William A Goddard

List of Publications by Year
in descending order

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647 papers	92,376 citations	266 141 h-index	364 282 g-index
653 all docs	653 docs citations	653 times ranked	68631 citing authors

#	Article	IF	Citations
1	DREIDING: a generic force field for molecular simulations. The Journal of Physical Chemistry, 1990, 94, 8897-8909.	2.9	5,555
2	ReaxFF:Â A Reactive Force Field for Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 9396-9409.	1.1	4,490
3	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.	4.4	3,032
4	Charge equilibration for molecular dynamics simulations. The Journal of Physical Chemistry, 1991, 95, 3358-3363.	2.9	2,910
5	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
6	Silicon nanowires as efficient thermoelectric materials. Nature, 2008, 451, 168-171.	13.7	2,493
7	ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation. Journal of Physical Chemistry A, 2008, 112, 1040-1053.	1.1	1,892
8	Catalysis Research of Relevance to Carbon Management:â€‰ Progress, Challenges, and Opportunities. Chemical Reviews, 2001, 101, 953-996.	23.0	1,311
9	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419.	6.0	1,292
10	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.	6.6	1,026
11	Thermal conductivity of carbon nanotubes. Nanotechnology, 2000, 11, 65-69.	1.3	988
12	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, 2673-2677.	3.3	863
13	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. Journal of Physical Chemistry A, 2003, 107, 3803-3811.	1.1	821
14	Covalent Organic Frameworks as Exceptional Hydrogen Storage Materials. Journal of the American Chemical Society, 2008, 130, 11580-11581.	6.6	746
15	Linear Artificial Molecular Muscles. Journal of the American Chemical Society, 2005, 127, 9745-9759.	6.6	660
16	Theoretical predictions for hot-carrier generation from surface plasmon decay. Nature Communications, 2014, 5, 5788.	5.8	600
17	Field-effect transistors made from solution-grown two-dimensional tellurene. Nature Electronics, 2018, 1, 228-236.	13.1	591
18	Predictions of Hole Mobilities in Oligoacene Organic Semiconductors from Quantum Mechanical Calculationsâ€. Journal of Physical Chemistry B, 2004, 108, 8614-8621.	1.2	586

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19	Excited States of H2O using improved virtual orbitals. Chemical Physics Letters, 1969, 3, 414-418.	1.2	579
20	Calculation of Solvation Free Energies of Charged Solutes Using Mixed Cluster/Continuum Models. Journal of Physical Chemistry B, 2008, 112, 9709-9719.	1.2	567
21	Self-assembly of carbon nanotubes into two-dimensional geometries using DNA origami templates. Nature Nanotechnology, 2010, 5, 61-66.	15.6	567
22	Temperature Dependence of Blue Phosphorescent Cyclometalated Ir(III) Complexes. Journal of the American Chemical Society, 2009, 131, 9813-9822.	6.6	558
23	Recent advances on simulation and theory of hydrogen storage in metalâ€“organic frameworks and covalent organic frameworks. Chemical Society Reviews, 2009, 38, 1460.	18.7	535
24	Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. ACS Nano, 2016, 10, 957-966.	7.3	534
25	Phosphofructokinase 1 Glycosylation Regulates Cell Growth and Metabolism. Science, 2012, 337, 975-980.	6.0	527
26	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
27	Starburst dendrimers. 5. Molecular shape control. Journal of the American Chemical Society, 1989, 111, 2339-2341.	6.6	500
28	Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. Physical Review Letters, 2003, 91, 098301.	2.9	495
29	Sulfation patterns of glycosaminoglycans encode molecular recognition and activity. Nature Chemical Biology, 2006, 2, 467-473.	3.9	494
30	Oxidative Aliphatic C-H Fluorination with Fluoride Ion Catalyzed by a Manganese Porphyrin. Science, 2012, 337, 1322-1325.	6.0	478
31	Starburstâ€Ðendrimere: Kontrolle von GrÃ¶ÃŸe, Gestalt, OberflÃchenchemie, Topologie und FlexibilitÃt beim Ãœbergang von Atomen zu makroskopischer Materie. Angewandte Chemie, 1990, 102, 119-157.	1.6	473
32	Generalized valence bond description of bonding in low-lying states of molecules. Accounts of Chemical Research, 1973, 6, 368-376.	7.6	467
33	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503.	16.1	464
34	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, 3735-3739.	3.3	462
35	Structure of PAMAM Dendrimers:Â Generations 1 through 11. Macromolecules, 2004, 37, 6236-6254.	2.2	455
36	A bonding model for gold(I) carbene complexes. Nature Chemistry, 2009, 1, 482-486.	6.6	451

