Niall J English

List of Publications by Year
in descending order

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263	7,492	44069	79698
papers	citations	48 h-index	73 g-index

266	266	266	6285
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gas hydrates in sustainable chemistry. Chemical Society Reviews, 2020, 49, 5225-5309.	38.1	443
2	Photo-induced Charge Separation across the Grapheneâ€“TiO₂ Interface Is Faster than Energy Losses: A Time-Domain ab Initio Analysis. Journal of the American Chemical Society, 2012, 134, 14238-14248.	13.7	226
3	Perspectives on external electric fields in molecular simulation: progress, prospects and challenges. Physical Chemistry Chemical Physics, 2015, 17, 12407-12440.	2.8	202
4	Perspectives on molecular simulation of clathrate hydrates: Progress, prospects and challenges. Chemical Engineering Science, 2015, 121, 133-156.	3.8	168
5	Molecular dynamics simulations of microwave heating of water. Journal of Chemical Physics, 2003, 118, 1589-1592.	3.0	141
6	Molecular-dynamics simulations of methane hydrate dissociation. Journal of Chemical Physics, 2005, 123, 244503.	3.0	136
7	Theoretical studies of the kinetics of methane hydrate crystallization in external electromagnetic fields. Journal of Chemical Physics, 2004, 120, 10247-10256.	3.0	135
8	Synergistic Effects on Band Gap-Narrowing in Titania by Codoping from First-Principles Calculations. Chemistry of Materials, 2010, 22, 1616-1623.	6.7	134
9	Thermal Conductivity of Methane Hydrate from Experiment and Molecular Simulation. Journal of Physical Chemistry B, 2007, 111, 13194-13205.	2.6	119
10	Hydrogen bonding and molecular mobility in liquid water in external electromagnetic fields. Journal of Chemical Physics, 2003, 119, 11806-11813.	3.0	115
11	First-principles calculation of nitrogen-tungsten codoping effects on the band structure of anatase-titania. Applied Physics Letters, 2009, 94, .	3.3	113
12	Band gap engineering of (N,Ta)-codoped TiO2: A first-principles calculation. Chemical Physics Letters, 2009, 478, 175-179.	2.6	95
13	Denaturation of hen egg white lysozyme in electromagnetic fields: A molecular dynamics study. Journal of Chemical Physics, 2007, 126, 091105.	3.0	94
14	A comprehensive review on the application of aerogels in CO2-adsorption: Materials and characterisation. Chemical Engineering Journal, 2021, 412, 128604.	12.7	92
15	Molecular dynamics study of thermal-driven methane hydrate dissociation. Journal of Chemical Physics, 2009, 131, 074704.	3.0	89
16	Structural and dynamical properties of methane clathrate hydrates. Journal of Computational Chemistry, 2003, 24, 1569-1581.	3.3	88
17	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 22847-22857.	3.1	87
18	Determining the appropriate exchange-correlation functional for time-dependent density functional theory studies of charge-transfer excitations in organic dyes. Journal of Chemical Physics, 2012, 136, 224301.	3.0	83

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19	Molecular dynamics study of water in contact with the TiO₂rutile-110, 100, 101, 001 and anatase-101, 001 surface. Molecular Physics, 2011, 109, 1649-1656.	1.7	82
20	Nonequilibrium molecular dynamics study of electric and low-frequency microwave fields on hen egg white lysozyme. Journal of Chemical Physics, 2009, 131, 035106.	3.0	79
21	Magnetic properties of first-row element-doped ZnS semiconductors: A density functional theory investigation. Physical Review B, 2009, 80, .	3.2	79
22	Mechanisms for Thermal Conduction in Methane Hydrate. Physical Review Letters, 2009, 103, 015901.	7.8	78
23	Controlled semiconductor nanorodassembly from solution: influence of concentration, charge and solvent nature. Journal of Materials Chemistry, 2012, 22, 1562-1569.	6.7	76
24	Diffusivity and Mobility of Adsorbed Water Layers at TiO2 Rutile and Anatase Interfaces. Crystals, 2016, 6, 1.	2.2	72
25	Massive generation of metastable bulk nanobubbles in water by external electric fields. Science Advances, 2020, 6, eaaz0094.	10.3	72
