Niall J English

List of Publications by Year in Descending Order

255 papers	5,764 citations	45 h-index	64 g-index
266 ext. papers	6,572 ext. citations	4.3 avg, IF	6.62 L-index

#	Paper	IF	Citations
255	A DFTB-Based Molecular Dynamics Investigation of an Explicitly Solvated Anatase Nanoparticle. *Applied Sciences (Switzerland)*, **2022**, 12, 780	2.6	0
254	Anti-gas hydrate surfaces: perspectives, progress and prospects. *Journal of Materials Chemistry A*, **2022**, 10, 379-406	13	5
253	Controlling hydrogen release from remaining-intact Clathrate hydrates by electromagnetic fields: molecular engineering microsecond non-equilibrium molecular dynamics.. *RSC Advances*, **2022**, 12, 4370-4376	3.7	0
252	Application of Porous Ceramics. *Engineering Materials*, **2022**, 499-537	0.4	
251	Characterization of Nanoporous Materials. *Engineering Materials*, **2022**, 319-351	0.4	0
250	Electric Field Effects on Photoelectrochemical Water Splitting: Perspectives and Outlook. *Energies*, **2022**, 15, 1553	3.1	
249	Double Life of Methanol: Experimental Studies and Nonequilibrium Molecular-Dynamics Simulation of Methanol Effects on Methane-Hydrate Nucleation.. *Journal of Physical Chemistry C*, **2022**, 126, 6075-6081	3.8	0
248	Sustainable Exploitation and Commercialization of Ultradense Nanobubbles: Reinventing Liquidity. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 3383-3386	8.3	0
247	Environmental Exploration of Ultra-Dense Nanobubbles: Rethinking Sustainability. *Environments - MDPI*, **2022**, 9, 33	3.2	0
246	Self-Diffusion of Individual Adsorbed Water Molecules at Rutile (110) and Anatase (101) TiO2 Interfaces from Molecular Dynamics. *Crystals*, **2022**, 12, 398	2.3	0
245	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	13.1	3
244	Onset of anharmonicity and thermal conductivity in SnSe. *Physical Review B*, **2021**, 104,	3.3	1
243	Molecular Simulation of External Electric Fields on the Crystal State: A Perspective. *Crystals*, **2021**, 11, 1405	2.3	
242	Unraveling Adhesion Strength between Gas Hydrate and Solid Surfaces. *Langmuir*, **2021**, 37, 13873-13884		3
241	Hydrogen Inter-Cage Hopping and Cage Occupancies inside Hydrogen Hydrate: Molecular-Dynamics Analysis. *Applied Sciences (Switzerland)*, **2021**, 11, 282	2.6	3
240	A -symmetric twisted organic salt as an efficient mechano-/thermo-responsive molecule: a reusable and sensitive fluorescent thermometer. *Chemical Communications*, **2021**, 57, 12321-12324	5.8	2
239	Density of Phonon States in Cubic Ice Ic. *Journal of Physical Chemistry C*, **2021**, 125, 23533-23538	3.8	1

238	Crystallisation competition between cubic and hexagonal ice structures: molecular-dynamics insight. *Molecular Simulation*, **2021**, 47, 18-26	2	2
237	Intra-Cage Structure, Vibrations and Tetrahedral-Site Hopping of H2 and D2 in Doubly-Occupied 51264 Cages in sII Clathrate Hydrates from Path-Integral and Classical Molecular Dynamics. *Applied Sciences (Switzerland)*, **2021**, 11, 54	2.6	1
236	Molecular Simulation of Crystallisation in External Electric Fields: A Review. *Crystals*, **2021**, 11, 316	2.3	2
235	Hydrogen and Deuterium Molecular Escape from Clathrate Hydrates: "Leaky" Microsecond-Molecular-Dynamics Predictions. *Journal of Physical Chemistry C*, **2021**, 125, 8430-8439	3.8	2
234	A comprehensive review on the application of aerogels in CO2-adsorption: Materials and characterisation. *Chemical Engineering Journal*, **2021**, 412, 128604	14.7	23
233	Structural and Electronic Properties of MgO/TiO2 Interfaces: A First-Principles Molecular-Simulation Study. *Journal of Physical Chemistry C*, **2021**, 125, 10795-10802	3.8	1
232	Water Breakup at FeO-Hematite/Water Interfaces: Influence of External Electric Fields from Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 6818-6826	6.4	3
231	Donor-acceptor structure and dynamics: Molecular dynamics simulation study of TIP4P/2005 water model. *Chemical Physics Letters*, **2021**, 775, 138581	2.5	
230	Electric-field-promoted photo-electrochemical production of hydrogen from water splitting. *Journal of Molecular Liquids*, **2021**, 342, 116949	6	3
229	Systematic Design-of-Experiments, factorial-design approaches for tuning simple empirical water models. *Molecular Simulation*, **2021**, 47, 119-130	2	1
228	Diverse morphologies of zinc oxide nanoparticles and their electrocatalytic performance in hydrogen production. *Journal of Energy Chemistry*, **2021**, 56, 162-170	12	7
227	Influence of external static and alternating electric fields on self-diffusion of water from molecular dynamics. *Journal of Molecular Liquids*, **2021**, 327, 114788	6	5
226	A Review of Reactor Designs for Hydrogen Storage in Clathrate Hydrates. *Applied Sciences (Switzerland)*, **2021**, 11, 469	2.6	4
225	The Importance of Precursors and Modification Groups of Aerogels in CO Capture. *Molecules*, **2021**, 26,	4.8	3
224	Machine-Learning-based Many-body Energy Analysis of Argon Clusters: fit for size?. *Chemical Physics*, **2021**, 552, 111347	2.3	1
223	Magnetic ferrite/carbonized cotton fiber composites for improving electromagnetic absorption properties at gigahertz frequencies. *Journal of Materials Science and Technology*, **2021**, 86, 127-138	9.1	8
222	Oxygen-evolution reactions (OER) on transition-metal-doped Fe3Co(PO4)4 iron-phosphate surfaces: a first-principles study. *Catalysis Science and Technology*, **2021**, 11, 4619-4626	5.5	1
221	Thermal Conductivity of High-Temperature Phases of Cu2S from Ab Initio Molecular Dynamics: Advent of Lattice-Site Hopping. *Journal of Physical Chemistry C*, **2020**, 124, 12318-12323	3.8	

