Debra Searles

List of Publications by Citations

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	The Fluctuation Theorem. *Advances in Physics*, **2002**, 51, 1529-1585	18.4	632
190	Experimental demonstration of violations of the second law of thermodynamics for small systems and short time scales. *Physical Review Letters*, **2002**, 89, 050601	7.4	628
189	Equilibrium microstates which generate second law violating steady states. *Physical Review E*, **1994**, 50, 1645-1648	2.4	547
188	Coordination of Atomic Co-Pt Coupling Species at Carbon Defects as Active Sites for Oxygen Reduction Reaction. *Journal of the American Chemical Society*, **2018**, 140, 10757-10763	16.4	301
187	Charge-controlled switchable CO2 capture on boron nitride nanomaterials. *Journal of the American Chemical Society*, **2013**, 135, 8246-53	16.4	239
186	Fluctuations and irreversibility: an experimental demonstration of a second-law-like theorem using a colloidal particle held in an optical trap. *Physical Review Letters*, **2004**, 92, 140601	7.4	189
185	Fluctuation theorems. *Annual Review of Physical Chemistry*, **2008**, 59, 603-33	15.7	176
184	Lithium Storage on Graphdiyne Predicted by DFT Calculations. *Journal of Physical Chemistry C*, **2012** , 116, 26222-26226	3.8	153
183	Anion Assisted Synthesis of Large Pore Hollow Dendritic Mesoporous Organosilica Nanoparticles: Understanding the Composition Gradient. *Chemistry of Materials*, **2016**, 28, 704-707	9.6	137
182	Thermostating highly confined fluids. *Journal of Chemical Physics*, **2010**, 132, 244706	3.9	109
181	Understanding the Origin of Li2MnO3 Activation in Li-Rich Cathode Materials for Lithium-Ion Batteries. *Advanced Functional Materials*, **2015**, 25, 7488-7496	15.6	104
180	Wall mediated transport in confined spaces: exact theory for low density. *Physical Review Letters*, **2003**, 91, 126102	7.4	93
179	Enhanced CO2 photocatalytic reduction on alkali-decorated graphitic carbon nitride. *Applied Catalysis B: Environmental*, **2017**, 216, 146-155	21.8	88
178	Steady states, invariant measures, and response theory. *Physical Review E*, **1995**, 52, 5839-5848	2.4	84
177	Hydrogen production from supercritical water gasification of chicken manure. *International Journal of Hydrogen Energy*, **2016**, 41, 22722-22731	6.7	81
176	Lithium and Sodium Storage on Graphitic Carbon Nitride. *Journal of Physical Chemistry C*, **2015**, 119, 21924-21927	4.8	79
175	Ab initio calculation of the deuterium quadrupole coupling in liquid water. *Journal of Chemical Physics*, **1992**, 97, 5898-5904	3.9	75

174	Evaluating the Catalytic Efficiency of Paired, Single-Atom Catalysts for the Oxygen Reduction Reaction. *ACS Catalysis*, **2019**, 9, 7660-7667	13.1	74
173	Ensemble dependence of the transient fluctuation theorem. *Journal of Chemical Physics*, **2000**, 113, 3503-3509	3.9	69
172	Carbon Dioxide Capture and Gas Separation on B80 Fullerene. *Journal of Physical Chemistry C*, **2014**, 118, 2170-2177	3.8	67
171	Fluctuation theorem for stochastic systems. *Physical Review E*, **1999**, 60, 159-64	2.4	66
170	Lithium storage on carbon nitride, graphenylene and inorganic graphenylene. *Physical Chemistry Chemical Physics*, **2016**, 18, 14205-15	3.6	65
169	Application of the Gallavotti-Cohen fluctuation relation to thermostated steady states near equilibrium. *Physical Review E*, **2005**, 71, 056120	2.4	60
168	Biphenylene and Phagraphene as Lithium Ion Battery Anode Materials. *ACS Applied Materials & Interfaces*, **2017**, 9, 20577-20584	9.5	59
167	Capacitance-enhanced sodium-ion storage in nitrogen-rich hard carbon. *Journal of Materials Chemistry A*, **2017**, 5, 22186-22192	13	59
166	Modeling molecular transport in slit pores. *Journal of Chemical Physics*, **2004**, 120, 5396-406	3.9	55
165	The fluctuation theorem and GreenKubo relations. *Journal of Chemical Physics*, **2000**, 112, 9727-9735	3.9	55