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37	Energetics, structure, mechanical and vibrational properties of single-walled carbon nanotubes. Nanotechnology, 1998, 9, 184-191.	1.3	448
38	Accurate Band Gaps for Semiconductors from Density Functional Theory. Journal of Physical Chemistry Letters, 2011, 2, 212-217.	2.1	444
39	Schottky-Barrier-Free Contacts with Two-Dimensional Semiconductors by Surface-Engineered MXenes. Journal of the American Chemical Society, 2016, 138, 15853-15856.	6.6	444
40	Mechanically bonded macromolecules. Chemical Society Reviews, 2010, 39, 17-29.	18.7	428
41	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.	1.2	426
42	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations:Â Effect of Monomeric Sequence. Journal of Physical Chemistry B, 2004, 108, 3149-3157.	1.2	425
43	Lithium-Doped Metal-Organic Frameworks for Reversible H₂ Storage at Ambient Temperature. Journal of the American Chemical Society, 2007, 129, 8422-8423.	6.6	418
44	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.	3.3	414
45	Acceleration of convergence for lattice sums. The Journal of Physical Chemistry, 1989, 93, 7320-7327.	2.9	405
46	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.	1.2	404
47	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, 11016-11022.	1.1	401
48	Oxidation of Methanol on 2nd and 3rd Row Group VIII Transition Metals (Pt, Ir, Os, Pd, Rh, and Ru):â€‰Application to Direct Methanol Fuel Cells. Journal of the American Chemical Society, 1999, 121, 10928-10941.	6.6	397
49	Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field. Journal of the American Chemical Society, 2005, 127, 7192-7202.	6.6	395
50	Oxygenâ€Vacancy Abundant Ultrafine Co₃O₄/Graphene Composites for Highâ€Rate Supercapacitor Electrodes. Advanced Science, 2018, 5, 1700659.	5.6	392
51	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, 493-499.	1.1	390
52	Effect of Solvent and pH on the Structure of PAMAM Dendrimers. Macromolecules, 2005, 38, 979-991.	2.2	389
53	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.	3.3	380
54	Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502.	1.2	366

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55	Subsurface oxide plays a critical role in CO ₂ activation by Cu(111) surfaces to form chemisorbed CO ₂ , the first step in reduction of CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6706-6711.	3.3	363
56	Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics, 2001, 115, 385-394.	1.2	345
57	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, 4963-4968.	3.3	332
58	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, 1016-1026.	2.3	326
59	Monolayer atomic crystal molecular superlattices. Nature, 2018, 555, 231-236.	13.7	323
60	Prediction of fullerene packing in C60 and C70 crystals. Nature, 1991, 351, 464-467.	13.7	312
61	Efficient hydrogen evolution by ternary molybdenum sulfoselenide particles on self-standing porous nickel diselenide foam. Nature Communications, 2016, 7, 12765.	5.8	312
62	Thermal conductivity of diamond and related materials from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6888-6900.	1.2	307
63	New Alkali Doped Pillared Carbon Materials Designed to Achieve Practical Reversible Hydrogen Storage for Transportation. Physical Review Letters, 2004, 92, 166103.	2.9	307
64	Toward a Lithiumâ€“â€œAirâ€•Battery: The Effect of CO₂ on the Chemistry of a Lithiumâ€“Oxygen Cell. Journal of the American Chemical Society, 2013, 135, 9733-9742.	6.6	307
65	Highly active and stable stepped Cu surface for enhanced electrochemical CO2 reduction to C2H4. Nature Catalysis, 2020, 3, 804-812.	16.1	298
66	First-Principles Investigation of Anistropic Hole Mobilities in Organic Semiconductors. Journal of Physical Chemistry B, 2009, 113, 8813-8819.	1.2	292
67	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. Journal of Physical Chemistry C, 2010, 114, 4939-4949.	1.5	288
68	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, 11794-11798.	3.3	287
69	Radically enhanced molecular recognition. Nature Chemistry, 2010, 2, 42-49.	6.6	280
70	Two-Phase Thermodynamic Model for Efficient and Accurate Absolute Entropy of Water from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 8191-8198.	1.2	277
71	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, 12622-12627.	3.3	276
72	In Silico Discovery of New Dopants for Fe-Doped Ni Oxyhydroxide (Ni_{1â€“x}Fe_xOOH) Catalysts for Oxygen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 6745-6748.	6.6	274

