# William Goddard

List of Publications by Year
in descending order



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|---|---|---|---|
| 765 papers | 84,293 citations | 416 132 h-index | 547 264 g-index |
| 786 all docs | 786 docs citations | 786 times ranked | 64743 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 | Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419. | 6.0 | 1,292 |
| 9 | 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 |
| 10 | ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. Journal of Physical Chemistry A, 2003, 107, 3803-3811. | 1.1 | 821 |
| 11 | High-performance bifunctional porous non-noble metal phosphide catalyst for overall water splitting. Nature Communications, 2018, 9, 2551. | 5.8 | 812 |
| 12 | Linear Artificial Molecular Muscles. Journal of the American Chemical Society, 2005, 127, 9745-9759. | 6.6 | 660 |
| 13 | Predictions of Hole Mobilities in Oligoacene Organic Semiconductors from Quantum Mechanical Calculationsâ€. Journal of Physical Chemistry B, 2004, 108, 8614-8621. | 1.2 | 586 |
| 14 | 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 |
| 15 | 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 |
| 16 | Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. ACS Nano, 2016, 10, 957-966. | 7.3 | 534 |
| 17 | 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 |
| 18 | Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. Physical Review Letters, 2003, 91, 098301. | 2.9 | 495 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Sulfation patterns of glycosaminoglycans encode molecular recognition and activity. Nature Chemical Biology, 2006, 2, 467-473. | 3.9 | 494 |
| 20 | Oxidative Aliphatic C-H Fluorination with Fluoride Ion Catalyzed by a Manganese Porphyrin. Science, 2012, 337, 1322-1325. | 6.0 | 478 |
| 21 | Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503. | 16.1 | 464 |
| 22 | 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 |
| 23 | Accurate Band Gaps for Semiconductors from Density Functional Theory. Journal of Physical Chemistry Letters, 2011, 2, 212-217. | 2.1 | 444 |
| 24 | 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 |
| 25 | Mechanically bonded macromolecules. Chemical Society Reviews, 2010, 39, 17-29. | 18.7 | 428 |
| 26 | 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 |
| 27 | 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 |
| 28 | Lithium-Doped Metal-Organic Frameworks for Reversible H2Storage at Ambient Temperature. Journal of the American Chemical Society, 2007, 129, 8422-8423. | 6.6 | 418 |
| 29 | 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 |
| 30 | 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 |
| 31 | 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 |
| 32 | 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 |
| 33 | 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 |
| 34 | Oxygenâ€Vacancy Abundant Ultrafine Co<sub>3</sub>O<sub>4</sub>/Graphene Composites for Highâ€Rate Supercapacitor Electrodes. Advanced Science, 2018, 5, 1700659. | 5.6 | 392 |
| 35 | 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 |
| 36 | Effect of Solvent and pH on the Structure of PAMAM Dendrimers. Macromolecules, 2005, 38, 979-991. | 2.2 | 389 |