220	Temperature-dependent kinetic pathways featuring distinctive thermal-activation mechanisms in structural evolution of ice VII. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 15437-15442	11.5	7
219	Gas hydrates in sustainable chemistry. *Chemical Society Reviews*, **2020**, 49, 5225-5309	58.5	186
218	Engineering Peptides to Catalyze and Control Stabilization of Gas Hydrates: Learning From Nature. *Journal of Physical Chemistry Letters*, **2020**, 11, 5068-5075	6.4	2
217	Dynamical properties of organo lead-halide perovskites and their interfaces to titania: insights from Density Functional Theory. *Heliyon*, **2020**, 6, e03427	3.6	2
216	Dynamical and structural properties of adsorbed water molecules at the TiO2 rutile-(110) surface: interfacial hydrogen bonding probed by ab-initio molecular dynamics. *Molecular Physics*, **2020**, 118, e1725166	1.7	3
215	In Situ Formation of Metal Hydrides Inside Carbon Aerogel Frameworks for Hydrogen Storage Applications. *Journal of Carbon Research*, **2020**, 6, 38	3.3	2
214	Dynamical and structural properties of adsorbed water molecules at the TiO2 anatase-(1□0□1) surface: Importance of interfacial hydrogen-bond rearrangements. *Chemical Physics Letters*, **2020**, 743, 137164	2.5	4
213	Stability-Ranking of Crystalline Ice Polymorphs Using Density-Functional Theory. *Crystals*, **2020**, 10, 40	2.3	1
212	Relaxation dynamics and power spectra of liquid water: a molecular dynamics simulation study. *Molecular Physics*, **2020**, 118, e1733117	1.7	
211	First-principles studies on □Fe2O3 surface slabs and mechanistic elucidation of a g-C3N4/□Fe2O3 heterojunction. *Catalysis Science and Technology*, **2020**, 10, 1376-1384	5.5	11
210	First-principles study of the structural, electronic, magnetic properties of orthorhombic PrCuO3 perovskites. *Chemical Physics Letters*, **2020**, 743, 137166	2.5	1
209	Massive generation of metastable bulk nanobubbles in water by external electric fields. *Science Advances*, **2020**, 6, eaaz0094	14.3	38
208	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	3.8	10
207	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. *Science Advances*, **2020**, 6, eaaz2915	14.3	9
206	Novel Superstructure-Phase Two-Dimensional Material 1-VSe at High Pressure. *Journal of Physical Chemistry Letters*, **2020**, 11, 380-386	6.4	11
205	Microbial Stabilization and Kinetic Enhancement of Marine Methane Hydrates. *Geomicrobiology Journal*, **2020**, 37, 279-286	2.5	3
204	Infrared spectra and density of states at the interface between water and protein: Insights from classical molecular dynamics. *Chemical Physics Letters*, **2020**, 757, 137867	2.5	0
203	Kinetic study on electro-nucleation of water in a heterogeneous propane nano-bubble system to form polycrystalline ice I. *Journal of Chemical Physics*, **2020**, 153, 084501	3.9	4