164	Electronic coupling and catalytic effect on H2 evolution of MoS2/graphene nanocatalyst. *Scientific Reports*, **2014**, 4, 6256	4.9	54
163	The Steady State Fluctuation Relation for the Dissipation Function. *Journal of Statistical Physics*, **2007**, 128, 1337-1363	1.5	53
162	Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. *Journal of Power Sources*, **2017**, 343, 354-363	8.9	51
161	Computational Evaluation of Lithium-Functionalized Carbon Nitride (g-C6N8) Monolayer as an Efficient Hydrogen Storage Material. *Journal of Physical Chemistry C*, **2016**, 120, 25180-25188	3.8	51
160	Causality, response theory, and the second law of thermodynamics. *Physical Review E*, **1996**, 53, 5808-5815	2.4	51
159	On the fluctuation theorem for the dissipation function and its connection with response theory. *Journal of Chemical Physics*, **2008**, 128, 014504	3.9	48
158	Ion-Responsive 19F MRI Contrast Agents for the Detection of Cancer Cells. *ACS Sensors*, **2016**, 1, 757-765	9.2	46
157	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. *Journal of Physical Chemistry C*, **2017**, 121, 14393-14400	3.8	46

156	PFPE-Based Polymeric 19F MRI Agents: A New Class of Contrast Agents with Outstanding Sensitivity. *Macromolecules*, **2017**, 50, 5953-5963	5.5	43
155	A local fluctuation theorem. *Journal of Chemical Physics*, **2001**, 115, 2033-2037	3.9	41
154	Conformation of Hydrophobically Modified Thermoresponsive Poly(OEGMA-co-TFEA) across the LCST Revealed by NMR and Molecular Dynamics Studies. *Macromolecules*, **2015**, 48, 3310-3317	5.5	36
153	Hydrogenated defective graphene as an anode material for sodium and calcium ion batteries: A density functional theory study. *Carbon*, **2018**, 136, 73-84	10.4	36
152	Independence of the transient fluctuation theorem to thermostatting details. *Physical Review E*, **2004**, 70, 066113	2.4	36
151	Fluctuations Relations for Nonequilibrium Systems. *Australian Journal of Chemistry*, **2004**, 57, 1119	1.2	36
150	Reversibility in nonequilibrium trajectories of an optically trapped particle. *Physical Review E*, **2004**, 70, 016111	2.4	35
149	Fluctuation theorem for Hamiltonian systems: Le Chatelier's principle. *Physical Review E*, **2001**, 63, 051105	2.4	35
148	Ab initio potential-energy surface of LiH2+ and its analytical representation. *Physical Review A*, **1991**, 43, 3365-3372	2.6	35
147	Graphyne and Graphdiyne: Versatile Catalysts for Dehydrogenation of Light Metal Complex Hydrides. *Journal of Physical Chemistry C*, **2013**, 117, 21643-21650	3.8	34
146	Nonequilibrium free-energy relations for thermal changes. *Physical Review Letters*, **2008**, 100, 250601	7.4	33
145	Reversible Hydrogen Uptake by BN and BC3 Monolayers Functionalized with Small Fe Clusters: A Route to Effective Energy Storage. *Journal of Physical Chemistry A*, **2016**, 120, 2009-13	2.8	32
144	Fluctuation Theorem for Heat Flow. *International Journal of Thermophysics*, **2001**, 22, 123-134	2.1	32
143	The use of molecular dynamics simulations with ab initio SCF calculations for the determination of the oxygen-17 quadrupole coupling constant in liquid water. *Molecular Physics*, **1993**, 80, 1177-1182	1.7	32
142	Improving Sensing of Sulfur-Containing Gas Molecules with ZnO Monolayers by Implanting Dopants and Defects. *Journal of Physical Chemistry C*, **2017**, 121, 24365-24375	3.8	30
141	Note on the Kaplan□Yorke Dimension and Linear Transport Coefficients. *Journal of Statistical Physics*, **2000**, 101, 17-34	1.5	30
140	Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne2. *Chemical Physics*, **1991**, 156, 395-401	2.3	30
139	M□ller□Plesset perturbation theory calculations of the pKa values for a range of carboxylic acids. *Computational and Theoretical Chemistry*, **2006**, 758, 275-278		29

138	Dissipation and the relaxation to equilibrium. *Journal of Statistical Mechanics: Theory and Experiment*, **2009**, 2009, P07029	1.9	28
137	Calculations of 17O nuclear quadrupole coupling constants. *Journal of Molecular Spectroscopy*, **1992**, 151, 474-481	1.3	28
