# Matthew D Wodrich

List of Publications by Year
in descending order



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|---|---|---|---|
| 76 papers | 4,347 citations | 87888 38 h-index | 106344 65 g-index |
| 84 all docs | 84 docs citations | 84 times ranked | 4321 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Systematic Errors in Computed Alkane Energies Using B3LYP and Other Popular DFT Functionals. Organic Letters, 2006, 8, 3631-3634. | 4.6 | 393 |
| 2 | How Accurate Are DFT Treatments of Organic Energies?. Organic Letters, 2007, 9, 1851-1854. | 4.6 | 260 |
| 3 | Bimetallic Oxidative Addition Involving Radical Intermediates in Nickel-Catalyzed Alkylâ€"Alkyl Kumada Coupling Reactions. Journal of the American Chemical Society, 2013, 135, 12004-12012. | 13.7 | 227 |
| 4 | Fast and Highly Chemoselective Alkynylation of Thiols with Hypervalent Iodine Reagents Enabled through a Low Energy Barrier Concerted Mechanism. Journal of the American Chemical Society, 2014, 136, 16563-16573. | 13.7 | 191 |
| 5 | The Concept of Protobranching and Its Many Paradigm Shifting Implications for Energy Evaluations. Chemistry - A European Journal, 2007, 13, 7731-7744. | 3.3 | 185 |
| 6 | Principles of electron capture and transfer dissociation mass spectrometry applied to peptide and protein structure analysis. Chemical Society Reviews, 2013, 42, 5014. | 38.1 | 175 |
| 7 | Room temperature decarboxylative cyanation of carboxylic acids using photoredox catalysis and cyanobenziodoxolones: a divergent mechanism compared to alkynylation. Chemical Science, 2017, 8, 1790-1800. | 7.4 | 146 |
| 8 | Evidence for d Orbital Aromaticity in Square Planar Coinage Metal Clusters. Journal of the American Chemical Society, 2005, 127, 5701-5705. | 13.7 | 143 |
| 9 | Axially Chiral Dibenzazepinones by a Palladium(0)â€Catalyzed Atropoâ€enantioselective Câˆ'H Arylation. Angewandte Chemie - International Edition, 2018, 57, 11040-11044. | 13.8 | 123 |
| 10 | Ligandâ€Controlled Regiodivergent Pathways of Rhodium(III)â€Catalyzed Dihydroisoquinolone Synthesis: Experimental and Computational Studies of Different Cyclopentadienyl Ligands. Chemistry - A European Journal, 2014, 20, 15409-15418. | 3.3 | 120 |
| 11 | Quantification of â€œfuzzyâ€•chemical concepts: a computational perspective. Chemical Society Reviews, 2012, 41, 4671. | 38.1 | 108 |
| 12 | Natural inspirations for metalâ€"ligand cooperative catalysis. Nature Reviews Chemistry, 2018, 2, . | 30.2 | 104 |
| 13 | Linear scaling relationships and volcano plots in homogeneous catalysis â€" revisiting the Suzuki reaction. Chemical Science, 2015, 6, 6754-6761. | 7.4 | 98 |
| 14 | Reconstitution of [Fe]-hydrogenase using model complexes. Nature Chemistry, 2015, 7, 995-1002. | 13.6 | 92 |
| 15 | How Large Is the Conjugative Stabilization of Diynes?. Journal of the American Chemical Society, 2004, 126, 15036-15037. | 13.7 | 85 |
| 16 | Covalent Capture of Nitrous Oxide by Nâ€Heterocyclic Carbenes. Angewandte Chemie - International Edition, 2012, 51, 232-234. | 13.8 | 84 |