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73	Mechanism of Câ˜F Reductive Elimination from Palladium(IV) Fluorides. Journal of the American Chemical Society, 2010, 132, 3793-3807.	6.6	273
74	Dendrimer Enhanced Ultrafiltration. 1. Recovery of Cu(II) from Aqueous Solutions Using PAMAM Dendrimers with Ethylene Diamine Core and Terminal NH2Groups. Environmental Science & Technology, 2005, 39, 1366-1377.	4.6	272
75	Improved Quantum Theory of Many-Electron Systems. II. The Basic Method. Physical Review, 1967, 157, 81-93.	2.7	269
76	Strain Rate Induced Amorphization in Metallic Nanowires. Physical Review Letters, 1999, 82, 2900-2903.	2.9	268
77	Source of Image Contrast in STM Images of Functionalized Alkanes on Graphite:Â A Systematic Functional Group Approach. Journal of Physical Chemistry B, 1997, 101, 5978-5995.	1.2	267
78	New surfactant classes for enhanced oil recovery and their tertiary oil recovery potential. Journal of Petroleum Science and Engineering, 2010, 71, 23-29.	2.1	264
79	Electronicâ˜Mechanical Coupling in Graphene from in situ Nanoindentation Experiments and Multiscale Atomistic Simulations. Nano Letters, 2011, 11, 1241-1246.	4.5	261
80	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, 10619-10640.	1.1	257
81	Antibody Catalysis of the Oxidation of Water. Science, 2001, 293, 1806-1811.	6.0	254
82	Ab initiostudies of the x-ray absorption edge in copper complexes. I. AtomicCu2+and Cu(ii)Cl2. Physical Review B, 1980, 22, 2767-2776.	1.1	252
83	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals:â€ƒCu-Ag and Cu-Ni. Physical Review B, 1999, 59, 3527-3533.	1.1	252
84	Olefin metathesis - a mechanistic study of high-valent Group VI catalysts. Journal of the American Chemical Society, 1982, 104, 448-456.	6.6	251
85	PAMAM Dendrimers Undergo pH Responsive Conformational Changes without Swelling. Journal of the American Chemical Society, 2009, 131, 2798-2799.	6.6	249
86	Molecular Dynamics Study of a Surfactant-Mediated Decaneâ˜Water Interface:â€‰ Effect of Molecular Architecture of Alkyl Benzene Sulfonate. Journal of Physical Chemistry B, 2004, 108, 12130-12140.	1.2	244
87	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.	1.1	241
88	Bimetallic Reductive Elimination from Dinuclear Pd(III) Complexes. Journal of the American Chemical Society, 2010, 132, 14092-14103.	6.6	237
89	ReaxFFMgHReactive Force Field for Magnesium Hydride Systems. Journal of Physical Chemistry A, 2005, 109, 851-859.	1.1	234
90	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.	1.1	228