136	Disproving the Iceberg Effect? A Study of the Deuteron Quadrupole Coupling Constant of Water in a Mixture with Dimethyl Sulfoxide via Computer Simulations. *Journal of the American Chemical Society*, **2000**, 122, 5379-5383	16.4	27
135	Influence of Constraints within a Cyclic Polymer on Solution Properties. *Biomacromolecules*, **2018**, 19, 616-625	6.9	26
134	Conformation Transitions of Thermoresponsive Dendronized Polymers across the Lower Critical Solution Temperature. *Macromolecules*, **2016**, 49, 900-908	5.5	26
133	A computational study of carbon dioxide adsorption on solid boron. *Physical Chemistry Chemical Physics*, **2014**, 16, 12695-702	3.6	26
132	Ab initio variational calculations of the vibrational properties of Li+3, Li2Na+, LiNa+2, and KLiNa+. *Journal of Chemical Physics*, **1991**, 95, 1107-1120	3.9	26
131	New observations regarding deterministic, time-reversible thermostats and Gauss's principle of least constraint. *Journal of Chemical Physics*, **2005**, 122, 194106	3.9	25
130	Basis set superposition errors in intermolecular structures and force constants. *Chemical Physics Letters*, **1991**, 183, 223-226	2.5	25
129	Origin of the Visible Light Absorption of Boron/Nitrogen Co-doped Anatase TiO2. *Journal of Physical Chemistry C*, **2013**, 117, 26454-26459	3.8	24
128	Unlocking the potential of commercial carbon nanofibers as free-standing positive electrodes for flexible aluminum ion batteries. *Journal of Materials Chemistry A*, **2019**, 7, 15123-15130	13	23
127	Low-Fouling Fluoropolymers for Bioconjugation and In Vivo Tracking. *Angewandte Chemie - International Edition*, **2020**, 59, 4729-4735	16.4	22
126	The conjugate-pairing rule for non-Hamiltonian systems. *Chaos*, **1998**, 8, 337-349	3.3	22
125	Gasification of diosgenin solid waste for hydrogen production in supercritical water. *International Journal of Hydrogen Energy*, **2017**, 42, 9448-9457	6.7	21
124	On the probability of violations of Fourier's law for heat flow in small systems observed for short times. *Journal of Chemical Physics*, **2010**, 132, 024501	3.9	21
123	Strain rate dependent properties of a simple fluid. *Molecular Physics*, **1998**, 95, 195-202	1.7	21
122	Thermodynamical and structural properties of neon in the liquid and supercritical states obtained from ab initio calculations and molecular dynamics simulations. *Journal of Chemical Physics*, **1993**, 99, 9163-9169	3.9	20
121	Ab initio rotationally resolved infrared spectrum of potassium-lithium (K2Li+). *The Journal of Physical Chemistry*, **1992**, 96, 6158-6165		20

120	How Low Nucleation Density of Graphene on CuNi Alloy is Achieved. *Advanced Science*, **2018**, 5, 1700961	13.6	19
119	The number dependence of the maximum Lyapunov exponent. *Physica A: Statistical Mechanics and Its Applications*, **1997**, 240, 96-104	3.3	19
118	Ab initio model of the Raman spectrum of Li+3: breathe mode frequencies. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1987**, 43, 699-701		19
117	Kinetic energy conserving integrators for Gaussian thermostatted SLLOD. *Journal of Chemical Physics*, **1999**, 111, 18-26	3.9	18
116	Use of molecular dynamics simulations with ab initio SCF calculations for the determination of the deuterium quadrupole coupling constant in liquid water and bond lengths in ice. *Journal of Computational Chemistry*, **1993**, 14, 1553-1560	3.5	18
115	Numerical experiments in quantum physics: Finite-element method. *American Journal of Physics*, **1988**, 56, 444-448	0.7	18
114	The link between the kinetics of gas hydrate formation and surface ion distribution in the low salt concentration regime. *Fuel*, **2019**, 240, 309-316	7.1	18
113	Switched Photocurrent on Tin Sulfide-Based Nanoplate Photoelectrodes. *ChemSusChem*, **2017**, 10, 670-674	8.4	17
112	Potassium-Ion Storage in Cellulose-Derived Hard Carbon: The Role of Functional Groups. *Batteries and Supercaps*, **2020**, 3, 953-960	5.6	17
