William A Goddard

List of Publications by Citations

645 papers	76,103 citations	130 h-index	258 g-index
653 ext. papers	83,955 ext. citations	8.3 avg, IF	8.16 L-index

#	Paper	IF	Citations
645	DREIDING: a generic force field for molecular simulations. *The Journal of Physical Chemistry*, **1990**, 94, 8897-8909		4645
644	ReaxFF: A Reactive Force Field for Hydrocarbons. *Journal of Physical Chemistry A*, **2001**, 105, 9396-9409	2.8	3390
643	Starburst Dendrimers: Molecular-Level Control of Size, Shape, Surface Chemistry, Topology, and Flexibility from Atoms to Macroscopic Matter. *Angewandte Chemie International Edition in English*, **1990**, 29, 138-175		2705
642	Charge equilibration for molecular dynamics simulations. *The Journal of Physical Chemistry*, **1991**, 95, 3358-3363		2479
641	Silicon nanowires as efficient thermoelectric materials. *Nature*, **2008**, 451, 168-71	50.4	2199
640	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
639	ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation. *Journal of Physical Chemistry A*, **2008**, 112, 1040-53	2.8	1392
638	Catalysis research of relevance to carbon management: progress, challenges, and opportunities. *Chemical Reviews*, **2001**, 101, 953-96	68.1	1188
637	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. *Science*, **2016**, 354, 1414-1419	33.3	986
636	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. *Journal of the American Chemical Society*, **1994**, 116, 11875-11882	16.4	953
635	Thermal conductivity of carbon nanotubes. *Nanotechnology*, **2000**, 11, 65-69	3.4	844
634	From The Cover: The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 2673-7	11.5	782
633	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. *Journal of Physical Chemistry A*, **2003**, 107, 3803-3811	2.8	682
632	Covalent organic frameworks as exceptional hydrogen storage materials. *Journal of the American Chemical Society*, **2008**, 130, 11580-1	16.4	643
631	Linear artificial molecular muscles. *Journal of the American Chemical Society*, **2005**, 127, 9745-59	16.4	617
630	Excited States of H2O using improved virtual orbitals. *Chemical Physics Letters*, **1969**, 3, 414-418	2.5	546
629	Predictions of Hole Mobilities in Oligoacene Organic Semiconductors from Quantum Mechanical Calculations *Journal of Physical Chemistry B*, **2004**, 108, 8614-8621	3.4	513

628	Self-assembly of carbon nanotubes into two-dimensional geometries using DNA origami templates. *Nature Nanotechnology*, **2010**, 5, 61-6	28.7	512
627	Recent advances on simulation and theory of hydrogen storage in metal-organic frameworks and covalent organic frameworks. *Chemical Society Reviews*, **2009**, 38, 1460-76	58.5	491
626	Temperature dependence of blue phosphorescent cyclometalated Ir(III) complexes. *Journal of the American Chemical Society*, **2009**, 131, 9813-22	16.4	482
625	Theoretical predictions for hot-carrier generation from surface plasmon decay. *Nature Communications*, **2014**, 5, 5788	17.4	475
624	Calculation of solvation free energies of charged solutes using mixed cluster/continuum models. *Journal of Physical Chemistry B*, **2008**, 112, 9709-19	3.4	459
623	Starburst dendrimers. 5. Molecular shape control. *Journal of the American Chemical Society*, **1989**, 111, 2339-2341	16.4	447
622	Generalized valence bond description of bonding in low-lying states of molecules. *Accounts of Chemical Research*, **1973**, 6, 368-376	24.3	427
621	Oxidative aliphatic C-H fluorination with fluoride ion catalyzed by a manganese porphyrin. *Science*, **2012**, 337, 1322-5	33.3	422
620	Sulfation patterns of glycosaminoglycans encode molecular recognition and activity. *Nature Chemical Biology*, **2006**, 2, 467-73	11.7	417
619	A bonding model for gold(I) carbene complexes. *Nature Chemistry*, **2009**, 1, 482-6	17.6	416
618	Shock waves in high-energy materials: the initial chemical events in nitramine RDX. *Physical Review Letters*, **2003**, 91, 098301	7.4	416
617	Energetics, structure, mechanical and vibrational properties of single-walled carbon nanotubes. *Nanotechnology*, **1998**, 9, 184-191	3.4	411
616	Structure of PAMAM Dendrimers: Generations 1 through 11. *Macromolecules*, **2004**, 37, 6236-6254	5.5	408
615	Lithium-doped metal-organic frameworks for reversible H2 storage at ambient temperature. *Journal of the American Chemical Society*, **2007**, 129, 8422-3	16.4	403
614	Phosphofructokinase 1 glycosylation regulates cell growth and metabolism. *Science*, **2012**, 337, 975-80	33.3	389
613	Starburst-Dendrimere: Kontrolle von Gr□, Gestalt, Oberfl□chenchemie, Topologie und Flexibilit□ beim □bergang von Atomen zu makroskopischer Materie. *Angewandte Chemie*, **1990**, 102, 119-157	3.6	387
612	Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. *ACS Nano*, **2016**, 10, 957-66	16.7	380
611	Mechanically bonded macromolecules. *Chemical Society Reviews*, **2010**, 39, 17-29	58.5	380