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91	Molecular dynamics study of the binaryCu46Zr54metallic glass motivated by experiments: Glass formation and atomic-level structure. Physical Review B, 2005, 71, .	1.1	227
92	Self-Assembled Monolayer Mechanism for Corrosion Inhibition of Iron by Imidazolines. Langmuir, 1996, 12, 6419-6428.	1.6	225
93	Formation of carbonâ€“nitrogen bonds in carbon monoxide electrolysis. Nature Chemistry, 2019, 11, 846-851.	6.6	223
94	Improved Quantum Theory of Many-Electron Systems. I. Construction of Eigenfunctions ofS^2Which Satisfy Pauli's Principle. Physical Review, 1967, 157, 73-80.	2.7	222
95	Configuration interaction studies of O3 and O+3. Ground and excited states. Journal of Chemical Physics, 1975, 62, 3912-3924.	1.2	221
96	Multiparadigm Modeling of Dynamical Crack Propagation in Silicon Using a Reactive Force Field. Physical Review Letters, 2006, 96, 095505.	2.9	214
97	Initiation Mechanisms and Kinetics of Pyrolysis and Combustion of JP-10 Hydrocarbon Jet Fuel. Journal of Physical Chemistry A, 2009, 113, 1740-1746.	1.1	213
98	Improved Designs of Metalâ€“Organic Frameworks for Hydrogen Storage. Angewandte Chemie - International Edition, 2007, 46, 6289-6292.	7.2	212
99	Phosphoramidite Gold(I)-Catalyzed Diastereo- and Enantioselective Synthesis of 3,4-Substituted Pyrrolidines. Journal of the American Chemical Society, 2011, 133, 5500-5507.	6.6	210
100	Improved Quantum Theory of Manyâ€Electron Systems. V. The Spinâ€Coupling Optimized GI Method. Journal of Chemical Physics, 1969, 51, 1073-1087.	1.2	207
101	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, 4767-4773.	2.1	206
102	Stabilizing Highly Active Ru Sites by Suppressing Lattice Oxygen Participation in Acidic Water Oxidation. Journal of the American Chemical Society, 2021, 143, 6482-6490.	6.6	204
103	Dendritic Chelating Agents. 1. Cu(II) Binding to Ethylene Diamine Core Poly(amidoamine) Dendrimers in Aqueous Solutions. Langmuir, 2004, 20, 2640-2651.	1.6	200
104	Resolution of the Band Gap Prediction Problem for Materials Design. Journal of Physical Chemistry Letters, 2016, 7, 1198-1203.	2.1	200
105	Poly(amidoamine) Dendrimers:â€‰ A New Class of High Capacity Chelating Agents for Cu(II) Ions. Environmental Science & Technology, 1999, 33, 820-824.	4.6	198
106	Theoretical Study of Solvent Effects on the Platinum-Catalyzed Oxygen Reduction Reaction. Journal of Physical Chemistry Letters, 2010, 1, 856-861.	2.1	195
107	pKaValues of Guanine in Water:Â Density Functional Theory Calculations Combined with Poissonâ^'Boltzmann Continuumâ^'Solvation Model. Journal of Physical Chemistry B, 2003, 107, 344-357.	1.2	193
108	The Self-Consistent Field Equations for Generalized Valence Bond and Open-Shell Hartreeâ€"Fock Wave Functions. , 1977, , 79-127.		193