111	Calculation of the deuteron quadrupole relaxation rate in a mixture of water and dimethyl sulfoxide. *Journal of the American Chemical Society*, **2004**, 126, 4704-10	16.4	17
110	Potential energy surface and vibrational band origins of the triatomic lithium cation. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1988**, 44, 505-515		17
109	Diffusion of lithium ions in Lithium-argyrodite solid-state electrolytes. *Npj Computational Materials*, **2020**, 6,	10.9	17
108	A proof of Clausius' theorem for time reversible deterministic microscopic dynamics. *Journal of Chemical Physics*, **2011**, 134, 204113	3.9	16
107	Comment on "Modified nonequilibrium molecular dynamics for fluid flows with energy conservation" [J. Chem. Phys. 106, 5615 (1997)]. *Journal of Chemical Physics*, **1998**, 108, 4351-4352	3.9	16
106	A fitting program for potential energy surfaces of bent triatomic molecules. *Computer Physics Communications*, **1992**, 67, 527-536	4.2	16
105	Three-Dimensional Silicon Carbide from Siligraphene as a High Capacity Lithium Ion Battery Anode Material. *Journal of Physical Chemistry C*, **2019**, 123, 27295-27304	3.8	15
104	Numerical study of the steady state fluctuation relations far from equilibrium. *Journal of Chemical Physics*, **2006**, 124, 194102	3.9	15
103	Insights into the trapping mechanism of light metals on C2N-h2D: Utilisation as an anode material for metal ion batteries. *Carbon*, **2020**, 160, 125-132	10.4	15

102	Computational Study on the Adsorption of Sodium and Calcium on Edge-Functionalized Graphene Nanoribbons. *Journal of Physical Chemistry C*, **2019**, 123, 14895-14908	3.8	14
101	Computational Studies of the Interaction of Carbon Dioxide with Graphene-Supported Titanium Dioxide. *Journal of Physical Chemistry C*, **2015**, 119, 29044-29051	3.8	14
100	Highly ordered macroporous dual-element-doped carbon from metal-organic frameworks for catalyzing oxygen reduction. *Chemical Science*, **2020**, 11, 9584-9592	9.4	14
99	Water diffusion in zeolite membranes: Molecular dynamics studies on effects of water loading and thermostat. *Journal of Membrane Science*, **2015**, 495, 322-333	9.6	13
98	Effect of Carbon Chain Length of Organic Salts on the Thermodynamic Stability of Methane Hydrate. *Journal of Chemical & Engineering Data*, **2016**, 61, 1952-1960	2.8	13
97	Effect of solvation and confinement on the trans-gauche isomerization reaction in n-butane. *Journal of Chemical Physics*, **2006**, 125, 164501	3.9	13
96	Variational calculations of rotationally resolved infrared properties of Li2Na+, LiNa2+ and KLiNa+. *Journal of Molecular Structure*, **1992**, 272, 73-93	3.4	13
95	Semiclathrate hydrates of methane + tetraalkylammonium hydroxides. *Fuel*, **2017**, 203, 618-626	7.1	12
94	On Typicality in Nonequilibrium Steady States. *Journal of Statistical Physics*, **2016**, 164, 842-857	1.5	12
93	Non-Hamiltonian molecular dynamics implementation of the Gibbs ensemble method. II. Molecular liquid-vapor results for carbon dioxide. *Journal of Chemical Physics*, **2007**, 126, 164105	3.9	12
92	Generalized fluctuation formula. *AIP Conference Proceedings*, **2000**,	0	12
91	Ab initio transition probabilities, band strengths and lifetimes for the lowest-lying vibrational states of Li+3. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1988**, 44, 985-989		12
90	Doping Effects on the Performance of Paired Metal Catalysts for the Hydrogen Evolution Reaction. *Journal of Chemical Information and Modeling*, **2019**, 59, 2242-2247	6.1	11
89	Shaping the Future of Solid-State Electrolytes through Computational Modeling. *Advanced Materials*, **2020**, 32, e1908041	24	11
88	Time Reversibility, Correlation Decay and the Steady State Fluctuation Relation for Dissipation. *Entropy*, **2013**, 15, 1503-1515	2.8	11
87	Molecular Dynamics and NMR Parameter Calculations **2004**, 175-189		11