610	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations: Effect of Monomeric Sequence. *Journal of Physical Chemistry B*, **2004**, 108, 3149-3157	3.4	375
609	Oxidation of Methanol on 2nd and 3rd Row Group VIII Transition Metals (Pt, Ir, Os, Pd, Rh, and Ru): Application to Direct Methanol Fuel Cells. *Journal of the American Chemical Society*, **1999**, 121, 10928-10941	16.4	370
608	Atomic level simulations on a million particles: The cell multipole method for Coulomb and London nonbond interactions. *Journal of Chemical Physics*, **1992**, 97, 4309-4315	3.9	366
607	Acceleration of convergence for lattice sums. *The Journal of Physical Chemistry*, **1989**, 93, 7320-7327		364
606	Field-effect transistors made from solution-grown two-dimensional tellurene. *Nature Electronics*, **2018**, 1, 228-236	28.4	358
605	Effect of Solvent and pH on the Structure of PAMAM Dendrimers. *Macromolecules*, **2005**, 38, 979-991	5.5	354
604	Accurate Band Gaps for Semiconductors from Density Functional Theory. *Journal of Physical Chemistry Letters*, **2011**, 2, 212-217	6.4	340
603	The two-phase model for calculating thermodynamic properties of liquids from molecular dynamics: Validation for the phase diagram of Lennard-Jones fluids. *Journal of Chemical Physics*, **2003**, 119, 11792-11805	3.9	334
602	Development of the ReaxFF reactive force field for describing transition metal catalyzed reactions, with application to the initial stages of the catalytic formation of carbon nanotubes. *Journal of Physical Chemistry A*, **2005**, 109, 493-9	2.8	332
601	Origin of low sodium capacity in graphite and generally weak substrate binding of Na and Mg among alkali and alkaline earth metals. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 3735-9	11.5	328
600	Simulations on the thermal decomposition of a poly(dimethylsiloxane) polymer using the ReaxFF reactive force field. *Journal of the American Chemical Society*, **2005**, 127, 7192-202	16.4	316
599	Melting and crystallization in Ni nanoclusters: The mesoscale regime. *Journal of Chemical Physics*, **2001**, 115, 385-394	3.9	314
598	Thermal decomposition of RDX from reactive molecular dynamics. *Journal of Chemical Physics*, **2005** , 122, 54502	3.9	313
597	Prediction of fullerene packing in C60 and C70 crystals. *Nature*, **1991**, 351, 464-467	50.4	292
596	New alkali doped pillared carbon materials designed to achieve practical reversible hydrogen storage for transportation. *Physical Review Letters*, **2004**, 92, 166103	7.4	286
595	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4963-8	11.5	280
594	Thermal conductivity of diamond and related materials from molecular dynamics simulations. *Journal of Chemical Physics*, **2000**, 113, 6888-6900	3.9	280
593	Schottky-Barrier-Free Contacts with Two-Dimensional Semiconductors by Surface-Engineered MXenes. *Journal of the American Chemical Society*, **2016**, 138, 15853-15856	16.4	278

