60
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382	Mean spherical approximation for a model liquid metal potential. <i>Molecular Physics</i> , 1981 , 43, 1267-1291	1.7	59
381	Evaluation of force fields for molecular simulation of polyhedral oligomeric silsesquioxanes. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 2502-10	3.4	58
380	Vapor-Liquid Phase Coexistence of Alkane-Carbon Dioxide and Perfluoroalkane-Carbon Dioxide Mixtures. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4485-4491	3.4	58
379	Interfacial ionic 'liquids': connecting static and dynamic structures. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 032101	1.8	57
378	Cellular Dynamics simulations of bacterial chemotaxis. <i>Chemical Engineering Science</i> , 1993 , 48, 687-699	4.4	57
377	A model for association in electrolytes. Analytic solution of the hypernetted-chain/mean spherical approximation. <i>Journal of Chemical Physics</i> , 1985 , 83, 317-325	3.9	57
376	Suppression of the dynamic transition in surface water at low hydration levels: a study of water on rutile. <i>Physical Review E</i> , 2009 , 79, 051504	2.4	56
375	Dynamic and structural properties of room-temperature ionic liquids near silica and carbon surfaces. <i>Langmuir</i> , 2013 , 29, 9744-9	4	55
374	Distinctive Nanoscale Organization of Dicationic versus Monocationic Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 18251-18257	3.8	55
373	Investigating the quartz (1010)/water interface using classical and ab initio molecular dynamics. <i>Langmuir</i> , 2011 , 27, 8700-9	4	55
372	Thermodynamic and transport properties of polyhedral oligomeric silsesquioxanes in poly(dimethylsiloxane). <i>Journal of Physical Chemistry B</i> , 2005 , 109, 14300-7	3.4	55

371	Liquid-gas transition for hard spheres with attractive Yukawa tail interactions. <i>Chemical Physics</i> , 1979 , 42, 241-247	2.3	55
370	Nonequilibrium molecular dynamics calculation of self-diffusion in a non-Newtonian fluid subject to a Couette strain field. <i>Journal of Chemical Physics</i> , 1991 , 94, 2149-2158	3.9	54
369	Molecular dynamics simulations of stretched gold nanowires: the relative utility of different semiempirical potentials. <i>Journal of Chemical Physics</i> , 2007 , 126, 144707	3.9	53
368	Ejection of atoms upon self-trapping of an atomic exciton in solid argon. <i>Physical Review B</i> , 1989 , 39, 9580-9583	3.3	53
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364	Algorithmic efficiency of simulated annealing for heat exchanger network design. <i>Computers and Chemical Engineering</i> , 1990 , 14, 1039-1050	4	52
363	Molecular-Based Modeling of Water and Aqueous Solutions at Supercritical Conditions. <i>Advances in Chemical Physics</i> , 2007 , 115-205		51
362	Vapor-liquid equilibrium simulations of the SCPDP model of water. <i>Chemical Physics Letters</i> , 2002 , 357, 189-194	2.5	50
361	Molecular dynamics simulation of the limiting conductance of NaCl in supercritical water. <i>Chemical Physics Letters</i> , 1998 , 293, 289-294	2.5	48
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358	In Situ Electrochemical Dilatometry of Onion-Like Carbon and Carbon Black. <i>Journal of the Electrochemical Society</i> , 2012 , 159, A1897-A1903	3.9	46
357	Molecular Simulation Study of Tetraalkylammonium Halides. 1. Solvation Structure and Hydrogen Bonding in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 3818-3826	3.4	46
356	Anomalies in the Solubility of Alkanes in Near-Critical Water. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 12307-12314	3.4	46
355	Molecular dynamics simulation of limiting conductances for LiCl, NaBr, and CsBr in supercritical water. <i>Journal of Chemical Physics</i> , 2000 , 112, 864-869	3.9	46
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353	Solution of the Ornstein-Zernike equation in the vicinity of the critical point of a simple fluid. <i>Journal of Chemical Physics</i> , 1985 , 82, 4303-4311	3.9	46
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349	Dielectric constant of dipolar hard sphere mixtures. <i>Journal of Chemical Physics</i> , 1986 , 85, 6658-6667	3.9	44
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347	Sintering of titanium dioxide nanoparticles: a comparison between molecular dynamics and phenomenological modeling. <i>Journal of Nanoparticle Research</i> , 2008 , 10, 1169-1182	2.3	43
346	Comment on "Structure and dynamics of liquid water on rutile TiO ₂ (110)" <i>Physical Review B</i> , 2012 , 85,	3.3	42
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344	Comment on "Near critical phase behaviour of dilute mixtures" <i>Molecular Physics</i> , 1995 , 84, 41-48	1.7	42
343	Fundamental aspects of electric double layer force-distance measurements at liquid-solid interfaces using atomic force microscopy. <i>Scientific Reports</i> , 2016 , 6, 32389	4.9	40
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340	Computational chemistry for molecular electronics. <i>Computational Materials Science</i> , 2003 , 28, 321-341	3.2	40
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332	Effective Interactions between Polyhedral Oligomeric Silsesquioxanes Dissolved in Normal Hexadecane from Molecular Simulation. <i>Macromolecules</i> , 2005 , 38, 8950-8959	5.5	38
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330	Configurational bias Gibbs ensemble Monte Carlo simulation of vapor-liquid equilibria of linear and short-branched alkanes. <i>Fluid Phase Equilibria</i> , 1997 , 141, 45-61	2.5	37
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328	Simulated Water Adsorption Isotherms in Hydrophilic and Hydrophobic Cylindrical Nanopores. <i>Adsorption</i> , 2005 , 11, 397-401	2.6	37
327	Shear viscosity of a simple fluid over a wide range of strain rates. <i>Molecular Physics</i> , 2002 , 100, 2735-2738	3.7	37
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325	Computer Simulation of the Dielectric Properties of Liquid Water. <i>Molecular Simulation</i> , 1989 , 2, 89-104	2	37
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- 3¹⁶ Modeling the interaction between integrin-binding peptide (RGD) and rutile surface: the effect of cation mediation on Asp adsorption. *Langmuir*, **2012**, 28, 2799-811 4 35
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- 3¹⁰ Analytic solution of the molecular Ornstein-Zernike equation for nonspherical molecules. Spheres with anisotropic surface adhesion. *Journal of Chemical Physics*, **1986**, 84, 1833-1842 3.9 35
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- 3⁰² Influence of Surface Oxidation on Ion Dynamics and Capacitance in Porous and Nonporous Carbon Electrodes. *Journal of Physical Chemistry C*, **2016**, 120, 8730-8741 3.8 34
- 3⁰¹ Adsorption of arginine-glycine-aspartate tripeptide onto negatively charged rutile (110) mediated by cations: the effect of surface hydroxylation. *ACS Applied Materials & Interfaces*, **2013**, 5, 2567-79 9.5 33
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