

# Debra Searles

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

191  
papers

6,761  
citations

37  
h-index

76  
g-index

214  
ext. papers

7,742  
ext. citations

5.5  
avg, IF

6.13  
L-index

#	Paper	IF	Citations
191	Fully periodic, computationally efficient constant potential molecular dynamics simulations of ionic liquid supercapacitors.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 184101	3.9	1
190	Thermoresponsive Supramolecular Assemblies from Dendronized Amphiphiles To Form Fluorescent Spheres with Tunable Chirality. <i>ACS Nano</i> , <b>2021</b> ,	16.7	2
189	Dendronized polydiacetylenes photo-polymerization of supramolecular assemblies showing thermally tunable chirality. <i>Chemical Communications</i> , <b>2021</b> , 57, 12780-12783	5.8	2
188	Bandgap engineering of two-dimensional C3N bilayers. <i>Nature Electronics</i> , <b>2021</b> , 4, 486-494	28.4	6
187	Sc, Ge co-doping NASICON boosts solid-state sodium ion batteries' performance. <i>Energy Storage Materials</i> , <b>2021</b> , 40, 282-291	19.4	11
186	Carbon nitrides as cathode materials for aluminium ion batteries. <i>Carbon</i> , <b>2021</b> , 183, 546-559	10.4	0
185	Effect of defects and defect distribution on Li-diffusion and elastic properties of anti-perovskite Li3OCl solid electrolyte. <i>Energy Storage Materials</i> , <b>2021</b> , 41, 614-622	19.4	2
184	Exploring the effect of interlayer distance of expanded graphite for sodium ion storage using first principles calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 3063-3070	3.6	7
183	Accurate prediction of binding energies for two-dimensional catalytic materials using machine learning. <i>ChemCatChem</i> , <b>2020</b> , 12, 5109-5120	5.2	7
182	Potassium-Ion Storage in Cellulose-Derived Hard Carbon: The Role of Functional Groups. <i>Batteries and Supercaps</i> , <b>2020</b> , 3, 953-960	5.6	17
181	Shaping the Future of Solid-State Electrolytes through Computational Modeling. <i>Advanced Materials</i> , <b>2020</b> , 32, e1908041	24	11
180	Graphdiyne and Hydrogen-Substituted Graphdiyne as Potential Cathode Materials for High-Capacity Aluminum-Ion Batteries. <i>ACS Applied Energy Materials</i> , <b>2020</b> , 3, 7404-7415	6.1	7
179	Low-Fouling Fluoropolymers for Bioconjugation and In Vivo Tracking. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 4759-4765	3.6	9
178	Low-Fouling Fluoropolymers for Bioconjugation and In Vivo Tracking. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 4729-4735	16.4	22
177	Insights into the trapping mechanism of light metals on C2N-h2D: Utilisation as an anode material for metal ion batteries. <i>Carbon</i> , <b>2020</b> , 160, 125-132	10.4	15
176	Highly ordered macroporous dual-element-doped carbon from metal-organic frameworks for catalyzing oxygen reduction. <i>Chemical Science</i> , <b>2020</b> , 11, 9584-9592	9.4	14
175	Sulfur-based redox chemistry for electrochemical energy storage. <i>Coordination Chemistry Reviews</i> , <b>2020</b> , 422, 213445	23.2	11