592	ReaxFF-lg: correction of the ReaxFF reactive force field for London dispersion, with applications to the equations of state for energetic materials. *Journal of Physical Chemistry A*, **2011**, 115, 11016-22	2.8	278
591	Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters. *Journal of Chemical Theory and Computation*, **2009**, 5, 1016-26	6.4	276
590	Oxygen-Vacancy Abundant Ultrafine CoO/Graphene Composites for High-Rate Supercapacitor Electrodes. *Advanced Science*, **2018**, 5, 1700659	13.6	274
589	Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from ab initio molecular dynamics free-energy calculations at 298 K. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 1795-1800	11.5	263
588	Toward a lithium-"air" battery: the effect of CO2 on the chemistry of a lithium-oxygen cell. *Journal of the American Chemical Society*, **2013**, 135, 9733-42	16.4	262
587	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. *Nature Catalysis*, **2019**, 2, 495-503	36.5	258
586	Subsurface oxide plays a critical role in CO activation by Cu(111) surfaces to form chemisorbed CO, the first step in reduction of CO. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6706-6711	11.5	253
585	Entropy and the driving force for the filling of carbon nanotubes with water. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 11794-8	11.5	251
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582	Radically enhanced molecular recognition. *Nature Chemistry*, **2010**, 2, 42-9	17.6	247
581	Mechanism of C-F reductive elimination from palladium(IV) fluorides. *Journal of the American Chemical Society*, **2010**, 132, 3793-807	16.4	247
580	Strain Rate Induced Amorphization in Metallic Nanowires. *Physical Review Letters*, **1999**, 82, 2900-2903	7.4	246
579	Dendrimer enhanced ultrafiltration. 1. Recovery of Cu(II) from aqueous solutions using PAMAM dendrimers with ethylene diamine core and terminal NH2 groups. *Environmental Science & Technology*, **2005**, 39, 1366-77	10.3	243
578	Prediction of structure and function of G protein-coupled receptors. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12622-7	11.5	243
577	First-principles investigation of anistropic hole mobilities in organic semiconductors. *Journal of Physical Chemistry B*, **2009**, 113, 8813-9	3.4	240
576	Synergy between Fe and Ni in the optimal performance of (Ni,Fe)OOH catalysts for the oxygen evolution reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5872-5877	11.5	237
575	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. *Journal of Physical Chemistry C*, **2010**, 114, 4939-4949	3.8	236

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573	Electronic--mechanical coupling in graphene from in situ nanoindentation experiments and multiscale atomistic simulations. *Nano Letters*, **2011**, 11, 1241-6	11.5	229
572	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals: Cu-Ag and Cu-Ni. *Physical Review B*, **1999**, 59, 3527-3533	3.3	228
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570	Ab initio studies of the x-ray absorption edge in copper complexes. I. Atomic Cu2+ and Cu(ii)Cl2. *Physical Review B*, **1980**, 22, 2767-2776	3.3	224
569	PAMAM dendrimers undergo pH responsive conformational changes without swelling. *Journal of the American Chemical Society*, **2009**, 131, 2798-9	16.4	222
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566	Bimetallic reductive elimination from dinuclear Pd(III) complexes. *Journal of the American Chemical Society*, **2010**, 132, 14092-103	16.4	219
565	Two-phase thermodynamic model for efficient and accurate absolute entropy of water from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 8191-8	3.4	218
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563	Improved designs of metal-organic frameworks for hydrogen storage. *Angewandte Chemie - International Edition*, **2007**, 46, 6289-92	16.4	210
562	ReaxFF(MgH) reactive force field for magnesium hydride systems. *Journal of Physical Chemistry A*, **2005**, 109, 851-9	2.8	209
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555	Self-Assembled Monolayer Mechanism for Corrosion Inhibition of Iron by Imidazolines. *Langmuir*, **1996**, 12, 6419-6428	4	190
554	Carbon cluster formation during thermal decomposition of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-triamino-2,4,6-trinitrobenzene high explosives from ReaxFF reactive molecular dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 10619-40	2.8	189
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