202	Magnetic-Field Manipulation of Naturally Occurring Microbial Chiral Peptides to Regulate Gas-Hydrate Formation. *Journal of Physical Chemistry Letters*, **2020**, 11, 9079-9085	6.4	2
201	Self-ordering water molecules at TiO interfaces: Advances in structural classification.. *Journal of Chemical Physics*, **2020**, 153, 064502	3.9	2
200	Hydrogen Storage in Propane-Hydrate: Theoretical and Experimental Study. *Applied Sciences (Switzerland)*, **2020**, 10, 8962	2.6	2
199	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from Schrödinger Equation Treatment. *Applied Sciences (Switzerland)*, **2020**, 10, 8504	2.6	1
198	Atmospheric oxidation mechanism and kinetics of 2-bromo-4,6-dinitroaniline by OH radicals - a theoretical study. *Physical Chemistry Chemical Physics*, **2019**, 21, 21109-21127	3.6	
197	Magnetic-field effects on methane-hydrate kinetics and potential geophysical implications: Insights from non-equilibrium molecular dynamics. *Science of the Total Environment*, **2019**, 661, 664-669	10.2	6
196	Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study. *Physical Chemistry Chemical Physics*, **2019**, 21, 3339-3346	3.6	11
195	Hydrogen-/propane-hydrate decomposition: thermodynamic and kinetic analysis. *Molecular Physics*, **2019**, 117, 2434-2442	1.7	8
194	Crystal Structure Prediction via Basin-Hopping Global Optimization Employing Tiny Periodic Simulation Cells, with Application to Water-Ice. *Journal of Chemical Theory and Computation*, **2019**, 15, 3889-3900	6.4	9
193	Orientational and Folding Thermodynamics via Electric Dipole Moment Restraining. *Journal of Physical Chemistry B*, **2019**, 123, 2599-2608	3.4	2
192	Mechanisms of Iodide?Triiodide Exchange Reactions in Ionic Liquids: A Reactive Molecular-Dynamics Exploration. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	2
191	Amplitude effects on seismic velocities: How low can we go?. *Journal of Chemical Physics*, **2019**, 150, 084101	3.9	1
190	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. *Molecular Physics*, **2019**, 117, 3241-3253	1.7	1
189	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	2.5	4
188	Hybrid versus global thermostatting in molecular-dynamics simulation of methane-hydrate crystallisation. *Chinese Journal of Chemical Engineering*, **2019**, 27, 2180-2188	3.2	1
187	Acoustic-propagation properties of methane clathrate hydrates from non-equilibrium molecular dynamics. *Journal of Chemical Physics*, **2019**, 151, 144505	3.9	3
186	Electric-Field Control of Neon Uptake and Release to and from Clathrate Hydrates. *Journal of Physical Chemistry C*, **2019**, 123, 27554-27560	3.8	6
185	A New Relatively Simple Approach to Multipole Interactions in Either Spherical Harmonics or Cartesians, Suitable for Implementation into Ewald Sums. *International Journal of Molecular Sciences*, **2019**, 21,	6.3	2

184	Ionic conductivity along transmembrane-electropores in human aquaporin 4: calcium effects from non-equilibrium molecular dynamics. *Molecular Physics*, **2019**, 117, 3783-3790	1.7	1
183	Electro-nucleation of water nano-droplets in No Man's Land to fault-free ice I. *Physical Chemistry Chemical Physics*, **2018**, 20, 8042-8053	3.6	15
182	Electro-suppression of water nano-droplets' solidification in no man's land: Electromagnetic fields' entropic trapping of supercooled water. *Journal of Chemical Physics*, **2018**, 148, 044503	3.9	3
181	Elastic Characterization of S- and P-Wave Velocities in Marinelike Silica: The Role of Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry C*, **2018**, 122, 3006-3013	3.8	2
180	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	3.9	16
179	Silicon-bridged triphenylamine-based organic dyes for efficient dye-sensitised solar cells. *Solar Energy*, **2018**, 160, 64-75	6.8	14
178	Thermal Conductivity of Solids from First-Principles Molecular Dynamics Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 10682-10690	3.8	14
177	Molecular Dynamics Study of Propane Hydrate Dissociation: Nonequilibrium Analysis in Externally Applied Electric Fields. *Journal of Physical Chemistry C*, **2018**, 122, 7504-7515	3.8	18
176	Molecular-dynamics study of propane-hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. *Journal of Chemical Physics*, **2018**, 148, 114504	3.9	16
175	A systematic study via ab-initio MD of the effect solvation by room temperature ionic liquid has on the structure of a chromophore-titania interface. *Computational Materials Science*, **2018**, 141, 193-206	3.2	3
174	System-density fluctuations and electro-dissociation of methane clathrate hydrates in externally-applied static electric fields. *Journal of Chemical Thermodynamics*, **2018**, 117, 68-80	2.9	19
173	Elucidating mysteries of phase-segregated membranes: mobile-lipid recruitment facilitates pores' passage to the fluid phase. *Physical Chemistry Chemical Physics*, **2018**, 20, 19234-19239	3.6	3
172	Pressure dependence of structural properties of ice VII: An ab initio molecular-dynamics study. *Journal of Chemical Physics*, **2018**, 148, 204505	3.9	6
171	Tweaking the Electronic and Optical Properties of □MoO by Sulphur and Selenium Doping - a Density Functional Theory Study. *Scientific Reports*, **2018**, 8, 10144	4.9	14
170	Vibrational Study of Iodide-Based Room-Temperature Ionic-Liquid Effects on Candidate N719-Chromophore/Titania Interfaces for Dye-Sensitised Solar-Cell Applications from Ab-Initio Based Molecular-Dynamics Simulation. *Energies*, **2018**, 11, 2570	3.1	2
169	Ab Initio Molecular Dynamics Studies of the Effect of Solvation by Room-Temperature Ionic Liquids on the Vibrational Properties of a N719-Chromophore/Titania Interface. *Journal of Physical Chemistry C*, **2018**, 122, 26464-26471	3.8	0
168	Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4. *ACS Omega*, **2018**, 3, 15361-15369	3.9	14
167	Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study. *Journal of Chemical Physics*, **2018**, 149, 245102	3.9	17