26	Photo-active and optical properties of bismuth ferrite (BiFeO3): An experimental and theoretical study. Chemical Physics Letters, 2013, 572, 78-84.	2.6	67
27	Highly Ordered Nanorod Assemblies Extending over Device Scale Areas and in Controlled Multilayers by Electrophoretic Deposition. Journal of Physical Chemistry B, 2013, 117, 1608-1615.	2.6	64
28	Density Fluctuations in Liquid Water. Physical Review Letters, 2011, 106, 037801.	7.8	63
29	Minimizing Electronâ€“Hole Recombination on TiO₂ Sensitized with PbSe Quantum Dots: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2014, 5, 2941-2946.	4.6	63
30	Prediction of Henry's Law Constants by a Quantitative Structure Property Relationship and Neural Networks. Journal of Chemical Information and Computer Sciences, 2001, 41, 1150-1161.	2.8	61
31	Mechanisms for thermal conduction in various polymorphs of methane hydrate. Physical Review B, 2009, 80, .	3.2	61
32	Human aquaporin 4 gating dynamics under and after nanosecond-scale static and alternating electric-field impulses: A molecular dynamics study of field effects and relaxation. Journal of Chemical Physics, 2013, 139, 205101.	3.0	61
33	Defects Are Needed for Fast Photo-Induced Electron Transfer from a Nanocrystal to a Molecule: Time-Domain Ab Initio Analysis. Journal of the American Chemical Society, 2013, 135, 18892-18900.	13.7	61
34	Molecular dynamics simulations of microwave effects on water using different long-range electrostatics methodologies. Molecular Physics, 2006, 104, 243-253.	1.7	60
35	Carbon nanotube assisted water self-diffusion across lipid membranes in the absence and presence of electric fields. Molecular Simulation, 2009, 35, 3-12.	2.0	57
36	Perspectives on atmospheric CO2 fixation in inorganic and biomimetic structures. Coordination Chemistry Reviews, 2014, 269, 85-95.	18.8	57

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37	Communication: Influence of external static and alternating electric fields on water from long-time non-equilibrium ab initio molecular dynamics. Journal of Chemical Physics, 2017, 147, 031102.	3.0	57
38	Hydrogen bond perturbation in hen egg white lysozyme by external electromagnetic fields: A nonequilibrium molecular dynamics study. Journal of Chemical Physics, 2010, 133, 235102.	3.0	56
39	Massively parallel molecular dynamics simulation of formation of clathrate-hydrate precursors at planar water-methane interfaces: Insights into heterogeneous nucleation. Journal of Chemical Physics, 2014, 140, 204714.	3.0	56
40	First-Principles Calculation of Synergistic (N, P)-Codoping Effects on the Visible-Light Photocatalytic Activity of Anatase TiO₂. Journal of Physical Chemistry C, 2010, 114, 11984-11990.	3.1	55
41	Diffusive hydrogen inter-cage migration in hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. Journal of Chemical Physics, 2013, 138, 094507.	3.0	55
42	Effect of electrostatics techniques on the estimation of thermal conductivity via equilibrium molecular dynamics simulation: application to methane hydrate. Molecular Physics, 2008, 106, 1887-1898.	1.7	53
43	Static and alternating electric field and distance-dependent effects on carbon nanotube-assisted water self-diffusion across lipid membranes. Journal of Chemical Physics, 2009, 131, 114508.	3.0	53
44	First-principles study of the excited-state properties of coumarin-derived dyes in dye-sensitized solar cells. Journal of Materials Chemistry, 2011, 21, 11101.	6.7	53
45	Molecular dynamics simulations of liquid water using various long-range electrostatics techniques. Molecular Physics, 2005, 103, 1945-1960.	1.7	52
46	Tailoring the electronic structure of TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>by cation codoping from hybrid density functional theory calculations. Physical Review B, 2011, 83, .	3.2	52
47	Atomistic simulations of liquid water using Lekner electrostatics. Molecular Physics, 2002, 100, 3753-3769.	1.7	50