174	New Epoxy Thermosets Derived from a Bisimidazolium Ionic Liquid Monomer: An Experimental and Modeling Investigation. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2020</b> , 8, 12208-12221	8.3	11
173	Investigation of the Ionic Liquid Graphene Electric Double Layer in Supercapacitors Using Constant Potential Simulations. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	9
172	Diffusion of lithium ions in Lithium-argyrodite solid-state electrolytes. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	17
171	Design of two-dimensional carbon-nitride structures by tuning the nitrogen concentration. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	9
170	Structural Electrolytes Based on Epoxy Resins and Ionic Liquids: A Molecular-Level Investigation. <i>Macromolecules</i> , <b>2020</b> , 53, 7635-7649	5.5	11
169	Three-Dimensional Silicon Carbide from Siligraphene as a High Capacity Lithium Ion Battery Anode Material. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 27295-27304	3.8	15
168	Computational Study on the Adsorption of Sodium and Calcium on Edge-Functionalized Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 14895-14908	3.8	14
167	Unlocking the potential of commercial carbon nanofibers as free-standing positive electrodes for flexible aluminum ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 15123-15130	13	23
166	Doping Effects on the Performance of Paired Metal Catalysts for the Hydrogen Evolution Reaction. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 2242-2247	6.1	11
165	Evaluating the Catalytic Efficiency of Paired, Single-Atom Catalysts for the Oxygen Reduction Reaction. <i>ACS Catalysis</i> , <b>2019</b> , 9, 7660-7667	13.1	74
164	The link between the kinetics of gas hydrate formation and surface ion distribution in the low salt concentration regime. <i>Fuel</i> , <b>2019</b> , 240, 309-316	7.1	18
163	Hydrogenated defective graphene as an anode material for sodium and calcium ion batteries: A density functional theory study. <i>Carbon</i> , <b>2018</b> , 136, 73-84	10.4	36
162	Influence of Constraints within a Cyclic Polymer on Solution Properties. <i>Biomacromolecules</i> , <b>2018</b> , 19, 616-625	6.9	26
161	Interaction of Boron Nitride Nanotubes with Aluminium: A Computational Study. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 15226-15240	3.8	2
160	How Low Nucleation Density of Graphene on CuNi Alloy is Achieved. <i>Advanced Science</i> , <b>2018</b> , 5, 1700961	13.6	19
159	Coordination of Atomic Co-Pt Coupling Species at Carbon Defects as Active Sites for Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 10757-10763	16.4	301
158	Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. <i>Journal of Power Sources</i> , <b>2017</b> , 343, 354-363	8.9	51
157	Gasification of diosgenin solid waste for hydrogen production in supercritical water. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 9448-9457	6.7	21

156	Semiclathrate hydrates of methane + tetraalkylammonium hydroxides. <i>Fuel</i> , <b>2017</b> , 203, 618-626	7.1	12
155	Enhanced CO <sub>2</sub> photocatalytic reduction on alkali-decorated graphitic carbon nitride. <i>Applied Catalysis B: Environmental</i> , <b>2017</b> , 216, 146-155	21.8	88
154	Biphenylene and Phagraphene as Lithium Ion Battery Anode Materials. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 20577-20584	9.5	59
153	Switched Photocurrent on Tin Sulfide-Based Nanoplate Photoelectrodes. <i>ChemSusChem</i> , <b>2017</b> , 10, 670-674	6.4	17
152	Water Structure and Transport in Zeolites with Pores in One or Three Dimensions from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 381-391	3.8	9
151	Capacitance-enhanced sodium-ion storage in nitrogen-rich hard carbon. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 22186-22192	13	59
150	Improving Sensing of Sulfur-Containing Gas Molecules with ZnO Monolayers by Implanting Dopants and Defects. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 24365-24375	3.8	30
149	PFPE-Based Polymeric 19F MRI Agents: A New Class of Contrast Agents with Outstanding Sensitivity. <i>Macromolecules</i> , <b>2017</b> , 50, 5953-5963	5.5	43
148	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 14393-14400	3.8	46
147	Local response in nanopores. <i>Molecular Simulation</i> , <b>2016</b> , 42, 463-473	2	1
146	Introduction to Time-Reversible, Thermostatted Dynamical Systems, and Statistical Mechanical Ensembles <b>2016</b> , 17-48		
145	The Evans-Searles Fluctuation Theorem <b>2016</b> , 49-64		1
144	The Dissipation Theorem <b>2016</b> , 65-76		
143	Equilibrium Relaxation Theorems <b>2016</b> , 77-108		
142	Nonequilibrium Steady States <b>2016</b> , 109-132		
141	Applications of the Fluctuation, Dissipation, and Relaxation Theorems <b>2016</b> , 133-154		
140	Nonequilibrium Work Relations, the Clausius Inequality, and Equilibrium Thermodynamics <b>2016</b> , 155-186		
139	Equilibrium binding energies from fluctuation theorems and force spectroscopy simulations. <i>Soft Matter</i> , <b>2016</b> , 12, 9803-9820	3.6	1