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| 37 | 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, 483-486. | 6.6 | 381 |
| 38 | 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 |
| 39 | Selfâ€Consistent Procedures for Generalized Valence Bond Wavefunctions. Applications H3, BH, H2O, C2H6, and O2. Journal of Chemical Physics, 1972, 57, 738-748. | 1.2 | 368 |
| 40 | Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502. | 1.2 | 366 |
| 41 | Subsurface oxide plays a critical role in CO <sub>2</sub> activation by Cu(111) surfaces to form chemisorbed CO <sub>2</sub> , the first step in reduction of CO <sub>2</sub>. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6706-6711. | 3.3 | 363 |
| 42 | Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics, 2001, 115, 385-394. | 1.2 | 345 |
| 43 | 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 |
| 44 | Hildebrand and Hansen solubility parameters from Molecular Dynamics with applications to electronic nose polymer sensors. Journal of Computational Chemistry, 2004, 25, 1814-1826. | 1.5 | 328 |
| 45 | 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 |
| 46 | Monolayer atomic crystal molecular superlattices. Nature, 2018, 555, 231-236. | 13.7 | 323 |
| 47 | Cu metal embedded in oxidized matrix catalyst to promote CO <sub>2</sub> activation and CO dimerization for electrochemical reduction of CO <sub>2</sub>. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6685-6688. | 3.3 | 322 |
| 48 | Atomistic Mechanisms Underlying Selectivities in C<sub>1</sub> and C<sub>2</sub> Products from Electrochemical Reduction of CO on Cu(111). Journal of the American Chemical Society, 2017, 139, 130-136. | 6.6 | 320 |
| 49 | Prediction of fullerene packing in C60 and C70 crystals. Nature, 1991, 351, 464-467. | 13.7 | 312 |
| 50 | Efficient hydrogen evolution by ternary molybdenum sulfoselenide particles on self-standing porous nickel diselenide foam. Nature Communications, 2016, 7, 12765. | 5.8 | 312 |
| 51 | Reaction Mechanisms for the Electrochemical Reduction of CO<sub>2</sub> 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. | 6.6 | 310 |
| 52 | Thermal conductivity of diamond and related materials from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6888-6900. | 1.2 | 307 |
| 53 | Unexpected discovery of low-cost maricite NaFePO<sub>4</sub>as a high-performance electrode for Na-ion batteries. Energy and Environmental Science, 2015, 8, 540-545. | 15.6 | 299 |
| 54 | Highly active and stable stepped Cu surface for enhanced electrochemical CO2 reduction to C2H4. Nature Catalysis, 2020, 3, 804-812. | 16.1 | 298 |

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| 55 | 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 |
| 56 | 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 |
| 57 | Radically enhanced molecular recognition. Nature Chemistry, 2010, 2, 42-49. | 6.6 | 280 |
| 58 | 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. | 6.6 | 279 |
| 59 | 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 |
| 60 | In Silico Discovery of New Dopants for Fe-Doped Ni Oxyhydroxide (Ni<sub>1â€“x</sub>Fe<sub>x</sub>OOH) Catalysts for Oxygen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 6745-6748. | 6.6 | 274 |
| 61 | Mechanism of Câ^'F Reductive Elimination from Palladium(IV) Fluorides. Journal of the American Chemical Society, 2010, 132, 3793-3807. | 6.6 | 273 |
| 62 | Improved Quantum Theory of Many-Electron Systems. II. The Basic Method. Physical Review, 1967, 157, 81-93. | 2.7 | 269 |
| 63 | Strain Rate Induced Amorphization in Metallic Nanowires. Physical Review Letters, 1999, 82, 2900-2903. | 2.9 | 268 |
| 64 | 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 |
| 65 | Hydrogen bonding in the benzeneâ€“ammonia dimer. Nature, 1993, 362, 735-737. | 13.7 | 254 |
| 66 | Olefin metathesis - a mechanistic study of high-valent Group VI catalysts. Journal of the American Chemical Society, 1982, 104, 448-456. | 6.6 | 251 |
| 67 | PAMAM Dendrimers Undergo pH Responsive Conformational Changes without Swelling. Journal of the American Chemical Society, 2009, 131, 2798-2799. | 6.6 | 249 |
| 68 | 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 |
| 69 | The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO<sub>2</sub> (110) Surface. Journal of the American Chemical Society, 2017, 139, 149-155. | 6.6 | 243 |
| 70 | 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 |
| 71 | ReaxFFMgHReactive Force Field for Magnesium Hydride Systems. Journal of Physical Chemistry A, 2005, 109, 851-859. | 1.1 | 234 |
| 72 | 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. | 6.6 | 234 |