48	Human aquaporin 4 gating dynamics in dc and ac electric fields: A molecular dynamics study. Journal of Chemical Physics, 2011, 134, 055110.	3.0	50
49	Synergistic Effects of Bi/S Codoping on Visible Light-Activated Anatase TiO₂ Photocatalysts from First Principles. Journal of Physical Chemistry C, 2009, 113, 8373-8377.	3.1	49
50	Functional Assessment for Predicting Charge-Transfer Excitations of Dyes in Complexed State: A Study of Triphenylamineâ€“Donor Dyes on Titania for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2013, 117, 2114-2124.	2.5	49
51	Molecular dynamics study of CO2 hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. Journal of Chemical Physics, 2013, 139, 094701.	3.0	48
52	Electromagnetic-field effects on structure and dynamics of amyloidogenic peptides. Journal of Chemical Physics, 2016, 144, 085101.	3.0	46
53	Dipolar response and hydrogen-bond kinetics in liquid water in square-wave time-varying electric fields. Molecular Physics, 2014, 112, 1870-1878.	1.7	44
54	Electric-Field Effects on Adsorbed-Water Structural and Dynamical Properties at Rutile- and Anatase-TiO₂ Surfaces. Journal of Physical Chemistry C, 2016, 120, 19603-19612.	3.1	42

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55	Exploring Rutile (110) and Anatase (101) TiO₂ Water Interfaces by Reactive Force-Field Simulations. Journal of Physical Chemistry C, 2017, 121, 6701-6711.	3.1	41
56	Free-Energy Calculations of the Intercage Hopping Barriers of Hydrogen Molecules in Clathrate Hydrates. Journal of Physical Chemistry C, 2016, 120, 16561-16567.	3.1	40
57	Band gap engineering of double-cation-impurity-doped anatase-titania for visible-light photocatalysts: a hybrid density functional theory approach. Physical Chemistry Chemical Physics, 2011, 13, 13698.	2.8	39
58	Power-to-X: Lighting the Path to a Net-Zero-Emission Future. ACS Sustainable Chemistry and Engineering, 2021, 9, 7179-7181.	6.7	39
59	Electronic structure of cation-codoped TiO2 for visible-light photocatalyst applications from hybrid density functional theory calculations. Applied Physics Letters, 2011, 98, 142103.	3.3	38
60	A TD-DFT study of the effects of structural variations on the photochemistry of polyenedyes. Chemical Science, 2012, 3, 416-424.	7.4	38
61	Translational and rotational diffusive motion in liquid water in square-wave time-varying electric fields. Chemical Physics Letters, 2013, 582, 60-65.	2.6	38
62	Density functional theory description of the mechanism of ferromagnetism in nitrogen-doped SnO2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 374, 319-322.	2.1	36
63	Dynamical cage behaviour and hydrogen migration in hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. Journal of Chemical Physics, 2012, 136, 044506.	3.0	36
64	Hybrid density functional theory description of N- and C-doping of NiO. Journal of Chemical Physics, 2011, 134, 224703.	3.0	34
65	Perspectives on ab initio molecular simulation of excited-state properties of organic dye molecules in dye-sensitised solar cells. Physical Chemistry Chemical Physics, 2012, 14, 12044.	2.8	33
66	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. Journal of Chemical Physics, 2015, 142, 244503.	3.0	33
67	Ionic liquids in external electric and electromagnetic fields: a molecular dynamics study. Molecular Physics, 2011, 109, 625-638.	1.7	32
68	Molecular Dynamics Study of Propane Hydrate Dissociation: Nonequilibrium Analysis in Externally Applied Electric Fields. Journal of Physical Chemistry C, 2018, 122, 7504-7515.	3.1	31
69	Ternary structure reveals mechanism of a membrane diacylglycerol kinase. Nature Communications, 2015, 6, 10140.	12.8	30
70	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 24223-24234.	3.1	30
71	System-density fluctuations and electro-dissociation of methane clathrate hydrates in externally-applied static electric fields. Journal of Chemical Thermodynamics, 2018, 117, 68-80.	2.0	30