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109	Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Goldâ€“Iron Coreâ€“Shell Nanoparticles. Journal of the American Chemical Society, 2017, 139, 15608-15611.	6.6	191
110	Oxygen evolution reaction over catalytic single-site Co in a well-defined brookite TiO2 nanorod surface. Nature Catalysis, 2021, 4, 36-45.	16.1	189
111	Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting. Nature Communications, 2018, 9, 1809.	5.8	188
112	First Principles Calculation of pKa Values for 5-Substituted Uracils. Journal of Physical Chemistry A, 2001, 105, 274-280.	1.1	185
113	Adhesion and nonwetting-wetting transition in theAl/Î±â^'Al2O3interface. Physical Review B, 2004, 69, .	1.1	184
114	Mechanism of Homogeneous Ir(III) Catalyzed Regioselective Arylation of Olefins. Journal of the American Chemical Society, 2004, 126, 352-363.	6.6	184
115	Early maturation processes in coal. Part 2: Reactive dynamics simulations using the ReaxFF reactive force field on Morwell Brown coal structures. Organic Geochemistry, 2009, 40, 1195-1209.	0.9	183
116	Antiferromagnetic band structure ofLa2CuO4:â€ƒBecke-3â€“Lee-Yang-Parr calculations. Physical Review B, 2001, 63, .	1.1	182
117	Development of a ReaxFF Reactive Force Field for Glycine and Application to Solvent Effect and Tautomerization. Journal of Physical Chemistry B, 2011, 115, 249-261.	1.2	182
118	Definitive Band Gaps for Single-Wall Carbon Nanotubes. Journal of Physical Chemistry Letters, 2010, 1, 2946-2950.	2.1	179
119	Outstanding hydrogen evolution reaction catalyzed by porous nickel diselenide electrocatalysts. Energy and Environmental Science, 2017, 10, 1487-1492.	15.6	176
120	Bonding Properties of the Water Dimer:Â A Comparative Study of Density Functional Theories. Journal of Physical Chemistry A, 2004, 108, 2305-2313.	1.1	174
121	Alkylgold complexes by the intramolecular aminoauration of unactivated alkenes. Chemical Science, 2010, 1, 226.	3.7	174
122	Morse Stretch Potential Charge Equilibrium Force Field for Ceramics: Application to the Quartz-Stishovite Phase Transition and to Silica Glass. Physical Review Letters, 1999, 82, 1708-1711.	2.9	173
123	The Reaction Mechanism with Free Energy Barriers for Electrochemical Dihydrogen Evolution on MoS₂. Journal of the American Chemical Society, 2015, 137, 6692-6698.	6.6	173
124	Effects of Surface Roughness on the Electrochemical Reduction of CO₂ over Cu. ACS Energy Letters, 2020, 5, 1206-1214.	8.8	172
125	Highly stable tetrathiafulvalene radical dimers in [3]catenanes. Nature Chemistry, 2010, 2, 870-879.	6.6	171
126	Metalâ^'Organic Frameworks Provide Large Negative Thermal Expansion Behavior. Journal of Physical Chemistry C, 2007, 111, 15185-15191.	1.5	170

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127	Electrochemical CO Reduction Builds Solvent Water into Oxygenate Products. Journal of the American Chemical Society, 2018, 140, 9337-9340.	6.6	170
128	The charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model. Journal of Chemical Physics, 2015, 142, 064107.	1.2	167
129	Stabilization of Coiled-Coil Peptide Domains by Introduction of Trifluoroleucineâ€. Biochemistry, 2001, 40, 2790-2796.	1.2	166
130	BrÃ¸nsted basicity of the airâ€“water interface. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 18679-18683.	3.3	159
131	A Radically Configurable Six-State Compound. Science, 2013, 339, 429-433.	6.0	158
132	The predicted 3D structure of the human D2 dopamine receptor and the binding site and binding affinities for agonists and antagonists. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 3815-3820.	3.3	157
133	Pressureâ€Dependent Polymorphism and Bandâ€Gap Tuning of Methylammonium Lead Iodide Perovskite. Angewandte Chemie - International Edition, 2016, 55, 6540-6544.	7.2	157
134	Development and Validation of a ReaxFF Reactive Force Field for Cu Cation/Water Interactions and Copper Metal/Metal Oxide/Metal Hydroxide Condensed Phases. Journal of Physical Chemistry A, 2010, 114, 9507-9514.	1.1	156
135	Mechanical properties and force field parameters for polyethylene crystal. The Journal of Physical Chemistry, 1991, 95, 2260-2272.	2.9	154
136	On the Impact of Steric and Electronic Properties of Ligands on Gold(I)-Catalyzed Cycloaddition Reactions. Organic Letters, 2009, 11, 4798-4801.	2.4	153
137	The extended Perdew-Burke-Ernzerhof functional with improved accuracy for thermodynamic and electronic properties of molecular systems. Journal of Chemical Physics, 2004, 121, 4068-4082.	1.2	150
138	Computational and experimental demonstrations of one-pot tandem catalysis for electrochemical carbon dioxide reduction to methane. Nature Communications, 2019, 10, 3340.	5.8	150
139	Atomistic-Scale Simulations of the Initial Chemical Events in the Thermal Initiation of Triacetonetriperoxide. Journal of the American Chemical Society, 2005, 127, 11053-11062.	6.6	147
140	Application of the ReaxFF Reactive Force Field to Reactive Dynamics of Hydrocarbon Chemisorption and Decomposition. Journal of Physical Chemistry C, 2010, 114, 5675-5685.	1.5	147
141	Mechanistic Analysis of Hydroarylation Catalysts. Journal of the American Chemical Society, 2004, 126, 11658-11665.	6.6	146
142	Alkyl polyglycoside surfactantâ€“alcohol cosolvent formulations for improved oil recovery. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2009, 339, 48-59.	2.3	146
143	Nature of the Active Sites for CO Reduction on Copper Nanoparticles; Suggestions for Optimizing Performance. Journal of the American Chemical Society, 2017, 139, 11642-11645.	6.6	146
144	Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 169-181.	1.3	144