86	How approximate is the experimental evaluation of quadrupole coupling constants in liquids? A novel computational study. *Journal of Chemical Physics*, **2003**, 119, 6184-6193	3.9	11
85	Calculation of transport properties of neon in the liquid, supercritical, and gaseous state by molecular dynamics simulations applying an ab initio pair potential. *The Journal of Physical Chemistry*, **1993**, 97, 1980-1984		11

84	Sulfur-based redox chemistry for electrochemical energy storage. *Coordination Chemistry Reviews*, **2020**, 422, 213445	23.2	11
83	New Epoxy Thermosets Derived from a Bisimidazolium Ionic Liquid Monomer: An Experimental and Modeling Investigation. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 12208-12221	8.3	11
82	Structural Electrolytes Based on Epoxy Resins and Ionic Liquids: A Molecular-Level Investigation. *Macromolecules*, **2020**, 53, 7635-7649	5.5	11
81	Sc, Ge co-doping NASICON boosts solid-state sodium ion batteries' performance. *Energy Storage Materials*, **2021**, 40, 282-291	19.4	11
80	Temporal asymmetry of fluctuations in nonequilibrium steady states. *Journal of Chemical Physics*, **2006**, 124, 114109	3.9	10
79	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	2.4	10
78	Ab initio calculation of the thermal conductivity of neon in the liquid and hypercritical state over a wide pressure range. *Molecular Physics*, **1992**, 76, 1213-1219	1.7	10
77	Ab initio calculation of the shear viscosity of neon in the liquid and hypercritical state over a wide pressure and temperature range. *Chemical Physics*, **1992**, 164, 321-329	2.3	10
76	Water Structure and Transport in Zeolites with Pores in One or Three Dimensions from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2017**, 121, 381-391	3.8	9
75	Low-Fouling Fluoropolymers for Bioconjugation and In Vivo Tracking. *Angewandte Chemie*, **2020**, 132, 4759-4765	3.6	9
74	Interaction of Al, Ti, and Cu Atoms with Boron Nitride Nanotubes: A Computational Investigation. *Journal of Physical Chemistry C*, **2016**, 120, 3509-3518	3.8	9
73	Comparison of the effect of hydrogen incorporation and oxygen vacancies on the properties of anatase TiO2: electronics, optical absorption, and interaction with water. *Science Bulletin*, **2014**, 59, 2175-2180		9
72	Symplectic properties of algorithms and simulation methods. *Physica A: Statistical Mechanics and Its Applications*, **1997**, 240, 105-114	3.3	9
71	Temporal asymmetry of fluctuations in nonequilibrium steady states: links with correlation functions and nonlinear response. *Journal of Chemical Physics*, **2008**, 128, 164515	3.9	9
70	Deterministic derivation of non-equilibrium free energy theorems for natural isothermal isobaric systems. *Molecular Physics*, **2007**, 105, 1059-1066	1.7	9
69	The fluctuation theorem and Lyapunov weights. *Physica D: Nonlinear Phenomena*, **2004**, 187, 326-337	3.3	9
68	Isobaric-isothermal fluctuation theorem. *Journal of Chemical Physics*, **2002**, 116, 6875-6879	3.9	9
67	Comment on Moeller-Plesset perturbative ab initio calculations of the neon dimer potential. *The Journal of Physical Chemistry*, **1992**, 96, 6104-6104		9

66	Investigation of the Ionic Liquid Graphene Electric Double Layer in Supercapacitors Using Constant Potential Simulations. *Nanomaterials*, **2020**, 10,	5.4	9
65	Design of two-dimensional carbon-nitride structures by tuning the nitrogen concentration. *Npj Computational Materials*, **2020**, 6,	10.9	9
64	Electronics, Vacancies, Optical Properties, and Band Engineering of Red Photocatalyst SrNbO3: A Computational Investigation. *Journal of Physical Chemistry C*, **2014**, 118, 11267-11270	3.8	8
63	Lyapunov spectra and conjugate-pairing rule for confined atomic fluids. *Journal of Chemical Physics*, **2010**, 132, 244508	3.9	8
62	On the entropy of relaxing deterministic systems. *Journal of Chemical Physics*, **2011**, 135, 194107	3.9	8
61	Communication: Beyond Boltzmann's H-theorem: demonstration of the relaxation theorem for a non-monotonic approach to equilibrium. *Journal of Chemical Physics*, **2012**, 136, 021101	3.9	8