72	Effects of an external electromagnetic field on rutile Tio2: A molecular dynamics study. Journal of Physics and Chemistry of Solids, 2006, 67, 1399-1409.	4.0	29

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73	Very Different Responses to Electromagnetic Fields in Binary Ionic Liquid-Water Solutions. Journal of Physical Chemistry B, 2009, 113, 10128-10134.	2.6	29
74	New Insights into the Bandâ€Gap Narrowing of (N, P)â€Codoped TiO₂ from Hybrid Density Functional Theory Calculations. ChemPhysChem, 2011, 12, 2604-2608.	2.1	29
75	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. Journal of Physical Chemistry C, 2017, 121, 3690-3696.	3.1	29
76	Magnetic ferrite/carbonized cotton fiber composites for improving electromagnetic absorption properties at gigahertz frequencies. Journal of Materials Science and Technology, 2021, 86, 127-138.	10.7	29
77	Firstâ€principles calculation of electronic structure of Vâ€doped anatase TiO₂. ChemPhysChem, 2010, 11, 2606-2611.	2.1	28
78	Study of translational, librational and intra-molecular motion of adsorbed liquid water monolayers at various TiO₂ interfaces. Molecular Physics, 2011, 109, 2645-2654.	1.7	28
79	Benchmark study for the application of density functional theory to the prediction of octahedral tilting in perovskites. Physical Review B, 2012, 86, .	3.2	28
80	Density functional theory investigations of bismuth vanadate: Effect of hybrid functionals. Computational Materials Science, 2013, 74, 33-39.	3.0	28
81	Hydrogen-bond dynamics at the bioâ€“water interface in hydrated proteins: a molecular-dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 318-329.	2.8	28
82	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. Physical Chemistry Chemical Physics, 2017, 19, 717-728.	2.8	28
83	Electronic structures of N- and C-doped NiO from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 1184-1187.	2.1	27
84	Perspectives on Hydrate Thermal Conductivity. Energies, 2010, 3, 1934-1942.	3.1	26
85	Band gap engineering of (N, Si)-codoped TiO₂from hybrid density functional theory calculations. New Journal of Physics, 2012, 14, 053007.	2.9	26
86	Photo-active and dynamical properties of hematite (Fe2O3)â€“water interfaces: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 14445.	2.8	26
87	Spatial distribution of adsorbed water layers at the TiO2 rutile and anatase interfaces. Chemical Physics Letters, 2012, 554, 102-106.	2.6	25
88	Study of clathrate hydrates via equilibrium molecular-dynamics simulation employing polarisable and non-polarisable, rigid and flexible water models. Journal of Chemical Physics, 2016, 144, 164503.	3.0	25
89	Molecular-dynamics study of propane-hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. Journal of Chemical Physics, 2018, 148, 114504.	3.0	25
90	Tweaking the Electronic and Optical Properties of Î±-MoO3 by Sulphur and Selenium Doping â€“ a Density Functional Theory Study. Scientific Reports, 2018, 8, 10144.	3.3	25

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91	Dynamical Properties of Hydrogen Sulphide Motion in its Clathrate Hydrate from Ab Initio and Classical Isobaricâ^'Isothermal Molecular Dynamics. Journal of Physical Chemistry A, 2011, 115, 6226-6232.	2.5	24
92	Hydrogen bond dynamical properties of adsorbed liquid water monolayers with various TiO2interfaces. Molecular Physics, 2012, 110, 2919-2925.	1.7	24
93	Mechanisms for thermal conduction in hydrogen hydrate. Journal of Chemical Physics, 2012, 136, 044501.	3.0	24
94	Effects of external electromagnetic fields on the conformational sampling of a short alanine peptide. Journal of Computational Chemistry, 2012, 33, 917-923.	3.3	24
95	Electronic properties of F/Zr co-doped anatase TiO2 photocatalysts from GGA +U calculations. Chemical Physics Letters, 2010, 498, 338-344.	2.6	23
96	Guest and host contributions towards thermal conduction in various polymorphs of methane hydrate. Computational Materials Science, 2010, 49, S176-S180.	3.0	23
