William Goddard

List of Publications by Citations

749 papers	67,293 citations	119 h-index	238 g-index
786 ext. papers	75,423 ext. citations	8.5 avg, IF	8.17 L-index

#	Paper	IF	Citations
749	DREIDING: a generic force field for molecular simulations. *The Journal of Physical Chemistry*, **1990**, 94, 8897-8909		4645
748	ReaxFF: A Reactive Force Field for Hydrocarbons. *Journal of Physical Chemistry A*, **2001**, 105, 9396-9409	2.8	3390
747	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
746	Charge equilibration for molecular dynamics simulations. *The Journal of Physical Chemistry*, **1991**, 95, 3358-3363		2479
745	Silicon nanowires as efficient thermoelectric materials. *Nature*, **2008**, 451, 168-71	50.4	2199
744	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
743	ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation. *Journal of Physical Chemistry A*, **2008**, 112, 1040-53	2.8	1392
742	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. *Science*, **2016**, 354, 1414-1419	33.3	986
741	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
740	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. *Journal of Physical Chemistry A*, **2003**, 107, 3803-3811	2.8	682
739	Linear artificial molecular muscles. *Journal of the American Chemical Society*, **2005**, 127, 9745-59	16.4	617
738	High-performance bifunctional porous non-noble metal phosphide catalyst for overall water splitting. *Nature Communications*, **2018**, 9, 2551	17.4	566
737	Predictions of Hole Mobilities in Oligoacene Organic Semiconductors from Quantum Mechanical Calculations *Journal of Physical Chemistry B*, **2004**, 108, 8614-8621	3.4	513
736	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
735	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
734	Oxidative aliphatic C-H fluorination with fluoride ion catalyzed by a manganese porphyrin. *Science*, **2012**, 337, 1322-5	33.3	422
733	Sulfation patterns of glycosaminoglycans encode molecular recognition and activity. *Nature Chemical Biology*, **2006**, 2, 467-73	11.7	417

732	Shock waves in high-energy materials: the initial chemical events in nitramine RDX. *Physical Review Letters*, **2003**, 91, 098301	7.4	416
731	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
730	Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. *ACS Nano*, **2016**, 10, 957-66	16.7	380
729	Mechanically bonded macromolecules. *Chemical Society Reviews*, **2010**, 39, 17-29	58.5	380
728	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
727	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
726	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
725	Effect of Solvent and pH on the Structure of PAMAM Dendrimers. *Macromolecules*, **2005**, 38, 979-991	5.5	354
724	Self-Consistent Procedures for Generalized Valence Bond Wavefunctions. Applications H3, BH, H2O, C2H6, and O2. *Journal of Chemical Physics*, **1972**, 57, 738-748	3.9	354
723	Accurate Band Gaps for Semiconductors from Density Functional Theory. *Journal of Physical Chemistry Letters*, **2011**, 2, 212-217	6.4	340
722	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
721	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
720	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
719	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
718	Melting and crystallization in Ni nanoclusters: The mesoscale regime. *Journal of Chemical Physics*, **2001**, 115, 385-394	3.9	314
717	Thermal decomposition of RDX from reactive molecular dynamics. *Journal of Chemical Physics*, **2005**, 122, 54502	3.9	313
716	Prediction of fullerene packing in C60 and C70 crystals. *Nature*, **1991**, 351, 464-467	50.4	292
715	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