60	The glass transition and the Jarzynski equality. *Journal of Chemical Physics*, **2008**, 129, 134504	3.9	8
59	On the wavevector dependent shear viscosity of a simple fluid. *Molecular Physics*, **1999**, 97, 415-422	1.7	8
58	Accurate prediction of binding energies for two-dimensional catalytic materials using machine learning. *ChemCatChem*, **2020**, 12, 5109-5120	5.2	7
57	Graphdiyne and Hydrogen-Substituted Graphdiyne as Potential Cathode Materials for High-Capacity Aluminum-Ion Batteries. *ACS Applied Energy Materials*, **2020**, 3, 7404-7415	6.1	7
56	On the relationship between dissipation and the rate of spontaneous entropy production from linear irreversible thermodynamics. *Molecular Simulation*, **2014**, 40, 208-217	2	7
55	Fine tuning the teaching methods used for second year university mathematics. *International Journal of Mathematical Education in Science and Technology*, **2012**, 43, 1-9	0.5	7
54	Local fluctuation theorem for large systems. *Physical Review Letters*, **2013**, 110, 260602	7.4	7
53	Different approaches for evaluating exponentially weighted nonequilibrium relations. *Journal of Chemical Physics*, **2010**, 133, 154108	3.9	7
52	Effect of terminal amino acids on the stability and specificity of PNA-DNA hybridisation. *Organic and Biomolecular Chemistry*, **2007**, 5, 917-23	3.9	7
51	Simulations of the Thermal Conductivity in the Vicinity of the Critical Point. *Molecular Simulation*, **1998**, 20, 385-395	2	7
50	Exploring the effect of interlayer distance of expanded graphite for sodium ion storage using first principles calculations. *Physical Chemistry Chemical Physics*, **2021**, 23, 3063-3070	3.6	7
49	The covariant dissipation function for transient nonequilibrium states. *Journal of Chemical Physics*, **2010**, 133, 054507	3.9	6

48	Is there an iceberg effect in the water/DMSO mixture? Some information from computational chemistry. *Journal of Molecular Liquids*, **2002**, 98-99, 71-77	6	6
47	Electric field gradients are highly pair-additive. *Chemical Physics Letters*, **2001**, 346, 160-162	2.5	6
46	The Dissipation Function: Its Relationship to Entropy Production, Theorems for Nonequilibrium Systems and Observations on Its Extrema. *Understanding Complex Systems*, **2014**, 31-47	0.4	6
45	Bandgap engineering of two-dimensional C3N bilayers. *Nature Electronics*, **2021**, 4, 486-494	28.4	6
44	System size effects on calculation of the viscosity of extended molecules. *Chemical Engineering Science*, **2015**, 121, 236-244	4.4	5
43	Applicability of optimal protocols and the Jarzynski equality. *Physica Scripta*, **2014**, 89, 048002	2.6	5
42	Response theory for confined systems. *Journal of Chemical Physics*, **2012**, 137, 074114	3.9	5
41	The Fluctuation Theorem and Dissipation Theorem for Poiseuille Flow. *Journal of Physics: Conference Series*, **2011**, 297, 012017	0.3	5
40	Nonequilibrium Umbrella Sampling and the Functional Crooks Fluctuation Theorem. *Journal of Statistical Physics*, **2011**, 145, 831-840	1.5	5
39	Musings on thermostats. *Journal of Chemical Physics*, **2010**, 133, 104106	3.9	5
38	On violations of Le Chatelier's principle for a temperature change in small systems observed for short times. *Journal of Chemical Physics*, **2009**, 131, 214503	3.9	5
37	SVD Analysis in Fitting Property Surfaces. *Journal of the Chinese Chemical Society*, **1992**, 39, 339-341	1.5	5
36	The free energy of expansion and contraction: treatment of arbitrary systems using the Jarzynski equality. *Journal of Chemical Physics*, **2012**, 136, 174111	3.9	4
35	Effects of the juxtaposition of carbonaceous slit pores on the overall transport behavior of adsorbed fluids. *Langmuir*, **2005**, 21, 229-39	4	4
34	Sieving of H 2 and D 2 Through End-to-End Nanotubes. *Communications in Theoretical Physics*, **2014**, 62, 541-549	2.4	3