166	Does Local Structure Bias How a Crystal Nucleus Evolves?. *Journal of Physical Chemistry Letters*, **2018**, 9, 6991-6998	6.4	12
165	Vibrational, energetic-dynamical and dissociation properties of water clusters in static electric fields: Non-equilibrium molecular-dynamics insights. *Chemical Physics Letters*, **2018**, 710, 207-214	2.5	3
164	Non-equilibrium molecular-dynamics study of electromagnetic-field-induced propane-hydrate dissociation. *Journal of Chemical Physics*, **2018**, 149, 124702	3.9	9
163	Pressure-Induced Densification of Ice I under Triaxial Mechanical Compression: Dissociation versus Retention of Crystallinity for Intermediate States in Atomistic and Coarse-Grained Water Models. *Journal of Physical Chemistry Letters*, **2018**, 9, 5267-5274	6.4	5
162	Formation and properties of water from quartz and hydrogen at high pressure and temperature. *Earth and Planetary Science Letters*, **2017**, 461, 54-60	5.3	8
161	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. *Journal of Physical Chemistry C*, **2017**, 121, 3690-3696	3.8	21
160	On the Mechanism of the Iodide-Triiodide Exchange Reaction in a Solid-State Ionic Liquid. *Journal of Physical Chemistry B*, **2017**, 121, 6436-6441	3.4	7
159	Ice-Amorphization of Supercooled Water Nanodroplets in No Man's Land. *ACS Earth and Space Chemistry*, **2017**, 1, 187-196	3.2	10
158	Exploring Rutile (110) and Anatase (101) TiO2 Water Interfaces by Reactive Force-Field Simulations. *Journal of Physical Chemistry C*, **2017**, 121, 6701-6711	3.8	32
157	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 24223-24234	3.8	21
156	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	6.4	8
155	Global-density fluctuations in methane clathrate hydrates in externally applied electromagnetic fields. *Journal of Chemical Physics*, **2017**, 147, 024506	3.9	14
154	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	3.9	34
153	optPBE-vdW density functional theory study of liquid water and pressure-induced structural evolution in ice Ih. *Canadian Journal of Chemistry*, **2017**, 95, 1205-1211	0.9	2
152	Equilibrium Born-Oppenheimer molecular-dynamics exploration of the lattice thermal conductivity of silicon clathrates. *Computational Materials Science*, **2017**, 126, 1-6	3.2	7
151	Understanding the interface between silicon-based materials and water: Molecular-dynamics exploration of infrared spectra. *AIP Advances*, **2017**, 7, 115105	1.5	14
150	Exploring Promising Catalysts for Chemical Hydrogen Storage in Ammonia Borane: A Density Functional Theory Study. *Catalysts*, **2017**, 7, 140	4	9
149	Organic Dyes Containing Coplanar Dihexyl-Substituted Dithienosilole Groups for Efficient Dye-Sensitised Solar Cells. *International Journal of Photoenergy*, **2017**, 2017, 1-14	2.1	6

148	Dynamics of hydrogen guests in ice XVII nanopores. *Physical Review Materials*, **2017**, 1,	3.2	6
147	Hydrogen-bond dynamics at the bio-water interface in hydrated proteins: a molecular-dynamics study. *Physical Chemistry Chemical Physics*, **2016**, 19, 318-329	3.6	21
146	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. *Physical Chemistry Chemical Physics*, **2016**, 19, 717-728	3.6	24
145	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	3.8	32
144	Thermal Properties of Methane Hydrate by Experiment and Modeling and Impacts Upon Technology **2016**, 680-686		
143	Free-Energy Calculations of the Intercage Hopping Barriers of Hydrogen Molecules in Clathrate Hydrates. *Journal of Physical Chemistry C*, **2016**, 120, 16561-16567	3.8	35
142	Role of Hydration Layer in Dynamical Transition in Proteins: Insights from Translational Self-Diffusivity. *Journal of Physical Chemistry B*, **2016**, 120, 12031-12039	3.4	9
141	Time-dependent density fluctuations in liquid water. *Chemical Physics Letters*, **2016**, 649, 119-122	2.5	2
140	Structural and dynamical properties of methane clathrate hydrates from molecular dynamics: Comparison of atomistic and more coarse-grained potential models. *Fluid Phase Equilibria*, **2016**, 413, 235-241	2.5	6
139	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	3.8	8
138	Verhulst and stochastic models for comparing mechanisms of MAb productivity in six CHO cell lines. *Cytotechnology*, **2016**, 68, 1499-511	2.2	2
137	Distortion induced magnetic phase transition in cubic BaFeO 3. *Journal of Magnetism and Magnetic Materials*, **2016**, 401, 1097-1105	2.8	5
136	Communication: Librational dynamics in water, sI and sII clathrate hydrates, and ice Ih: Molecular-dynamics insights. *Journal of Chemical Physics*, **2016**, 144, 051101	3.9	10
135	Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	20
134	Diffusivity and Mobility of Adsorbed Water Layers at TiO2 Rutile and Anatase Interfaces. *Crystals*, **2016**, 6, 1	2.3	64
133	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	3.9	7
132	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	3.9	5
131	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	3.9	22