138	Computational Evaluation of Lithium-Functionalized Carbon Nitride (g-C <sub>6</sub> N <sub>8</sub> ) Monolayer as an Efficient Hydrogen Storage Material. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 25180-25188	3.8	51
137	Effect of Carbon Chain Length of Organic Salts on the Thermodynamic Stability of Methane Hydrate. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2016</b> , 61, 1952-1960	2.8	13
136	Ion-Responsive 19F MRI Contrast Agents for the Detection of Cancer Cells. <i>ACS Sensors</i> , <b>2016</b> , 1, 757-765	5.2	46
135	On Typicality in Nonequilibrium Steady States. <i>Journal of Statistical Physics</i> , <b>2016</b> , 164, 842-857	1.5	12
134	Conformation Transitions of Thermoresponsive Dendronized Polymers across the Lower Critical Solution Temperature. <i>Macromolecules</i> , <b>2016</b> , 49, 900-908	5.5	26
133	Anion Assisted Synthesis of Large Pore Hollow Dendritic Mesoporous Organosilica Nanoparticles: Understanding the Composition Gradient. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 704-707	9.6	137
132	Interaction of Al, Ti, and Cu Atoms with Boron Nitride Nanotubes: A Computational Investigation. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 3509-3518	3.8	9
131	Reversible Hydrogen Uptake by BN and BC <sub>3</sub> Monolayers Functionalized with Small Fe Clusters: A Route to Effective Energy Storage. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 2009-13	2.8	32
130	Lithium storage on carbon nitride, graphenylene and inorganic graphenylene. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 14205-15	3.6	65
129	Hydrogen production from supercritical water gasification of chicken manure. <i>International Journal of Hydrogen Energy</i> , <b>2016</b> , 41, 22722-22731	6.7	81
128	A Derivation of the Gibbs Equation and the Determination of Change in Gibbs Entropy from Calorimetry. <i>Australian Journal of Chemistry</i> , <b>2016</b> , 69, 1413	1.2	1
127	Conformation of Hydrophobically Modified Thermoresponsive Poly(OEGMA-co-TFEA) across the LCST Revealed by NMR and Molecular Dynamics Studies. <i>Macromolecules</i> , <b>2015</b> , 48, 3310-3317	5.5	36
126	Water diffusion in zeolite membranes: Molecular dynamics studies on effects of water loading and thermostat. <i>Journal of Membrane Science</i> , <b>2015</b> , 495, 322-333	9.6	13
125	Lithium and Sodium Storage on Graphitic Carbon Nitride. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 21923-21927	3.8	19
124	Understanding the Origin of Li <sub>2</sub> MnO <sub>3</sub> Activation in Li-Rich Cathode Materials for Lithium-Ion Batteries. <i>Advanced Functional Materials</i> , <b>2015</b> , 25, 7488-7496	15.6	104
123	Computational Studies of the Interaction of Carbon Dioxide with Graphene-Supported Titanium Dioxide. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 29044-29051	3.8	14
122	System size effects on calculation of the viscosity of extended molecules. <i>Chemical Engineering Science</i> , <b>2015</b> , 121, 236-244	4.4	5
121	Electronic coupling and catalytic effect on H <sub>2</sub> evolution of MoS <sub>2</sub> /graphene nanocatalyst. <i>Scientific Reports</i> , <b>2014</b> , 4, 6256	4.9	54