| 17 | General and Practical Formation of Thiocyanates from Thiols. Chemistry - A European Journal, 2015, 21, 2662-2668. | 3.3 | 82 |
| 18 | Mild complexation protocol for chiral Cp<sup>x</sup>Rh and Ir complexes suitable for <i>in situ</i> catalysis. Chemical Science, 2019, 10, 781-787. | 7.4 | 82 |

| # | ARTICLE | IF | CITATIONS |
|---|---|---|---|
| 19 | A Generalized Picture of Câ€“C Cross-Coupling. ACS Catalysis, 2017, 7, 5643-5653. | 11.2 | 68 |
| 20 | A Functional Model of [Fe]-Hydrogenase. Journal of the American Chemical Society, 2016, 138, 3270-3273. | 13.7 | 66 |
| 21 | Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots. Chemical Science, 2016, 7, 5723-5735. | 7.4 | 65 |
| 22 | Bimetallic Oxidative Addition in Nickel-Catalyzed Alkylâ€“Aryl Kumada Coupling Reactions. Organometallics, 2014, 33, 5708-5715. | 2.3 | 64 |
| 23 | Double Aromaticity in Monocyclic Carbon, Boron, and Borocarbon Rings Based on Magnetic Criteria. Chemistry - A European Journal, 2007, 13, 4582-4593. | 3.3 | 60 |
| 24 | Stereoselective synthesis of alkyl-, aryl-, vinyl- and alkynyl-substituted <i>Z</i>-enamides and enol ethers. Chemical Science, 2019, 10, 3223-3230. | 7.4 | 58 |
| 25 | A catalytically active [Mn]-hydrogenase incorporating a non-native metal cofactor. Nature Chemistry, 2019, 11, 669-675. | 13.6 | 55 |
| 26 | Iron Pincer Complexes as Catalysts and Intermediates in Alkylâ€“Aryl Kumada Coupling Reactions. Organometallics, 2015, 34, 289-298. | 2.3 | 54 |
| 27 | The atomic-resolution crystal structure of activated [Fe]-hydrogenase. Nature Catalysis, 2019, 2, 537-543. | 34.4 | 54 |
| 28 | The Genesis of Molecular Volcano Plots. Accounts of Chemical Research, 2021, 54, 1107-1117. | 15.6 | 54 |
| 29 | Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. Chemical Science, 2021, 12, 6879-6889. | 7.4 | 54 |
| 30 | A Î²-Carbon elimination strategy for convenient in situ access to cyclopentadienyl metal complexes. Chemical Science, 2017, 8, 7174-7179. | 7.4 | 53 |
| 31 | Alkynylation of Thiols with Ethynylbenziodoxolone (EBX) Reagents: Î±- or Î²- Ï€-Addition?. Organic Letters, 2016, 18, 60-63. | 4.6 | 52 |
| 32 | Overcoming systematic DFT errors for hydrocarbon reaction energies. Theoretical Chemistry Accounts, 2010, 127, 429-442. | 1.4 | 51 |
| 33 | Empirical Corrections to Density Functional Theory Highlight the Importance of Nonbonded Intramolecular Interactions in Alkanes. Journal of Physical Chemistry A, 2008, 112, 11495-11500. | 2.5 | 48 |
| 34 | Activity-Based Screening of Homogeneous Catalysts through the Rapid Assessment of Theoretically Derived Turnover Frequencies. ACS Catalysis, 2019, 9, 5716-5725. | 11.2 | 48 |
| 35 | New Additivity Schemes for Hydrocarbon Energies. Organic Letters, 2006, 8, 2135-2138. | 4.6 | 45 |
| 36 | Sequential Nâ€“O and Nâ€“N Bond Cleavage of N-Heterocyclic Carbene-Activated Nitrous Oxide with a Vanadium Complex. Journal of the American Chemical Society, 2012, 134, 1471-1473. | 13.7 | 44 |

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|---|---|---|---|
| 37 | Neutral Aminyl Radicals Derived from Azoimidazolium Dyes. Journal of the American Chemical Society, 2016, 138, 15126-15129. | 13.7 | 40 |