130	Electromagnetic-field effects on structure and dynamics of amyloidogenic peptides. *Journal of Chemical Physics*, **2016**, 144, 085101	3.9	32
129	Oscillating electric-field effects on adsorbed-water at rutile- and anatase-TiO surfaces. *Journal of Chemical Physics*, **2016**, 145, 204706	3.9	14
128	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	3.9	19
127	Perspectives on external electric fields in molecular simulation: progress, prospects and challenges. *Physical Chemistry Chemical Physics*, **2015**, 17, 12407-40	3.6	140
126	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. *Journal of Chemical Physics*, **2015**, 142, 244503	3.9	26
125	Perspectives on molecular simulation of clathrate hydrates: Progress, prospects and challenges. *Chemical Engineering Science*, **2015**, 121, 133-156	4.4	137
124	Revisiting Verhulst and Monod models: analysis of batch and fed-batch cultures. *Cytotechnology*, **2015**, 67, 515-30	2.2	12
123	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	2.4	12
122	Hydrogen-bond vibrational and energetic dynamical properties in sI and sII clathrate hydrates and in ice Ih: Molecular dynamics insights. *Journal of Chemical Physics*, **2015**, 143, 154504	3.9	6
121	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	19
120	Electric field-controlled semiconductor nanorod assembly in solution: mechanistic insights from non-equilibrium molecular dynamics. *Canadian Journal of Chemistry*, **2015**, 93, 888-890	0.9	1
119	Ternary structure reveals mechanism of a membrane diacylglycerol kinase. *Nature Communications*, **2015**, 6, 10140	17.4	27
118	Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. *Journal of Photochemistry and Photobiology A: Chemistry*, **2015**, 301, 20-31	4.7	4
117	Modelling of Mammalian Cell Cultures. *Cell Engineering*, **2015**, 259-326		7
116	Prediction of Henry's Law Constants via group-specific quantitative structure property relationships. *Chemosphere*, **2015**, 127, 1-9	8.4	9
115	Implicit and explicit solvent models for modeling a bifunctional arene ruthenium hydrogen-storage catalyst: a classical and ab initio molecular simulation study. *Journal of Computational Chemistry*, **2014**, 35, 683-91	3.5	5
114	Perspectives on atmospheric CO2 fixation in inorganic and biomimetic structures. *Coordination Chemistry Reviews*, **2014**, 269, 85-95	23.2	49
113	Towards the design of novel boron- and nitrogen-substituted ammonia-borane and bifunctional arene ruthenium catalysts for hydrogen storage. *Journal of Computational Chemistry*, **2014**, 35, 891-903	3.5	6

112	Theoretical studies of separation of cis-trans isomers using dinuclear (Cu(2+)- and Zn(2+)-based) cryptates. *Journal of Molecular Modeling*, **2014**, 20, 2328	2	1
111	Thermal Conductivity of Supercooled Water: An Equilibrium Molecular Dynamics Exploration. *Journal of Physical Chemistry Letters*, **2014**, 5, 3819-24	6.4	11
110	Photo-active and dynamical properties of hematite (Fe2O3)-water interfaces: an experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2014**, 16, 14445-54	3.6	24
109	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 22847-22857	3.8	72
108	Reversible pressure-induced crystal-amorphous structural transformation in ice Ih. *Chemical Physics Letters*, **2014**, 609, 54-58	2.5	9
107	Density functional theory calculations of catalytic mechanistic pathways for the formation of O2 involving triazolylidene iridium complexes. *New Journal of Chemistry*, **2014**, 38, 4060	3.6	5
106	Minimizing Electron-Hole Recombination on TiO2 Sensitized with PbSe Quantum Dots: Time-Domain Ab Initio Analysis. *Journal of Physical Chemistry Letters*, **2014**, 5, 2941-6	6.4	55
105	Process control of particle deposition systems using acoustic and electrical response signals. *Advanced Powder Technology*, **2014**, 25, 1560-1570	4.6	
104	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	3.9	20
103	Dipolar response and hydrogen-bond kinetics in liquid water in square-wave time-varying electric fields. *Molecular Physics*, **2014**, 112, 1870-1878	1.7	33
102	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	3.9	48
101	The influence of Ti- and Si-doping on the structure, morphology and photo-response properties of □-Fe2O3 for efficient water-splitting: Insights from experiment and first-principles calculations. *Chemical Physics Letters*, **2014**, 592, 242-246	2.5	17
100	Molecular dynamics study of CO2 hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. *Journal of Chemical Physics*, **2013**, 139, 094701	3.9	33
99	Comparative studies for evaluation of CO□fixation in the cavity of the Rubisco enzyme using QM, QM/MM and linear-scaling DFT methods. *Journal of Molecular Modeling*, **2013**, 19, 2329-34	2	10
98	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	3.9	49
97	Photo-active and optical properties of bismuth ferrite (BiFeO3): An experimental and theoretical study. *Chemical Physics Letters*, **2013**, 572, 78-84	2.5	47
96	Fabrication of nano-structured TiO2 coatings using a microblast deposition technique. *Applied Surface Science*, **2013**, 275, 316-323	6.7	8
95	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, 18892-900	16.4	58