120	A computational study of carbon dioxide adsorption on solid boron. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 12695-702	3.6	26
119	Electronics, Vacancies, Optical Properties, and Band Engineering of Red Photocatalyst SrNbO <sub>3</sub> : A Computational Investigation. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 11267-11270	3.8	8
118	Comparison of the effect of hydrogen incorporation and oxygen vacancies on the properties of anatase TiO <sub>2</sub> : electronics, optical absorption, and interaction with water. <i>Science Bulletin</i> , <b>2014</b> , 59, 2175-2180 <sup>9</sup>		
117	Carbon Dioxide Capture and Gas Separation on B <sub>80</sub> Fullerene. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 2170-2177	3.8	67
116	Applicability of optimal protocols and the Jarzynski equality. <i>Physica Scripta</i> , <b>2014</b> , 89, 048002	2.6	5
115	On the relationship between dissipation and the rate of spontaneous entropy production from linear irreversible thermodynamics. <i>Molecular Simulation</i> , <b>2014</b> , 40, 208-217	2	7
114	Sieving of H <sub>2</sub> and D <sub>2</sub> Through End-to-End Nanotubes. <i>Communications in Theoretical Physics</i> , <b>2014</b> , 62, 541-549	2.4	3
113	The Dissipation Function: Its Relationship to Entropy Production, Theorems for Nonequilibrium Systems and Observations on Its Extrema. <i>Understanding Complex Systems</i> , <b>2014</b> , 31-47	0.4	6
112	Graphyne and Graphdiyne: Versatile Catalysts for Dehydrogenation of Light Metal Complex Hydrides. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 21643-21650	3.8	34
111	Free Energy Calculations with Reduced Potential Cutoff Radii. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 2083-9	6.4	0
110	Charge-controlled switchable CO <sub>2</sub> capture on boron nitride nanomaterials. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 8246-53	16.4	239
109	Origin of the Visible Light Absorption of Boron/Nitrogen Co-doped Anatase TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 26454-26459	3.8	24
108	Time Reversibility, Correlation Decay and the Steady State Fluctuation Relation for Dissipation. <i>Entropy</i> , <b>2013</b> , 15, 1503-1515	2.8	11
107	Local fluctuation theorem for large systems. <i>Physical Review Letters</i> , <b>2013</b> , 110, 260602	7.4	7
106	Lithium Storage on Graphdiyne Predicted by DFT Calculations. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 26222-26226	3.8	153
105	Fine tuning the teaching methods used for second year university mathematics. <i>International Journal of Mathematical Education in Science and Technology</i> , <b>2012</b> , 43, 1-9	0.5	7
104	Response theory for confined systems. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 074114	3.9	5
103	The free energy of expansion and contraction: treatment of arbitrary systems using the Jarzynski equality. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 174111	3.9	4

102	A local dissipation theorem. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 214110	3.9	0
101	Communication: Beyond Boltzmann's H-theorem: demonstration of the relaxation theorem for a non-monotonic approach to equilibrium. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 021101	3.9	8
100	Contribution of the stochastic forces to the fluctuation theorem. <i>Physical Review E</i> , <b>2012</b> , 85, 042102	2.4	
99	Transient violation of Le Chatelier's principle for a network of water molecules. <i>Journal of the Iranian Chemical Society</i> , <b>2011</b> , 8, 424-432	2	
98	The Fluctuation Theorem and Dissipation Theorem for Poiseuille Flow. <i>Journal of Physics: Conference Series</i> , <b>2011</b> , 297, 012017	0.3	5
97	Nonequilibrium Umbrella Sampling and the Functional Crooks Fluctuation Theorem. <i>Journal of Statistical Physics</i> , <b>2011</b> , 145, 831-840	1.5	5
96	A proof of Clausius' theorem for time reversible deterministic microscopic dynamics. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 204113	3.9	16
95	Planar mixed flow and chaos: Lyapunov exponents and the conjugate-pairing rule. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 114112	3.9	
94	On the entropy of relaxing deterministic systems. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 194107	3.9	8
93	On the probability of violations of Fourier's law for heat flow in small systems observed for short times. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 024501	3.9	21
92	Thermostating highly confined fluids. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 244706	3.9	109
91	Lyapunov spectra and conjugate-pairing rule for confined atomic fluids. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 244508	3.9	8
90	The covariant dissipation function for transient nonequilibrium states. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 054507	3.9	6
89	Musings on thermostats. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 104106	3.9	5
88	Different approaches for evaluating exponentially weighted nonequilibrium relations. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 154108	3.9	7
87	Thermodynamics of Small Systems <b>2010</b> , 75-109		1
86	Applying Bi-directional Jarzynski Methods to Quasi-equilibrium States. <i>Australian Journal of Chemistry</i> , <b>2010</b> , 63, 357	1.2	1
85	On violations of Le Chatelier's principle for a temperature change in small systems observed for short times. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 214503	3.9	5