33	Chaotic properties of isokinetic-isobaric atomic systems under planar shear and elongational flows. *Physical Review E*, **2008**, 77, 056217	2.4	3
32	High-Performance Supercapacitor Materials Based on Hierarchically Porous Carbons Derived from Artocarpus heterophyllus Seed. *ACS Applied Energy Materials*,	6.1	3
31	Interaction of Boron Nitride Nanotubes with Aluminium: A Computational Study. *Journal of Physical Chemistry C*, **2018**, 122, 15226-15240	3.8	2

30	The effect of confinement and wall structure on the kinetics of isomerisation of n-butane. *Molecular Simulation*, **2009**, 35, 172-185	2	2
29	Non-equilibrium molecular dynamics integrators using Maple. *Mathematics and Computers in Simulation*, **1998**, 45, 147-162	3.3	2
28	Boundary condition independence of molecular dynamics simulations of planar elongational flow. *Physical Review E*, **2007**, 75, 066702	2.4	2
27	Thermoresponsive Supramolecular Assemblies from Dendronized Amphiphiles To Form Fluorescent Spheres with Tunable Chirality. *ACS Nano*, **2021**,	16.7	2
26	Dendronized polydiacetylenes photo-polymerization of supramolecular assemblies showing thermally tunable chirality. *Chemical Communications*, **2021**, 57, 12780-12783	5.8	2
25	Effect of defects and defect distribution on Li-diffusion and elastic properties of anti-perovskite Li3OCl solid electrolyte. *Energy Storage Materials*, **2021**, 41, 614-622	19.4	2
24	Local response in nanopores. *Molecular Simulation*, **2016**, 42, 463-473	2	1
23	The EvansSearles Fluctuation Theorem **2016**, 49-64		1
22	Equilibrium binding energies from fluctuation theorems and force spectroscopy simulations. *Soft Matter*, **2016**, 12, 9803-9820	3.6	1
21	Thermodynamics of Small Systems **2010**, 75-109		1
20	Applying Bi-directional Jarzynski Methods to Quasi-equilibrium States. *Australian Journal of Chemistry*, **2010**, 63, 357	1.2	1
19	A Derivation of the Gibbs Equation and the Determination of Change in Gibbs Entropy from Calorimetry. *Australian Journal of Chemistry*, **2016**, 69, 1413	1.2	1
18	Fluctuation Relations and the Foundations of Statistical Thermodynamics: A Deterministic Approach and Numerical Demonstration57-82		1
17	Fully periodic, computationally efficient constant potential molecular dynamics simulations of ionic liquid supercapacitors.. *Journal of Chemical Physics*, **2022**, 156, 184101	3.9	1
16	Free Energy Calculations with Reduced Potential Cutoff Radii. *Journal of Chemical Theory and Computation*, **2013**, 9, 2083-9	6.4	0
15	A local dissipation theorem. *Journal of Chemical Physics*, **2012**, 137, 214110	3.9	0
14	Carbon nitrides as cathode materials for aluminium ion batteries. *Carbon*, **2021**, 183, 546-559	10.4	0
13	Introduction to Time-Reversible, Thermostatted Dynamical Systems, and Statistical Mechanical Ensembles **2016**, 17-48		

12	The Dissipation Theorem **2016**, 65-76	
11	Equilibrium Relaxation Theorems **2016**, 77-108	
10	Nonequilibrium Steady States **2016**, 109-132	
9	Applications of the Fluctuation, Dissipation, and Relaxation Theorems **2016**, 133-154	
8	Nonequilibrium Work Relations, the Clausius Inequality, and Equilibrium Thermodynamics **2016**, 155-186	
7	Transient violation of Le Chatelier's principle for a network of water molecules. *Journal of the Iranian Chemical Society*, **2011**, 8, 424-432	2
6	Planar mixed flow and chaos: Lyapunov exponents and the conjugate-pairing rule. *Journal of Chemical Physics*, **2011**, 134, 114112	3.9
5	Contribution of the stochastic forces to the fluctuation theorem. *Physical Review E*, **2012**, 85, 042102	2.4
4	Potential Energy Functions. *Lecture Notes in Quantum Chemistry II*, **1993**, 57-81	0.6
3	Finite-Element Solution of One-Dimensional Schrödinger Equations. *Lecture Notes in Quantum Chemistry II*, **1993**, 82-106	0.6
2	Applications to Bent Triatomic Molecules. *Lecture Notes in Quantum Chemistry II*, **1993**, 157-190	0.6
1	Dipole Moment Surfaces and Radiative Properties. *Lecture Notes in Quantum Chemistry II*, **1993**, 146-156	0.6