| 38 | Data-Driven Advancement of Homogeneous Nickel Catalyst Activity for Aryl Ether Cleavage. ACS Catalysis, 2020, 10, 7021-7031. | 11.2 | 40 |
| 39 | Nickel pincer model of the active site of lactate racemase involves ligand participation in hydride transfer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1242-1245. | 7.1 | 39 |
| 40 | Oneâ€Step Multigramâ€Scale Biomimetic Synthesis of Psiguadialâ€…B. Angewandte Chemie - International Edition, 2017, 56, 13776-13780. | 13.8 | 36 |
| 41 | Branched Alkanes Have Contrasting Stabilities. Organic Letters, 2010, 12, 3070-3073. | 4.6 | 34 |
| 42 | Accurate Thermochemistry of Hydrocarbon Radicals via an Extended Generalized Bond Separation Reaction Scheme. Journal of Physical Chemistry A, 2012, 116, 3436-3447. | 2.5 | 33 |
| 43 | Unraveling Metal/Pincer Ligand Effects in the Catalytic Hydrogenation of Carbon Dioxide to Formate. Organometallics, 2018, 37, 4568-4575. | 2.3 | 32 |
| 44 | On the Generality of Molecular Volcano Plots. ChemCatChem, 2018, 10, 1586-1591. | 3.7 | 29 |
| 45 | Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. Journal of Computational Chemistry, 2016, 37, 83-92. | 3.3 | 27 |
| 46 | On the Advantages of Hydrocarbon Radical Stabilization Energies Based on Râˆ'H Bond Dissociation Energies. Journal of Organic Chemistry, 2011, 76, 2439-2447. | 3.2 | 23 |
| 47 | Data-powered augmented volcano plots for homogeneous catalysis. Chemical Science, 2020, 11, 12070-12080. | 7.4 | 23 |
| 48 | How Strained are Carbomeric-Cycloalkanes?. Journal of Physical Chemistry A, 2010, 114, 6705-6712. | 2.5 | 22 |
| 49 | Improving the Thermodynamic Profiles of Prospective Suzukiâ€"Miyaura Crossâ€Coupling Catalysts by Altering the Electrophilic Coupling Component. ChemCatChem, 2018, 10, 1592-1597. | 3.7 | 21 |
| 50 | Toward Functional Typeâ€…III [Fe]â€Hydrogenase Biomimics for H<sub>2</sub> Activation: Insights from Computation. Chemistry - A European Journal, 2015, 21, 3987-3996. | 3.3 | 20 |
| 51 | A Monometallic Iron(I) Organoferrate. Organometallics, 2017, 36, 499-501. | 2.3 | 20 |
| 52 | Reaction Enthalpies Using the Neural-Network-Based X1 Approach: The Important Choice of Input Descriptors. Journal of Physical Chemistry A, 2009, 113, 3285-3290. | 2.5 | 19 |
| 53 | Heterolytic Nâ€"CÎ± Bond Cleavage in Electron Capture and Transfer Dissociation of Peptide Cations. Journal of Physical Chemistry B, 2012, 116, 10807-10815. | 2.6 | 19 |
| 54 | Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction. Helvetica Chimica Acta, 2018, 101, e1800107. | 1.6 | 19 |

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| 55 | Lowâ€Temperature Intramolecular [4+2] Cycloaddition of Allenes with Arenes for the Synthesis of Diene Ligands. Angewandte Chemie - International Edition, 2021, 60, 5475-5481. | 13.8 | 18 |
| 56 | Effects of halogen substitution on the properties of eight- and nine-vertex closo-boranes. Dalton Transactions, 2008, , 1745. | 3.3 | 15 |
| 57 | Data Mining the Câ^'C Crossâ€Coupling Genome. ChemCatChem, 2019, 11, 4096-4107. | 3.7 | 15 |