84	Dissipation and the relaxation to equilibrium. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , <b>2009</b> , 2009, P07029	1.9	28
83	The effect of confinement and wall structure on the kinetics of isomerisation of n-butane. <i>Molecular Simulation</i> , <b>2009</b> , 35, 172-185	2	2
82	Temporal asymmetry of fluctuations in nonequilibrium steady states: links with correlation functions and nonlinear response. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 164515	3.9	9
81	The glass transition and the Jarzynski equality. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 134504	3.9	8
80	Chaotic properties of isokinetic-isobaric atomic systems under planar shear and elongational flows. <i>Physical Review E</i> , <b>2008</b> , 77, 056217	2.4	3
79	Nonequilibrium free-energy relations for thermal changes. <i>Physical Review Letters</i> , <b>2008</b> , 100, 250601	7.4	33
78	On the fluctuation theorem for the dissipation function and its connection with response theory. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 014504	3.9	48
77	Fluctuation theorems. <i>Annual Review of Physical Chemistry</i> , <b>2008</b> , 59, 603-33	15.7	176
76	Deterministic derivation of non-equilibrium free energy theorems for natural isothermal isobaric systems. <i>Molecular Physics</i> , <b>2007</b> , 105, 1059-1066	1.7	9
75	The Steady State Fluctuation Relation for the Dissipation Function. <i>Journal of Statistical Physics</i> , <b>2007</b> , 128, 1337-1363	1.5	53
74	Non-Hamiltonian molecular dynamics implementation of the Gibbs ensemble method. II. Molecular liquid-vapor results for carbon dioxide. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 164105	3.9	12
73	Boundary condition independence of molecular dynamics simulations of planar elongational flow. <i>Physical Review E</i> , <b>2007</b> , 75, 066702	2.4	2
72	Effect of terminal amino acids on the stability and specificity of PNA-DNA hybridisation. <i>Organic and Biomolecular Chemistry</i> , <b>2007</b> , 5, 917-23	3.9	7
71	Effect of solvation and confinement on the trans-gauche isomerization reaction in n-butane. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 164501	3.9	13
70	Temporal asymmetry of fluctuations in nonequilibrium steady states. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 114109	3.9	10
69	Numerical study of the steady state fluctuation relations far from equilibrium. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 194102	3.9	15
68	Chaotic properties of planar elongational flow and planar shear flow: Lyapunov exponents, conjugate-pairing rule, and phase space contraction. <i>Physical Review E</i> , <b>2006</b> , 73, 046206	2.4	10
67	Müller-Blesset perturbation theory calculations of the pKa values for a range of carboxylic acids. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 758, 275-278		29