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| 73 | Selective Oxidation of Methane to Methanol Catalyzed, with Cï£¿H Activation, by Homogeneous, Cationic Gold. Angewandte Chemie - International Edition, 2004, 43, 4626-4629. | 7.2 | 229 |
| 74 | Isolation of a Structural Mechanism for Uncoupling T Cell Receptor Signaling from Peptide-MHC Binding. Cell, 2018, 174, 672-687.e27. | 13.5 | 229 |
| 75 | 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 |
| 76 | Force fields, structures, and properties of poly(vinylidene fluoride) crystals. Macromolecules, 1992, 25, 7268-7281. | 2.2 | 227 |
| 77 | Molecular dynamics study of the binaryCu46Zr54metallic glass motivated by experiments: Glass formation and atomic-level structure. Physical Review B, 2005, 71, . | 1.1 | 227 |
| 78 | Formation of carbonâ€“nitrogen bonds in carbon monoxide electrolysis. Nature Chemistry, 2019, 11, 846-851. | 6.6 | 223 |
| 79 | 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 |
| 80 | Configuration interaction studies of O3 and O+3. Ground and excited states. Journal of Chemical Physics, 1975, 62, 3912-3924. | 1.2 | 221 |
| 81 | 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 |
| 82 | Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. Journal of Chemical Physics, 2017, 146, 114104. | 1.2 | 211 |
| 83 | 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 |
| 84 | 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 |
| 85 | An extended hybrid density functional (X3LYP) with improved descriptions of nonbond interactions and thermodynamic properties of molecular systems. Journal of Chemical Physics, 2005, 122, 014105. | 1.2 | 204 |
| 86 | 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 |
| 87 | The hindered rotor density-of-states interpolation function. Journal of Chemical Physics, 1997, 106, 6675-6680. | 1.2 | 203 |
| 88 | Resolution of the Band Gap Prediction Problem for Materials Design. Journal of Physical Chemistry Letters, 2016, 7, 1198-1203. | 2.1 | 200 |
| 89 | 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 |
| 90 | Theoretical Study of Solvent Effects on the Platinum-Catalyzed Oxygen Reduction Reaction. Journal of Physical Chemistry Letters, 2010, 1, 856-861. | 2.1 | 195 |

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| 91 | Embedding Covalency into Metal Catalysts for Efficient Electrochemical Conversion of CO<sub>2</sub>. Journal of the American Chemical Society, 2014, 136, 11355-11361. | 6.6 | 192 |
| 92 | Engineering bacteria for production of rhamnolipid as an agent for enhanced oil recovery. Biotechnology and Bioengineering, 2007, 98, 842-853. | 1.7 | 191 |
| 93 | 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 |
| 94 | 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 |
| 95 | Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting. Nature Communications, 2018, 9, 1809. | 5.8 | 188 |
| 96 | Mechanism of Homogeneous Ir(III) Catalyzed Regioselective Arylation of Olefins. Journal of the American Chemical Society, 2004, 126, 352-363. | 6.6 | 184 |
| 97 | Antiferromagnetic band structure ofLa2CuO4:â€ƒBecke-3â€“Lee-Yang-Parr calculations. Physical Review B, 2001, 63, . | 1.1 | 182 |
| 98 | Design and study of homogeneous catalysts for the selective, low temperature oxidation of hydrocarbons. Journal of Molecular Catalysis A, 2006, 251, 8-23. | 4.8 | 181 |
| 99 | Electronic correlation and the Si(100) surface: Buckling versus nonbuckling. Journal of Vacuum Science and Technology, 1982, 21, 344-350. | 1.9 | 180 |
| 100 | Definitive Band Gaps for Single-Wall Carbon Nanotubes. Journal of Physical Chemistry Letters, 2010, 1, 2946-2950. | 2.1 | 179 |
| 101 | Contact Resistance for â€œEnd-Contactedâ€•Metalâˆ’Graphene and Metalâˆ’Nanotube Interfaces from Quantum Mechanics. Journal of Physical Chemistry C, 2010, 114, 17845-17850. | 1.5 | 177 |
| 102 | Outstanding hydrogen evolution reaction catalyzed by porous nickel diselenide electrocatalysts. Energy and Environmental Science, 2017, 10, 1487-1492. | 15.6 | 176 |
| 103 | Alkylgold complexes by the intramolecular aminoauration of unactivated alkenes. Chemical Science, 2010, 1, 226. | 3.7 | 174 |
| 104 | Low-frequency and rare exome chip variants associate with fasting glucose and type 2 diabetes susceptibility. Nature Communications, 2015, 6, 5897. | 5.8 | 173 |
| 105 | The Reaction Mechanism with Free Energy Barriers for Electrochemical Dihydrogen Evolution on MoS<sub>2</sub>. Journal of the American Chemical Society, 2015, 137, 6692-6698. | 6.6 | 173 |
| 106 | Effects of Surface Roughness on the Electrochemical Reduction of CO<sub>2</sub> over Cu. ACS Energy Letters, 2020, 5, 1206-1214. | 8.8 | 172 |
| 107 | Highly stable tetrathiafulvalene radical dimers in [3]catenanes. Nature Chemistry, 2010, 2, 870-879. | 6.6 | 171 |
| 108 | Metalâˆ’Organic Frameworks Provide Large Negative Thermal Expansion Behavior. Journal of Physical Chemistry C, 2007, 111, 15185-15191. | 1.5 | 170 |