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145	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 19896-19900.	3.3	143
146	Mechanical and Transport Properties of the Poly(ethylene oxide)â^'Poly(acrylic acid) Double Network Hydrogel from Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2007, 111, 1729-1737.	1.2	142
147	Reaction mechanism and kinetics for CO2 reduction on nickel single atom catalysts from quantum mechanics. Nature Communications, 2020, 11, 2256.	5.8	140
148	Flexible d basis sets for scandium through copper. The Journal of Physical Chemistry, 1981, 85, 2607-2611.	2.9	139
149	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. Journal of Physical Chemistry C, 2008, 112, 14645-14654.	1.5	138
150	Water adsorption on stepped ZnO surfaces from MD simulation. Surface Science, 2010, 604, 741-752.	0.8	138
151	Ab InitioEffective Potentials for Use in Molecular Calculations. Journal of Chemical Physics, 1972, 56, 2685-2701.	1.2	134
152	Accurate Energies and Structures for Large Water Clusters Using the X3LYP Hybrid Density Functional. Journal of Physical Chemistry A, 2004, 108, 10518-10526.	1.1	134
153	A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials. Advanced Materials, 2019, 31, e1805405.	11.1	134
154	Electrocatalysis at Organicâ€"Metal Interfaces: Identification of Structureâ€"Reactivity Relationships for CO₂ Reduction at Modified Cu Surfaces. Journal of the American Chemical Society, 2019, 141, 7355-7364.	6.6	133
155	Dynamics and Thermodynamics of Water in PAMAM Dendrimers at Subnanosecond Time Scales. Journal of Physical Chemistry B, 2005, 109, 8663-8672.	1.2	131
156	pKa Calculations of Aliphatic Amines, Diamines, and Aminoamides via Density Functional Theory with a Poissonâ^'Boltzmann Continuum Solvent Model. Journal of Physical Chemistry A, 2007, 111, 4422-4430.	1.1	131
157	New pseudospectral algorithms for electronic structure calculations: Length scale separation and analytical twoâ€electron integral corrections. Journal of Chemical Physics, 1994, 101, 4028-4041.	1.2	129
158	Dynamic Transition in the Structure of an Energetic Crystal during Chemical Reactions at Shock Front Prior to Detonation. Physical Review Letters, 2007, 99, 148303.	2.9	129
159	The Inner-Sphere Process in the Enantioselective Tsuji Allylation Reaction with (S)-t-Bu-phosphinooxazoline Ligands. Journal of the American Chemical Society, 2007, 129, 11876-11877.	6.6	129
160	Density-Dependent Liquid Nitromethane Decomposition: Molecular Dynamics Simulations Based on ReaxFF. Journal of Physical Chemistry A, 2011, 115, 10181-10202.	1.1	129
161	Decomposition of Condensed Phase Energetic Materials: Interplay between Uni- and Bimolecular Mechanisms. Journal of the American Chemical Society, 2014, 136, 4192-4200.	6.6	126
162	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. Journal of the American Chemical Society, 2018, 140, 6288-6297.	6.6	126

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163	Modified Generalized Valence-Bond Method: A Simple Correction for the Electron Correlation Missing in Generalized Valence-Bond Wave Functions; Prediction of Double-Well States forCr2andMo2. Physical Review Letters, 1985, 54, 661-664.	2.9	124
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