66	Effects of the juxtaposition of carbonaceous slit pores on the overall transport behavior of adsorbed fluids. <i>Langmuir</i> , <b>2005</b> , 21, 229-39	4	4
65	New observations regarding deterministic, time-reversible thermostats and Gauss's principle of least constraint. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 194106	3.9	25
64	Application of the Gallavotti-Cohen fluctuation relation to thermostated steady states near equilibrium. <i>Physical Review E</i> , <b>2005</b> , 71, 056120	2.4	60
63	Reversibility in nonequilibrium trajectories of an optically trapped particle. <i>Physical Review E</i> , <b>2004</b> , 70, 016111	2.4	35
62	Molecular Dynamics and NMR Parameter Calculations <b>2004</b> , 175-189		11
61	The fluctuation theorem and Lyapunov weights. <i>Physica D: Nonlinear Phenomena</i> , <b>2004</b> , 187, 326-337	3.3	9
60	Modeling molecular transport in slit pores. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 5396-406	3.9	55
59	Fluctuations and irreversibility: an experimental demonstration of a second-law-like theorem using a colloidal particle held in an optical trap. <i>Physical Review Letters</i> , <b>2004</b> , 92, 140601	7.4	189
58	Independence of the transient fluctuation theorem to thermostatting details. <i>Physical Review E</i> , <b>2004</b> , 70, 066113	2.4	36
57	Calculation of the deuteron quadrupole relaxation rate in a mixture of water and dimethyl sulfoxide. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 4704-10	16.4	17
56	Fluctuations Relations for Nonequilibrium Systems. <i>Australian Journal of Chemistry</i> , <b>2004</b> , 57, 1119	1.2	36
55	Wall mediated transport in confined spaces: exact theory for low density. <i>Physical Review Letters</i> , <b>2003</b> , 91, 126102	7.4	93
54	How approximate is the experimental evaluation of quadrupole coupling constants in liquids? A novel computational study. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 6184-6193	3.9	11
53	Is there an iceberg effect in the water/DMSO mixture? Some information from computational chemistry. <i>Journal of Molecular Liquids</i> , <b>2002</b> , 98-99, 71-77	6	6
52	Isobaric Isothermal fluctuation theorem. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 6875-6879	3.9	9
51	The Fluctuation Theorem. <i>Advances in Physics</i> , <b>2002</b> , 51, 1529-1585	18.4	632
50	Experimental demonstration of violations of the second law of thermodynamics for small systems and short time scales. <i>Physical Review Letters</i> , <b>2002</b> , 89, 050601	7.4	628
49	Electric field gradients are highly pair-additive. <i>Chemical Physics Letters</i> , <b>2001</b> , 346, 160-162	2.5	6

48	Fluctuation Theorem for Heat Flow. <i>International Journal of Thermophysics</i> , <b>2001</b> , 22, 123-134	2.1	32
47	A local fluctuation theorem. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 2033-2037	3.9	41
46	Fluctuation theorem for Hamiltonian systems: Le Chatelier's principle. <i>Physical Review E</i> , <b>2001</b> , 63, 051105	2.4	35
45	Note on the Kaplan-Yorke Dimension and Linear Transport Coefficients. <i>Journal of Statistical Physics</i> , <b>2000</b> , 101, 17-34	1.5	30
44	Generalized fluctuation formula. <i>AIP Conference Proceedings</i> , <b>2000</b> ,	0	12
43	Ensemble dependence of the transient fluctuation theorem. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 3503-3509	3.9	69
42	The fluctuation theorem and Green-Kubo relations. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 9727-9735	3.9	55
41	Disproving the Iceberg Effect? A Study of the Deuteron Quadrupole Coupling Constant of Water in a Mixture with Dimethyl Sulfoxide via Computer Simulations. <i>Journal of the American Chemical Society</i> , <b>2000</b> , 122, 5379-5383	16.4	27
40	Fluctuation theorem for stochastic systems. <i>Physical Review E</i> , <b>1999</b> , 60, 159-64	2.4	66
39	Kinetic energy conserving integrators for Gaussian thermostatted SLLOD. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 18-26	3.9	18
38	On the wavevector dependent shear viscosity of a simple fluid. <i>Molecular Physics</i> , <b>1999</b> , 97, 415-422	1.7	8
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