| 58 | Functional Models of the Nickel Pincer Nucleotide Cofactor of Lactate Racemase. Angewandte Chemie - International Edition, 2019, 58, 16869-16872. | 13.8 | 12 |
| 59 | Probing Substrate Scope with Molecular Volcanoes. Organic Letters, 2020, 22, 7936-7941. | 4.6 | 12 |
| 60 | Diversifying Metalâ€"Ligand Cooperative Catalysis in Semiâ€Synthetic [Mn]â€Hydrogenases. Angewandte Chemie - International Edition, 2021, 60, 13350-13357. | 13.8 | 11 |
| 61 | Structure and Reactivity of Nâ€Heterocyclic Alkynyl Hypervalent Iodine Reagents. Chemistry - A European Journal, 2021, 27, 10979-10986. | 3.3 | 11 |
| 62 | What governs nitrogen configuration in substituted aminophosphines?. Journal of Physical Organic Chemistry, 2009, 22, 101-109. | 1.9 | 8 |
| 63 | Structureâ€"Correlation Principles Connecting Ground State Properties and Reaction Barrier Heights for the Cope Rearrangement of Semibullvalenes. Journal of Organic Chemistry, 2012, 77, 2548-2552. | 3.2 | 8 |
| 64 | On the Viability of Heterolytic Peptide Nâ€"CÎ± Bond Cleavage in Electron Capture and Transfer Dissociation Mass Spectrometry. Journal of Physical Chemistry B, 2014, 118, 2985-2992. | 2.6 | 8 |
| 65 | Electronic Elements Governing the Binding of Small Molecules to a [Fe]-Hydrogenase Mimic. European Journal of Inorganic Chemistry, 2013, 2013, 3993-3999. | 2.0 | 7 |
| 66 | Ping-Pong Protons: How Hydrogen-Bonding Networks Facilitate Heterolytic Bond Cleavage in Peptide Radical Cations. Journal of Physical Chemistry B, 2014, 118, 2628-2637. | 2.6 | 7 |
| 67 | Reply to â€œComment on â€˜Accurate Thermochemistry of Hydrocarbon Radicals via an Extended Generalized Bond Separation Reaction Schemeâ€™â€. Journal of Physical Chemistry A, 2012, 116, 8794-8796. | 2.5 | 6 |
| 68 | Lowâ€Temperature Intramolecular [4+2] Cycloaddition of Allenes with Arenes for the Synthesis of Diene Ligands. Angewandte Chemie, 2021, 133, 5535-5541. | 2.0 | 6 |
| 69 | The (not so) simple prediction of enantioselectivity â€" a pipeline for high-fidelity computations. Chemical Science, 2022, 13, 6858-6864. | 7.4 | 6 |
| 70 | Oneâ€Step Multigramâ€Scale Biomimetic Synthesis of Psiguadialâ€…B. Angewandte Chemie, 2017, 129, 13964-13968. | 2.0 | 4 |
| 71 | 1,1â€²-Bi(trishomobarrelenyl) - Synthesis and Chiroptic Properties. European Journal of Organic Chemistry, 2009, 2009, 1048-1052. | 2.4 | 2 |
| 72 | Methoxycyclization of 1,5â€Enynes by Coinage Metal Catalysts: Is Gold Always Superior?. Helvetica Chimica Acta, 2021, 104, e2100134. | 1.6 | 2 |

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|---|---|---|---|
| 73 | Mapping Catalystâ€Solvent Interplay in Competing Carboamination/Cyclopropanation Reactions. Chemistry - A European Journal, 2022, , . | 3.3 | 1 |
| 74 | Evidence for d Orbital Aromaticity in Square Planar Coinage Metal Clusters.. ChemInform, 2005, 36, no. | 0.0 | 0 |
| 75 | Functional Models of the Nickel Pincer Nucleotide Cofactor of Lactate Racemase. Angewandte Chemie, 2019, 131, 17025-17028. | 2.0 | 0 |
| 76 | Diversifying Metalâ€"Ligand Cooperative Catalysis in Semiâ€Synthetic [Mn]â€Hydrogenases. Angewandte Chemie, 2021, 133, 13462-13469. | 2.0 | 0 |