Matthew J Mcgrath

List of Publications by Year
in descending order

28	3,068	304743	526287
papers	citations	22 h-index	27 g-index

30	30	30	4690
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular understanding of sulphuric acidâ€“amine particle nucleation in the atmosphere. Nature, 2013, 502, 359-363.	27.8	774
2	Land management and land-cover change haveÂimpacts of similar magnitude on surfaceÂtemperature. Nature Climate Change, 2014, 4, 389-393.	18.8	404
3	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	2.6	327
4	Europeâ€™s forest management did not mitigate climate warming. Science, 2016, 351, 597-600.	12.6	290
5	Trade-offs in using European forests to meet climate objectives. Nature, 2018, 562, 259-262.	27.8	149
6	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	2.5	128
7	Structure and Dynamics of the Aqueous Liquidâ^'Vapor Interface:Â A Comprehensive Particle-Based Simulation StudyâŠ¥. Journal of Physical Chemistry B, 2006, 110, 3738-3746.	2.6	115
8	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	2.1	99
9	The Structure and Stability of Biological Metaphosphate, Phosphate, and Phosphorane Compounds in the Gas Phase and in Solution. Journal of the American Chemical Society, 2004, 126, 1654-1665.	13.7	94
10	Re-examining the properties of the aqueous vaporâ€“liquid interface using dispersion corrected density functional theory. Journal of Chemical Physics, 2011, 135, 124712.	3.0	82
11	Time-Dependent Properties of Liquid Water:â€‰ A Comparison of Carâ^'Parrinello and Bornâ^'Oppenheimer Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1274-1281.	5.3	77
12	Liquid structures of water, methanol, and hydrogen fluoride at ambient conditions from first principles molecular dynamics simulations with a dispersion corrected density functional. Physical Chemistry Chemical Physics, 2011, 13, 19943.	2.8	63
13	Adenosine Triphosphate Hydrolysis Mechanism in Kinesin Studied by Combined Quantum-Mechanical/Molecular-Mechanical Metadynamics Simulations. Journal of the American Chemical Society, 2013, 135, 8908-8919.	13.7	56
14	Excited State Hydrogen Bond Dynamics:â€‰ Coumarin 102 in Acetonitrileâ^'Water Binary Mixtures. Journal of Physical Chemistry A, 2008, 112, 2511-2514.	2.5	48
15	Evaluating the performance of land surface model ORCHIDEE-CANÂv1.0 on water and energy flux estimation with a single- and multi-layer energy budget scheme. Geoscientific Model Development, 2016, 9, 2951-2972.	3.6	43
16	Calculation of the Gibbs free energy of solvation and dissociation of HCl in water via Monte Carlo simulations and continuum solvation models. Physical Chemistry Chemical Physics, 2013, 15, 13578.	2.8	39
17	Vaporâ€“Liquid Coexistence Curves for Methanol and Methane Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2011, 115, 11688-11692.	2.6	38
18	Rethinking the application of the first nucleation theorem to particle formation. Journal of Chemical Physics, 2012, 136, 094107.	3.0	35

#	Article	IF	Citations
19	Representing anthropogenic gross land use change, wood harvest, and forest age dynamics in a global vegetation model ORCHIDEE-MICT v8.4.2. Geoscientific Model Development, 2018, 11, 409-428.	3.6	30
20	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	7.5	29
21	Structural Rearrangements and Magic Numbers in Reactions between Pyridine-Containing Water Clusters and Ammonia. Journal of Physical Chemistry A, 2012, 116, 4902-4908.	2.5	25
22	Simulating damage for wind storms in the land surface model ORCHIDEE-CAN (revision 4262). Geoscientific Model Development, 2018, 11, 771-791.	3.6	24
23	Structure of the Methanol Liquidâ^'Vapor Interface: A Comprehensive Particle-Based Simulation Study. Journal of Physical Chemistry C, 2008, 112, 15412-15418.	3.1	23
24	The consolidated European synthesis of CO₂ emissions and removals for the European Union and United Kingdom: 1990â€“2018. Earth System Science Data, 2021, 13, 2363-2406.	9.9	23
25	Vapor-liquid nucleation of argon: Exploration of various intermolecular potentials. Journal of Chemical Physics, 2010, 133, 084106.	3.0	20
26	First principles Monte Carlo simulations of aggregation in the vapor phase of hydrogen fluoride. Physical Chemistry Chemical Physics, 2010, 12, 7678.	2.8	18
27	Vaporâ€“liquid phase equilibria of water modelled by a Kimâ€“Gordon potential. Chemical Physics Letters, 2009, 479, 60-64.	2.6	2
28	Large-Scale Monte Carlo Simulations for Aggregation, Self-Assembly, and Phase Equilibria. , 0, , 189-199.		0