714	Thermal conductivity of diamond and related materials from molecular dynamics simulations. *Journal of Chemical Physics*, **2000**, 113, 6888-6900	3.9	280
713	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
712	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
711	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
710	Oxygen-Vacancy Abundant Ultrafine CoO/Graphene Composites for High-Rate Supercapacitor Electrodes. *Advanced Science*, **2018**, 5, 1700659	13.6	274
709	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
708	Hildebrand and Hansen solubility parameters from molecular dynamics with applications to electronic nose polymer sensors. *Journal of Computational Chemistry*, **2004**, 25, 1814-26	3.5	261
707	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. *Nature Catalysis*, **2019**, 2, 495-503	36.5	258
706	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
705	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
704	Efficient hydrogen evolution by ternary molybdenum sulfoselenide particles on self-standing porous nickel diselenide foam. *Nature Communications*, **2016**, 7, 12765	17.4	248
703	Radically enhanced molecular recognition. *Nature Chemistry*, **2010**, 2, 42-9	17.6	247
702	Mechanism of C-F reductive elimination from palladium(IV) fluorides. *Journal of the American Chemical Society*, **2010**, 132, 3793-807	16.4	247
701	Mechanistic Explanation of the pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu (111). *Journal of the American Chemical Society*, **2016**, 138, 483-6	16.4	246
700	Strain Rate Induced Amorphization in Metallic Nanowires. *Physical Review Letters*, **1999**, 82, 2900-2903	7.4	246
699	Theoretical studies of oxidative addition and reductive elimination. 3. Carbon-hydrogen and carbon-carbon reductive coupling from palladium and platinum bis(phosphine) complexes. *Journal of the American Chemical Society*, **1986**, 108, 6115-6128	16.4	243
698	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
697	Unexpected discovery of low-cost maricite NaFePO4 as a high-performance electrode for Na-ion batteries. *Energy and Environmental Science*, **2015**, 8, 540-545	35.4	236

696	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
695	Hydrogen bonding in the benzene–ammonia dimer. *Nature*, **1993**, 362, 735-737	50.4	236
694	Improved Quantum Theory of Many-Electron Systems. II. The Basic Method. *Physical Review*, **1967**, 157, 81-93		236
693	Reaction Mechanisms for the Electrochemical Reduction of CO to CO and Formate on the Cu(100) Surface at 298 K from Quantum Mechanics Free Energy Calculations with Explicit Water. *Journal of the American Chemical Society*, **2016**, 138, 13802-13805	16.4	229
692	PAMAM dendrimers undergo pH responsive conformational changes without swelling. *Journal of the American Chemical Society*, **2009**, 131, 2798-9	16.4	222
691	Monolayer atomic crystal molecular superlattices. *Nature*, **2018**, 555, 231-236	50.4	220
690	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
689	Atomistic Mechanisms Underlying Selectivities in C(1) and C(2) Products from Electrochemical Reduction of CO on Cu(111). *Journal of the American Chemical Society*, **2017**, 139, 130-136	16.4	214
688	The Mechanism for Unimolecular Decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab Initio Study. *Journal of Physical Chemistry A*, **2000**, 104, 2261-2272	2.8	214
687	ReaxFF(MgH) reactive force field for magnesium hydride systems. *Journal of Physical Chemistry A*, **2005**, 109, 851-9	2.8	209
686	Theoretical studies of oxidative addition and reductive elimination. 2. Reductive coupling of hydrogen-hydrogen, hydrogen-carbon, and carbon-carbon bonds from palladium and platinum complexes. *Organometallics*, **1986**, 5, 609-622	3.8	209
685	Configuration interaction studies of O3 and O+3. Ground and excited states. *Journal of Chemical Physics*, **1975**, 62, 3912-3924	3.9	206
684	Improved Quantum Theory of Many-Electron Systems. I. Construction of Eigenfunctions ofS^2Which Satisfy Pauli's Principle. *Physical Review*, **1967**, 157, 73-80		206
683	Olefin metathesis - a mechanistic study of high-valent Group VI catalysts. *Journal of the American Chemical Society*, **1982**, 104, 448-456	16.4	203
682	Selective oxidation of methane to methanol catalyzed, with C-H activation, by homogeneous, cationic gold. *Angewandte Chemie - International Edition*, **2004**, 43, 4626-9	16.4	202
681	Molecular dynamics study of the binary Cu46Zr54 metallic glass motivated by experiments: Glass formation and atomic-level structure. *Physical Review B*, **2005**, 71,	3.3	199
680	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
679	Molecular Dynamics Study of a Surfactant-Mediated Decane–Water Interface: Effect of Molecular Architecture of Alkyl Benzene Sulfonate. *Journal of Physical Chemistry B*, **2004**, 108, 12130-12140	3.4	187