97	Influence of doping on the photoactive properties of magnetron-sputtered titania coatings: Experimental and theoretical study. Physical Review B, 2012, 86, .	3.2	23
98	Mechanism of Atmospheric CO2Fixation in the Cavities of a Dinuclear Cryptate. Inorganic Chemistry, 2012, 51, 5282-5288.	4.0	23
99	Communication: Influence of nanosecond-pulsed electric fields on water and its subsequent relaxation: Dipolar effects and debunking memory. Journal of Chemical Physics, 2015, 142, 141101.	3.0	23
100	Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study. Journal of Chemical Physics, 2018, 149, 245102.	3.0	23
101	Thermal conductivity in amorphous ices from molecular dynamics. Physical Review B, 2010, 82, .	3.2	22
102	Massively parallel molecular-dynamics simulation of ice crystallisation and melting: The roles of system size, ensemble, and electrostatics. Journal of Chemical Physics, 2014, 141, 234501.	3.0	22
103	Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study. International Journal of Molecular Sciences, 2016, 17, 1133.	4.1	22
104	Global-density fluctuations in methane clathrate hydrates in externally applied electromagnetic fields. Journal of Chemical Physics, 2017, 147, 024506.	3.0	22
105	Triplet Harvesting Using Two-Photon Absorption in Substituted Naphthalimides for Their Application as Heavy-Atom-Free Photosensitizers. Journal of Physical Chemistry C, 2020, 124, 8178-8185.	3.1	22
106	Electromagnetic field effects on binary dimethylimidazolium-based ionic liquid/water solutions. Physical Chemistry Chemical Physics, 2009, 11, 9370.	2.8	21
107	Dynamical and energetic properties of hydrogen and hydrogenâ€“tetrahydrofuran clathrate hydrates. Physical Chemistry Chemical Physics, 2011, 13, 19780.	2.8	21
108	Coupling of translational and rotational motion in chiral liquids in electromagnetic and circularly polarised electric fields. Journal of Chemical Physics, 2012, 136, 094508.	3.0	21

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109	Structural Properties of Liquid Water and Ice Ih from Ab-Initio Molecular Dynamics with a Non-Local Correlation Functional. Energies, 2015, 8, 9383-9391.	3.1	20
110	Understanding the interface between silicon-based materials and water: Molecular-dynamics exploration of infrared spectra. AIP Advances, 2017, 7, .	1.3	20
111	Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4. ACS Omega, 2018, 3, 15361-15369.	3.5	20
112	Non-equilibrium molecular-dynamics study of electromagnetic-field-induced propane-hydrate dissociation. Journal of Chemical Physics, 2018, 149, 124702.	3.0	20
113	First-principles studies on Î±-Fe₂O₃ surface slabs and mechanistic elucidation of a g-C₃N₄/Î±-Fe₂O₃ heterojunction. Catalysis Science and Technology, 2020, 10, 1376-1384.	4.1	20
114	First-Principles Study of S Doping at the Rutile TiO₂ (110) Surface. Journal of Physical Chemistry C, 2009, 113, 17464-17470.	3.1	19
115	Electronic properties of anatase-TiO2 codoped by cation-pairs from hybrid density functional theory calculations. Chemical Physics Letters, 2011, 513, 218-223.	2.6	19
116	Does Local Structure Bias How a Crystal Nucleus Evolves?. Journal of Physical Chemistry Letters, 2018, 9, 6991-6998.	4.6	19
117	Energetic and Electronic Properties of P Doping at the Rutile TiO₂ (110) Surface from First Principles. Journal of Physical Chemistry C, 2009, 113, 9423-9430.	3.1	18
118	Density equalisation in supercooled high- and low-density water mixtures. Journal of Chemical Physics, 2013, 139, 084508.	3.0	18
119	Dynamical properties of physically adsorbed water molecules at the TiO2 rutile-(110) surface. Chemical Physics Letters, 2013, 583, 125-130.	2.6	18
120	The influence of Ti- and Si-doping on the structure, morphology and photo-response properties of Î±-Fe2O3 for efficient water-splitting: Insights from experiment and first-principles calculations. Chemical Physics Letters, 2014, 592, 242-246.	2.6	18
121	Revisiting Verhulst and Monod models: analysis of batch and fed-batch cultures. Cytotechnology, 2015, 67, 515-530.	1.6	18