94	Density equalisation in supercooled high- and low-density water mixtures. *Journal of Chemical Physics*, **2013**, 139, 084508	3.9	18
93	Translational and rotational diffusive motion in liquid water in square-wave time-varying electric fields. *Chemical Physics Letters*, **2013**, 582, 60-65	2.5	28
92	Dynamical properties of physically adsorbed water molecules at the TiO2 rutile-(1 1 0) surface. *Chemical Physics Letters*, **2013**, 583, 125-130	2.5	17
91	Density functional theory investigations of bismuth vanadate: Effect of hybrid functionals. *Computational Materials Science*, **2013**, 74, 33-39	3.2	27
90	Functional assessment for predicting charge-transfer excitations of dyes in complexed state: a study of triphenylamine-donor dyes on titania for dye-sensitized solar cells. *Journal of Physical Chemistry A*, **2013**, 117, 2114-24	2.8	47
89	Highly ordered nanorod assemblies extending over device scale areas and in controlled multilayers by electrophoretic deposition. *Journal of Physical Chemistry B*, **2013**, 117, 1608-15	3.4	55
88	Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. *Photochemical and Photobiological Sciences*, **2013**, 12, 1220-31	4.2	12
87	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	5.5	9
86	Diffusive hydrogen inter-cage migration in hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. *Journal of Chemical Physics*, **2013**, 138, 094507	3.9	41
85	Massively-Parallel Molecular Dynamics Simulation of Clathrate Hydrates on Blue Gene Platforms. *Energies*, **2013**, 6, 3072-3081	3.1	10
84	Application of statistical techniques for elucidating flow cytometric data of batch and fed-batch cultures. *Biotechnology and Applied Biochemistry*, **2013**, 60, 536-45	2.8	4
83	Effects of external electromagnetic fields on the conformational sampling of a short alanine peptide. *Journal of Computational Chemistry*, **2012**, 33, 917-23	3.5	19
82	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, 12044-56	3.6	27
81	Spatial distribution of adsorbed water layers at the TiO2 rutile and anatase interfaces. *Chemical Physics Letters*, **2012**, 554, 102-106	2.5	21
80	A TD-DFT study of the effects of structural variations on the photochemistry of polyene dyes. *Chemical Science*, **2012**, 3, 416-424	9.4	38
79	Photo-induced charge separation across the graphene-TiO2 interface is faster than energy losses: a time-domain ab initio analysis. *Journal of the American Chemical Society*, **2012**, 134, 14238-48	16.4	206
78	Controlled semiconductor nanorod assembly from solution: influence of concentration, charge and solvent nature. *Journal of Materials Chemistry*, **2012**, 22, 1562-1569		72
77	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	3.9	8