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| 109 | Electrochemical CO Reduction Builds Solvent Water into Oxygenate Products. Journal of the American Chemical Society, 2018, 140, 9337-9340. | 6.6 | 170 |
| 110 | Dynamics of Lithium Dendrite Growth and Inhibition: Pulse Charging Experiments and Monte Carlo Calculations. Journal of Physical Chemistry Letters, 2014, 5, 1721-1726. | 2.1 | 169 |
| 111 | Mechanistic Study of Gold(I)-Catalyzed Intermolecular Hydroamination of Allenes. Journal of the American Chemical Society, 2010, 132, 13064-13071. | 6.6 | 168 |
| 112 | The charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model. Journal of Chemical Physics, 2015, 142, 064107. | 1.2 | 167 |
| 113 | Efficient photocatalytic reduction of dinitrogen to ammonia on bismuth monoxide quantum dots. Journal of Materials Chemistry A, 2017, 5, 201-209. | 5.2 | 160 |
| 114 | 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 |
| 115 | A Radically Configurable Six-State Compound. Science, 2013, 339, 429-433. | 6.0 | 158 |
| 116 | Pressureâ€Dependent Polymorphism and Bandâ€Gap Tuning of Methylammonium Lead Iodide Perovskite. Angewandte Chemie - International Edition, 2016, 55, 6540-6544. | 7.2 | 157 |
| 117 | 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 |
| 118 | Mechanism for Unimolecular Decomposition of HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazocine), an ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 1302-1314. | 1.1 | 152 |
| 119 | Non-conventional fluorescent biogenic and synthetic polymers without aromatic rings. Polymer Chemistry, 2017, 8, 1722-1727. | 1.9 | 152 |
| 120 | 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 |
| 121 | Computational and experimental demonstrations of one-pot tandem catalysis for electrochemical carbon dioxide reduction to methane. Nature Communications, 2019, 10, 3340. | 5.8 | 150 |
| 122 | Atomic H-Induced Mo<sub>2</sub>C Hybrid as an Active and Stable Bifunctional Electrocatalyst. ACS Nano, 2017, 11, 384-394. | 7.3 | 149 |
| 123 | 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 |
| 124 | Mechanistic Analysis of Hydroarylation Catalysts. Journal of the American Chemical Society, 2004, 126, 11658-11665. | 6.6 | 146 |
| 125 | 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 |
| 126 | Correlationâ€consistent singletâ€“triplet gaps in substituted carbenes. Journal of Chemical Physics, 1988, 88, 1752-1763. | 1.2 | 144 |