122	Oscillating electric-field effects on adsorbed-water at rutile- and anatase-TiO2 surfaces. Journal of Chemical Physics, 2016, 145, 204706.	3.0	18
123	Study of hydrogen-molecule guests in type II clathrate hydrates using a force-matched potential model parameterised from ab initio molecular dynamics. Journal of Chemical Physics, 2018, 148, 102323.	3.0	18
124	Silicon-bridged triphenylamine-based organic dyes for efficient dye-sensitised solar cells. Solar Energy, 2018, 160, 64-75.	6.1	18
125	Diverse morphologies of zinc oxide nanoparticles and their electrocatalytic performance in hydrogen production. Journal of Energy Chemistry, 2021, 56, 162-170.	12.9	18
126	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. Science Advances, 2020, 6, eaaz2915.	10.3	18

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127	Electro-nucleation of water nano-droplets in No Man's Land to fault-free ice I_c. Physical Chemistry Chemical Physics, 2018, 20, 8042-8053.	2.8	17
128	Novel Superstructure-Phase Two-Dimensional Material 1T-VSe2 at High Pressure. Journal of Physical Chemistry Letters, 2020, 11, 380-386.	4.6	17
129	Molecular Dynamics Simulations of Clathrate Hydrates on Specialised Hardware Platforms. Energies, 2012, 5, 3526-3533.	3.1	16
130	Thermal Conductivity of Solids from First-Principles Molecular Dynamics Calculations. Journal of Physical Chemistry C, 2018, 122, 10682-10690.	3.1	16
131	Estimation of zeta potentials of titania nanoparticles by molecular simulation. Physica A: Statistical Mechanics and Its Applications, 2009, 388, 4091-4096.	2.6	15
132	Electrical conductivity and dipolar relaxation of binary dimethylimidazolium chlorideâ€“water solutions: A molecular dynamics study. Journal of Molecular Liquids, 2010, 157, 163-167.	4.9	15
133	Pressure-induced amorphization of methane hydrate. Physical Review B, 2012, 86, .	3.2	15
134	Thermal Conductivity of Supercooled Water: An Equilibrium Molecular Dynamics Exploration. Journal of Physical Chemistry Letters, 2014, 5, 3819-3824.	4.6	15
135	Opto-electronic properties of stable blue photosensitisers on a TiO2 anatase-101 surface for efficient dye-sensitised solar cells. Chemical Physics Letters, 2019, 731, 136624.	2.6	15
136	Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study. Physical Chemistry Chemical Physics, 2019, 21, 3339-3346.	2.8	15
137	Electro-Oxidation Reaction of Methanol over La_{2â€“x}Sr_xNiO_{4+Î´} Ruddlesdenâ€“Popper Oxides. ACS Applied Energy Materials, 2022, 5, 503-515.	5.1	15
138	Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. Photochemical and Photobiological Sciences, 2013, 12, 1220-1231.	2.9	14
139	Role of Hydration Layer in Dynamical Transition in Proteins: Insights from Translational Self-Diffusivity. Journal of Physical Chemistry B, 2016, 120, 12031-12039.	2.6	14
140	Unraveling Adhesion Strength between Gas Hydrate and Solid Surfaces. Langmuir, 2021, 37, 13873-13881.	3.5	14
141	Anti-gas hydrate surfaces: perspectives, progress and prospects. Journal of Materials Chemistry A, 2022, 10, 379-406.	10.3	14
142	Massively parallel molecular dynamics simulation of formation of ice-crystallite precursors in supercooled water: Incipient-nucleation behavior and role of system size. Physical Review E, 2015, 92, 032132.	2.1	13
143	Near-microsecond human aquaporin 4 gating dynamics in static and alternating external electric fields: Non-equilibrium molecular dynamics. Journal of Chemical Physics, 2016, 145, 085102.	3.0	13
144	Formation and properties of water from quartz and hydrogen at high pressure and temperature. Earth and Planetary Science Letters, 2017, 461, 54-60.	4.4	13

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145	Crystal Structure Prediction via Basin-Hopping Global Optimization Employing Tiny Periodic Simulation Cells, with Application to Waterâ€“Ice. Journal of Chemical Theory and Computation, 2019, 15, 3889-3900.	5.3	13