76	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	3.9	70
75	Mechanism of atmospheric CO2 fixation in the cavities of a dinuclear cryptate. *Inorganic Chemistry*, **2012**, 51, 5282-8	5.1	22
74	Hydrogen bond dynamical properties of adsorbed liquid water monolayers with various TiO2 interfaces. *Molecular Physics*, **2012**, 110, 2919-2925	1.7	23
73	Molecular Dynamics Simulations of Clathrate Hydrates on Specialised Hardware Platforms. *Energies* , **2012**, 5, 3526-3533	3.1	14
72	Dynamical cage behaviour and hydrogen migration in hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. *Journal of Chemical Physics*, **2012**, 136, 044506	3.9	31
71	Mechanisms for thermal conduction in hydrogen hydrate. *Journal of Chemical Physics*, **2012**, 136, 044501	3.9	19
70	Coupling of translational and rotational motion in chiral liquids in electromagnetic and circularly polarised electric fields. *Journal of Chemical Physics*, **2012**, 136, 094508	3.9	20
69	Influence of doping on the photoactive properties of magnetron-sputtered titania coatings: Experimental and theoretical study. *Physical Review B*, **2012**, 86,	3.3	22
68	Benchmark study for the application of density functional theory to the prediction of octahedral tilting in perovskites. *Physical Review B*, **2012**, 86,	3.3	26
67	Pressure-induced amorphization of methane hydrate. *Physical Review B*, **2012**, 86,	3.3	12
66	Ab initio study on optoelectronic properties of interstitially versus substitutionally doped titania. *Physical Review B*, **2012**, 86,	3.3	5
65	Band gap engineering of (N, Si)-codoped TiO2from hybrid density functional theory calculations. *New Journal of Physics*, **2012**, 14, 053007	2.9	23
64	Dynamical properties of hydrogen sulphide motion in its clathrate hydrate from ab initio and classical isobaric-isothermal molecular dynamics. *Journal of Physical Chemistry A*, **2011**, 115, 6226-32	2.8	21
63	Density fluctuations in liquid water. *Physical Review Letters*, **2011**, 106, 037801	7.4	58
62	Electrophoretic deposition of poly(3-decylthiophene) onto gold-mounted cadmium selenide nanorods. *Langmuir*, **2011**, 27, 13506-13	4	6
61	Hybrid density functional theory description of N- and C-doping of NiO. *Journal of Chemical Physics*, **2011**, 134, 224703	3.9	27
60	Human aquaporin 4 gating dynamics in dc and ac electric fields: a molecular dynamics study. *Journal of Chemical Physics*, **2011**, 134, 055110	3.9	45
59	Tailoring the electronic structure of TiO2 by cation codoping from hybrid density functional theory calculations. *Physical Review B*, **2011**, 83,	3.3	48

58	Electronic properties of anatase-TiO2 codoped by cation-pairs from hybrid density functional theory calculations. *Chemical Physics Letters*, **2011**, 513, 218-223	2.5	14
57	Molecular dynamics study of water in contact with the TiO2 rutile-110, 100, 101, 001 and anatase-101, 001 surface. *Molecular Physics*, **2011**, 109, 1649-1656	1.7	72
56	A theoretical thermodynamic investigation of cascade reactions in dinuclear octa-azacryptates involving carbon dioxide. *Journal of Molecular Modeling*, **2011**, 17, 3151-62	2	6
55	New insights into the band-gap narrowing of (N, P)-codoped TiO2 from hybrid density functional theory calculations. *ChemPhysChem*, **2011**, 12, 2604-8	3.2	27
54	First-principles study of the excited-state properties of coumarin-derived dyes in dye-sensitized solar cells. *Journal of Materials Chemistry*, **2011**, 21, 11101		51
53	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, 13698-703	3.6	36
52	Dynamical and energetic properties of hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. *Physical Chemistry Chemical Physics*, **2011**, 13, 19780-7	3.6	18
51	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	24
50	Electronic structure of cation-codoped TiO2 for visible-light photocatalyst applications from hybrid density functional theory calculations. *Applied Physics Letters*, **2011**, 98, 142103	3.4	35
49	Ionic liquids in external electric and electromagnetic fields: a molecular dynamics study. *Molecular Physics*, **2011**, 109, 625-638	1.7	28
48	Thermal conduction and phonon propagation in pressure-amorphized ices. *Physical Review B*, **2011**, 83,	3.3	12
47	Synergistic effects on band gap-narrowing in titania by doping from first-principles calculations: density functional theory studies. *Materials Research Society Symposia Proceedings*, **2011**, 1352, 9		
46	Perspectives on Hydrate Thermal Conductivity. *Energies*, **2010**, 3, 1934-1942	3.1	20
45	Hydrogen bond perturbation in hen egg white lysozyme by external electromagnetic fields: a nonequilibrium molecular dynamics study. *Journal of Chemical Physics*, **2010**, 133, 235102	3.9	52
44	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	3.8	51
43	Synergistic Effects on Band Gap-Narrowing in Titania by Codoping from First-Principles Calculations. *Chemistry of Materials*, **2010**, 22, 1616-1623	9.6	118
42	Electronic Structure and Origin of Visible-Light Activity of C-Doped Cubic In2O3 from First-Principles Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 13942-13946	3.8	8
41	Guest and host contributions towards thermal conduction in various polymorphs of methane hydrate. *Computational Materials Science*, **2010**, 49, S176-S180	3.2	17