678	An extended hybrid density functional (X3LYP) with improved descriptions of nonbond interactions and thermodynamic properties of molecular systems. *Journal of Chemical Physics*, **2005**, 122, 14105	3.9	187
677	In Silico Discovery of New Dopants for Fe-Doped Ni Oxyhydroxide (NiFe OOH) Catalysts for Oxygen Evolution Reaction. *Journal of the American Chemical Society*, **2018**, 140, 6745-6748	16.4	186
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675	Initiation mechanisms and kinetics of pyrolysis and combustion of JP-10 hydrocarbon jet fuel. *Journal of Physical Chemistry A*, **2009**, 113, 1740-6	2.8	184
674	Force fields, structures, and properties of poly(vinylidene fluoride) crystals. *Macromolecules*, **1992**, 25, 7268-7281	5.5	183
673	Poly(amidoamine) Dendrimers: A New Class of High Capacity Chelating Agents for Cu(II) Ions. *Environmental Science & Technology*, **1999**, 33, 820-824	10.3	175
672	Electronic correlation and the Si(100) surface: Buckling versus nonbuckling. *Journal of Vacuum Science and Technology*, **1982**, 21, 344-350		174
671	Theoretical Study of Solvent Effects on the Platinum-Catalyzed Oxygen Reduction Reaction. *Journal of Physical Chemistry Letters*, **2010**, 1, 856-861	6.4	172
670	Mechanism of homogeneous Ir(III) catalyzed regioselective arylation of olefins. *Journal of the American Chemical Society*, **2004**, 126, 352-63	16.4	172
669	The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO(2) (110) Surface. *Journal of the American Chemical Society*, **2017**, 139, 149-155	16.4	168
668	The hindered rotor density-of-states interpolation function. *Journal of Chemical Physics*, **1997**, 106, 6675-6680	3.9	168
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664	Mechanistic study of gold(I)-catalyzed intermolecular hydroamination of allenes. *Journal of the American Chemical Society*, **2010**, 132, 13064-71	16.4	160
663	Highly stable tetrathiafulvalene radical dimers in [3]catenanes. *Nature Chemistry*, **2010**, 2, 870-9	17.6	159
662	Embedding covalency into metal catalysts for efficient electrochemical conversion of CO2. *Journal of the American Chemical Society*, **2014**, 136, 11355-61	16.4	157
661	Contact Resistance for End-Contacted Metal-Graphene and Metal-Nanotube Interfaces from Quantum Mechanics. *Journal of Physical Chemistry C*, **2010**, 114, 17845-17850	3.8	155

660	Metal□Organic Frameworks Provide Large Negative Thermal Expansion Behavior. *Journal of Physical Chemistry C*, **2007**, 111, 15185-15191	3.8	154
659	Free-Energy Barriers and Reaction Mechanisms for the Electrochemical Reduction of CO on the Cu(100) Surface, Including Multiple Layers of Explicit Solvent at pH 0. *Journal of Physical Chemistry Letters*, **2015**, 6, 4767-73	6.4	152
658	Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Gold-Iron Core-Shell Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 15608-15611	16.4	151
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655	Explanation of Dramatic pH-Dependence of Hydrogen Binding on Noble Metal Electrode: Greatly Weakened Water Adsorption at High pH. *Journal of the American Chemical Society*, **2018**, 140, 7787-7790	16.4	148
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652	The Reaction Mechanism with Free Energy Barriers for Electrochemical Dihydrogen Evolution on MoS2. *Journal of the American Chemical Society*, **2015**, 137, 6692-8	16.4	146
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629	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. *Journal of Chemical Physics*, **2017**, 146, 114104	3.9	117
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