146	A Review of Reactor Designs for Hydrogen Storage in Clathrate Hydrates. Applied Sciences (Switzerland), 2021, 11, 469.	2.5	13
147	Communication: Librational dynamics in water, sI and sII clathrate hydrates, and ice Ih: Molecular-dynamics insights. Journal of Chemical Physics, 2016, 144, 051101.	3.0	13
148	Understanding Competitive Photo-Induced Molecular Oxygen Dissociation and Desorption Dynamics atop a Reduced Rutile TiO₂(110) Surface: A Time-Domain Ab Initio Study. ACS Catalysis, 2022, 12, 6702-6711.	11.2	13
149	Density functional theory studies of doping in titania. Molecular Simulation, 2010, 36, 618-632.	2.0	12
150	Thermal conduction and phonon propagation in pressure-amorphized ices. Physical Review B, 2011, 83, .	3.2	12
151	Comparative studies for evaluation of CO2 fixation in the cavity of the Rubisco enzyme using QM, QM/MM and linear-scaling DFT methods. Journal of Molecular Modeling, 2013, 19, 2329-2334.	1.8	12
152	Massively-Parallel Molecular Dynamics Simulation of Clathrate Hydrates on Blue Gene Platforms. Energies, 2013, 6, 3072-3081.	3.1	12
153	Prediction of Henryâ€™s Law Constants via group-specific quantitative structure property relationships. Chemosphere, 2015, 127, 1-9.	8.2	12
154	Influence of external static and alternating electric fields on self-diffusion of water from molecular dynamics. Journal of Molecular Liquids, 2021, 327, 114788.	4.9	12
155	The Importance of Precursors and Modification Groups of Aerogels in CO2 Capture. Molecules, 2021, 26, 5023.	3.8	12
156	Fabrication of nano-structured TiO2 coatings using a microblast deposition technique. Applied Surface Science, 2013, 275, 316-323.	6.1	11
157	Ice-Amorphization of Supercooled Water Nanodroplets in No Manâ€™s Land. ACS Earth and Space Chemistry, 2017, 1, 187-196.	2.7	11
158	Electropumping of Water Through Human Aquaporin 4 by Circularly Polarized Electric Fields: Dramatic Enhancement and Control Revealed by Non-Equilibrium Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 4646-4651.	4.6	11
159	Exploring Promising Catalysts for Chemical Hydrogen Storage in Ammonia Borane: A Density Functional Theory Study. Catalysts, 2017, 7, 140.	3.5	11
160	Engineering Peptides to Catalyze and Control Stabilization of Gas Hydrates: Learning From Nature. Journal of Physical Chemistry Letters, 2020, 11, 5068-5075.	4.6	11
161	Electric-field-promoted photo-electrochemical production of hydrogen from water splitting. Journal of Molecular Liquids, 2021, 342, 116949.	4.9	11
162	Perturbation of hydration layer in solvated proteins by external electric and electromagnetic fields: Insights from non-equilibrium molecular dynamics. Journal of Chemical Physics, 2016, 145, 205101.	3.0	10

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163	Electric-Field Control of Neon Uptake and Release to and from Clathrate Hydrates. Journal of Physical Chemistry C, 2019, 123, 27554-27560.	3.1	10
164	Hydrogen Inter-Cage Hopping and Cage Occupancies inside Hydrogen Hydrate: Molecular-Dynamics Analysis. Applied Sciences (Switzerland), 2021, 11, 282.	2.5	10
165	Diffusion and interactions of carbon dioxide and oxygen in the vicinity of the active site of Rubisco: Molecular dynamics and quantum chemical studies. Journal of Chemical Physics, 2012, 137, 145103.	3.0	9
166	Effect of space linkers in dinuclear copper cryptates on the efficiency of atmospheric CO2 uptake: a DFT study. Catalysis Science and Technology, 2013, 3, 2234.	4.1	9
167	Reversible pressure-induced crystal-amorphous structural transformation in ice Ih. Chemical Physics Letters, 2014, 609, 54-58.	2.6	9
168	Modelling of Mammalian Cell Cultures. Cell Engineering, 2015, , 259-326.	0.4	9
169	Dispersion and Solvation Effects on the Structure and Dynamics of N719 Adsorbed to Anatase Titania (101) Surfaces in Room-Temperature Ionic Liquids: An ab Initio Molecular Simulation Study. Journal of Physical Chemistry C, 2016, 120, 21-30.	3.1	9
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