Niall J English

List of Publications by Citations

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

#	Paper	IF	Citations
255	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
254	Gas hydrates in sustainable chemistry. *Chemical Society Reviews*, **2020**, 49, 5225-5309	58.5	186
253	Perspectives on external electric fields in molecular simulation: progress, prospects and challenges. *Physical Chemistry Chemical Physics*, **2015**, 17, 12407-40	3.6	140
252	Perspectives on molecular simulation of clathrate hydrates: Progress, prospects and challenges. *Chemical Engineering Science*, **2015**, 121, 133-156	4.4	137
251	Synergistic Effects on Band Gap-Narrowing in Titania by Codoping from First-Principles Calculations. *Chemistry of Materials*, **2010**, 22, 1616-1623	9.6	118
250	Molecular dynamics simulations of microwave heating of water. *Journal of Chemical Physics*, **2003**, 118, 1589-1592	3.9	115
249	Molecular-dynamics simulations of methane hydrate dissociation. *Journal of Chemical Physics*, **2005**, 123, 244503	3.9	114
248	Theoretical studies of the kinetics of methane hydrate crystallization in external electromagnetic fields. *Journal of Chemical Physics*, **2004**, 120, 10247-56	3.9	112
247	First-principles calculation of nitrogen-tungsten codoping effects on the band structure of anatase-titania. *Applied Physics Letters*, **2009**, 94, 132102	3.4	104
246	Hydrogen bonding and molecular mobility in liquid water in external electromagnetic fields. *Journal of Chemical Physics*, **2003**, 119, 11806-11813	3.9	96
245	Thermal conductivity of methane hydrate from experiment and molecular simulation. *Journal of Physical Chemistry B*, **2007**, 111, 13194-205	3.4	90
244	Band gap engineering of (N,Ta)-codoped TiO2: A first-principles calculation. *Chemical Physics Letters*, **2009**, 478, 175-179	2.5	86
243	Structural and dynamical properties of methane clathrate hydrates. *Journal of Computational Chemistry*, **2003**, 24, 1569-81	3.5	83
242	Denaturation of hen egg white lysozyme in electromagnetic fields: a molecular dynamics study. *Journal of Chemical Physics*, **2007**, 126, 091105	3.9	74
241	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 22847-22857	3.8	72
240	Controlled semiconductor nanorod assembly from solution: influence of concentration, charge and solvent nature. *Journal of Materials Chemistry*, **2012**, 22, 1562-1569		72
239	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

238	Magnetic properties of first-row element-doped ZnS semiconductors: A density functional theory investigation. *Physical Review B*, **2009**, 80,	3.3	72
237	Molecular dynamics study of thermal-driven methane hydrate dissociation. *Journal of Chemical Physics*, **2009**, 131, 074704	3.9	71
236	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
235	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
234	Mechanisms for thermal conduction in methane hydrate. *Physical Review Letters*, **2009**, 103, 015901	7.4	64
233	Diffusivity and Mobility of Adsorbed Water Layers at TiO2 Rutile and Anatase Interfaces. *Crystals*, **2016**, 6, 1	2.3	64
232	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
231	Density fluctuations in liquid water. *Physical Review Letters*, **2011**, 106, 037801	7.4	58
230	Molecular dynamics simulations of microwave effects on water using different long-range electrostatics methodologies. *Molecular Physics*, **2006**, 104, 243-253	1.7	57
229	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
228	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
227	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
226	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
225	Mechanisms for thermal conduction in various polymorphs of methane hydrate. *Physical Review B*, **2009**, 80,	3.3	52
224	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
223	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
222	Perspectives on atmospheric CO2 fixation in inorganic and biomimetic structures. *Coordination Chemistry Reviews*, **2014**, 269, 85-95	23.2	49
221	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

220	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
219	Tailoring the electronic structure of TiO2 by cation codoping from hybrid density functional theory calculations. *Physical Review B*, **2011**, 83,	3.3	48
218	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
217	Photo-active and optical properties of bismuth ferrite (BiFeO3): An experimental and theoretical study. *Chemical Physics Letters*, **2013**, 572, 78-84	2.5	47
216	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
215	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
214	Molecular dynamics simulations of liquid water using various long-range electrostatics techniques. *Molecular Physics*, **2005**, 103, 1945-1960	1.7	46
213	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
212	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
211	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
210	Atomistic simulations of liquid water using Lekner electrostatics. *Molecular Physics*, **2002**, 100, 3753-3769	1.7	42
209	Diffusive hydrogen inter-cage migration in hydrogen and hydrogen-tetrahydrofuran clathrate hydrates. *Journal of Chemical Physics*, **2013**, 138, 094507	3.9	41
208	Massive generation of metastable bulk nanobubbles in water by external electric fields. *Science Advances*, **2020**, 6, eaaz0094	14.3	38
207	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
206	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
205	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
204	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
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202	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
201	Molecular dynamics study of CO2 hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. *Journal of Chemical Physics*, **2013**, 139, 094701	3.9	33
200	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
199	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
198	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
197	Electromagnetic-field effects on structure and dynamics of amyloidogenic peptides. *Journal of Chemical Physics*, **2016**, 144, 085101	3.9	32
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195	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
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187	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. *Journal of Chemical Physics*, **2015**, 142, 244503	3.9	26
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182	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
181	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
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173	Influence of doping on the photoactive properties of magnetron-sputtered titania coatings: Experimental and theoretical study. *Physical Review B*, **2012**, 86,	3.3	22
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171	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
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160	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
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150	First-Principles Study of S Doping at the Rutile TiO2 (110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 17464-17470	3.8	17
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147	Molecular-dynamics study of propane-hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. *Journal of Chemical Physics*, **2018**, 148, 114504	3.9	16
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