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| 127 | 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 |
| 128 | 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 |
| 129 | Engineering the Composition and Crystallinity of Molybdenum Sulfide for High-Performance Electrocatalytic Hydrogen Evolution. ACS Catalysis, 2015, 5, 448-455. | 5.5 | 141 |
| 130 | Reaction mechanism and kinetics for CO2 reduction on nickel single atom catalysts from quantum mechanics. Nature Communications, 2020, 11, 2256. | 5.8 | 140 |
| 131 | Atomistic Explanation of Shear-Induced Amorphous Band Formation in Boron Carbide. Physical Review Letters, 2014, 113, 095501. | 2.9 | 138 |
| 132 | Mechanistic Analysis of Iridium Heteroatom Câ^'H Activation:â€‰ Evidence for an Internal Electrophilic Substitution Mechanism. Organometallics, 2007, 26, 1565-1567. | 1.1 | 135 |
| 133 | Ab InitioEffective Potentials for Use in Molecular Calculations. Journal of Chemical Physics, 1972, 56, 2685-2701. | 1.2 | 134 |
| 134 | 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 |
| 135 | A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials. Advanced Materials, 2019, 31, e1805405. | 11.1 | 134 |
| 136 | Novel Family of Chiral-Based Topological Insulators: Elemental Tellurium under Strain. Physical Review Letters, 2013, 110, 176401. | 2.9 | 133 |
| 137 | Electrocatalysis at Organicâ€“Metal Interfaces: Identification of Structureâ€“Reactivity Relationships for CO<sub>2</sub> Reduction at Modified Cu Surfaces. Journal of the American Chemical Society, 2019, 141, 7355-7364. | 6.6 | 133 |
| 138 | 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 |
| 139 | Density-Dependent Liquid Nitromethane Decomposition: Molecular Dynamics Simulations Based on ReaxFF. Journal of Physical Chemistry A, 2011, 115, 10181-10202. | 1.1 | 129 |
| 140 | CH Activation with an O-Donor Iridiumâ^'Methoxo Complex. Journal of the American Chemical Society, 2005, 127, 14172-14173. | 6.6 | 128 |
| 141 | Mechanism for Degradation of Nafion in PEM Fuel Cells from Quantum Mechanics Calculations. Journal of the American Chemical Society, 2011, 133, 19857-19863. | 6.6 | 128 |
| 142 | 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 |
| 143 | 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 |
| 144 | Contact Resistance Properties between Nanotubes and Various Metals from Quantum Mechanics. Journal of Physical Chemistry C, 2007, 111, 11113-11116. | 1.5 | 125 |

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| 145 | Product Protection, the Key to Developing High Performance Methane Selective Oxidation Catalysts. Journal of the American Chemical Society, 2009, 131, 17110-17115. | 6.6 | 124 |
| 146 | Atomistic Description of Ionic Diffusion in PEOâ€“LiTFSI: Effect of Temperature, Molecular Weight, and Ionic Concentration. Macromolecules, 2018, 51, 8987-8995. | 2.2 | 124 |
| 147 | Solution-Phase Mechanistic Study and Solid-State Structure of a Tris(bipyridinium radical cation) Inclusion Complex. Journal of the American Chemical Society, 2012, 134, 3061-3072. | 6.6 | 123 |
| 148 | The Hessian biased force field for silicon nitride ceramics: Predictions of thermodynamic and mechanical properties for Î±â€•and Î²â€Si3N4. Journal of Chemical Physics, 1992, 97, 5048-5062. | 1.2 | 122 |
| 149 | Stability and Thermodynamics of the PtCl2Type Catalyst for Activating Methane to Methanol:Â A Computational Study. Organometallics, 2002, 21, 511-525. | 1.1 | 121 |
| 150 | Prediction of Vapor Pressures and Enthalpies of Vaporization Using a COSMO Solvation Model. Journal of Physical Chemistry A, 2004, 108, 7429-7439. | 1.1 | 120 |
| 151 | The ferroelectric and cubic phases in BaTiO3 ferroelectrics are also antiferroelectric. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 14695-14700. | 3.3 | 119 |
| 152 | Dynamics of the Dissociation of Hydrogen on Stepped Platinum Surfaces Using the ReaxFF Reactive Force Field. Journal of Physical Chemistry B, 2006, 110, 4274-4282. | 1.2 | 116 |
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