40	Density functional theory studies of doping in titania. *Molecular Simulation*, **2010**, 36, 618-632	2	9
39	Thermal conductivity in amorphous ices from molecular dynamics. *Physical Review B*, **2010**, 82,	3.3	22
38	Electronic properties of F/Zr co-doped anatase TiO2 photocatalysts from GGA + U calculations. *Chemical Physics Letters*, **2010**, 498, 338-344	2.5	23
37	First-principles calculation of electronic structure of V-doped anatase TiO2. *ChemPhysChem*, **2010**, 11, 2606-11	3.2	25
36	Electrical conductivity and dipolar relaxation of binary dimethylimidazolium chloride/water solutions: A molecular dynamics study. *Journal of Molecular Liquids*, **2010**, 157, 163-167	6	13
35	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	2.3	26
34	Mechanisms for thermal conduction in various polymorphs of methane hydrate. *Physical Review B*, **2009**, 80,	3.3	52
33	Nonequilibrium molecular dynamics study of electric and low-frequency microwave fields on hen egg white lysozyme. *Journal of Chemical Physics*, **2009**, 131, 035106	3.9	66
32	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	2.3	36
31	Estimation of zeta potentials of titania nanoparticles by molecular simulation. *Physica A: Statistical Mechanics and Its Applications*, **2009**, 388, 4091-4096	3.3	13
30	Band gap engineering of (N,Ta)-codoped TiO2: A first-principles calculation. *Chemical Physics Letters*, **2009**, 478, 175-179	2.5	86
29	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	3.8	16
28	Electromagnetic field effects on binary dimethylimidazolium-based ionic liquid/water solutions. *Physical Chemistry Chemical Physics*, **2009**, 11, 9370-4	3.6	19
27	Very different responses to electromagnetic fields in binary ionic liquid-water solutions. *Journal of Physical Chemistry B*, **2009**, 113, 10128-34	3.4	28
26	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	3.9	45
25	Magnetic properties of first-row element-doped ZnS semiconductors: A density functional theory investigation. *Physical Review B*, **2009**, 80,	3.3	72
24	First-principles calculation of nitrogen-tungsten codoping effects on the band structure of anatase-titania. *Applied Physics Letters*, **2009**, 94, 132102	3.4	104
23	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	3.8	46

22	Molecular dynamics study of thermal-driven methane hydrate dissociation. *Journal of Chemical Physics*, **2009**, 131, 074704	3.9	71
21	Carbon nanotube assisted water self-diffusion across lipid membranes in the absence and presence of electric fields. *Molecular Simulation*, **2009**, 35, 3-12	2	53
20	Mechanisms for thermal conduction in methane hydrate. *Physical Review Letters*, **2009**, 103, 015901	7.4	64
19	First-Principles Study of S Doping at the Rutile TiO2 (110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 17464-17470	3.8	17
18	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	45
17	Denaturation of hen egg white lysozyme in electromagnetic fields: a molecular dynamics study. *Journal of Chemical Physics*, **2007**, 126, 091105	3.9	74
16	Thermal conductivity of methane hydrate from experiment and molecular simulation. *Journal of Physical Chemistry B*, **2007**, 111, 13194-205	3.4	90
15	Calculation of binding affinities of HIV-1 RT and beta-secretase inhibitors using the linear interaction energy method with explicit and continuum solvation approaches. *Journal of Molecular Modeling*, **2007**, 13, 1081-97	2	5
14	Response to Comment on Denaturation of hen egg white lysozyme in electromagnetic fields: A molecular dynamics study [J. Chem. Phys. 126, 091105 (2007)]. *Journal of Chemical Physics*, **2007**, 127, 117102	3.9	0
13	Molecular dynamics simulations of microwave effects on water using different long-range electrostatics methodologies. *Molecular Physics*, **2006**, 104, 243-253	1.7	57
12	Effects of an external electromagnetic field on rutile Tio2: A molecular dynamics study. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 1399-1409	3.9	23
11	Molecular dynamics simulations of liquid water using various long-range electrostatics techniques. *Molecular Physics*, **2005**, 103, 1945-1960	1.7	46
10	Molecular-dynamics simulations of methane hydrate dissociation. *Journal of Chemical Physics*, **2005**, 123, 244503	3.9	114
9	Theoretical studies of the kinetics of methane hydrate crystallization in external electromagnetic fields. *Journal of Chemical Physics*, **2004**, 120, 10247-56	3.9	112
8	Structural and dynamical properties of methane clathrate hydrates. *Journal of Computational Chemistry*, **2003**, 24, 1569-81	3.5	83
7	Hydrogen bonding and molecular mobility in liquid water in external electromagnetic fields. *Journal of Chemical Physics*, **2003**, 119, 11806-11813	3.9	96
6	Molecular dynamics simulations of microwave heating of water. *Journal of Chemical Physics*, **2003**, 118, 1589-1592	3.9	115
5	Atomistic simulations of liquid water using Lekner electrostatics. *Molecular Physics*, **2002**, 100, 3753-3762	1.7	42

4	Prediction of Henry's law constants by a quantitative structure property relationship and neural networks. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1150-61		48
3	Electro-Oxidation Reaction of Methanol over La2−xSrxNiO4+δ Ruddlesden−Popper Oxides. *ACS Applied Energy Materials*,	6.1	1
2	Coherency spectral analysis of interfacial water at TiO2 surfaces. *Molecular Simulation*,1-10	2	3
1	Molecular simulation of water adsorption on hydrophilic and hydrophobic surfaces of silicon: IR-spectral explorations. *Molecular Simulation*,1-8	2	1