# Alexis T Bell

## List of Publications by Year in Descending Order



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| 523 papers | 47,147 citations | 100 h-index | 199 g-index |
| 560 ext. papers | 52,445 ext. citations | 7.6 avg, IF | 8.06 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 523 | Engineering Catalyst-Electrolyte Microenvironments to Optimize the Activity and Selectivity for the Electrochemical Reduction of CO on Cu and Ag.. *Accounts of Chemical Research*, **2022**, | 24.3 | 11 |
| 522 | Investigation of the modes of NO adsorption in Pd/H-CHA. *Applied Catalysis B: Environmental*, **2022**, 304, 120992 | 21.8 | 1 |
| 521 | Mechanistic understanding of pH effects on the oxygen evolution reaction. *Electrochimica Acta*, **2022**, 405, 139810 | 6.7 | 3 |
| 520 | Mechanism and Kinetics of n-Butane Dehydrogenation to 1,3-Butadiene Catalyzed by Isolated Pt Sites Grafted onto ?SiOZnOH Nests in Dealuminated Zeolite Beta. *ACS Catalysis*, **2022**, 12, 3333-3345 | 13.1 | 3 |
| 519 | Highly selective and productive reduction of carbon dioxide to multicarbon products via in situ CO management using segmented tandem electrodes. *Nature Catalysis*, **2022**, 5, 202-211 | 36.5 | 8 |
| 518 | On the Nature of Field-Enhanced Water Dissociation in Bipolar Membranes. *Journal of Physical Chemistry C*, **2021**, 125, 24974-24987 | 3.8 | 2 |
| 517 | Propane Dehydrogenation and Cracking over Zn/H-MFI Prepared by Solid-State Ion Exchange of ZnCl2. *ACS Catalysis*, **2021**, 11, 14489-14506 | 13.1 | 11 |
| 516 | Mechanism and Kinetics of Acetone Conversion to Isobutene over Isolated Hf Sites Grafted to Silicalite-1 and SiO. *Journal of the American Chemical Society*, **2021**, 143, 8352-8366 | 16.4 | 10 |
| 515 | Siloxyaluminate and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. *Chemistry - A European Journal*, **2021**, 27, 307-315 | 4.8 | 2 |
| 514 | Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. *Physical Chemistry Chemical Physics*, **2021**, 23, 9394-9406 | 3.6 | 8 |
| 513 | Mechanism and Kinetics of Light Alkane Dehydrogenation and Cracking over Isolated Ga Species in Ga/H-MFI. *ACS Catalysis*, **2021**, 11, 2062-2075 | 13.1 | 15 |
| 512 | Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. *Jacs Au*, **2021**, 1, 1708-1718 | | 5 |
| 511 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801 | 3.9 | 115 |
| 510 | Few-Unit-Cell MFI Zeolite Synthesized using a Simple Di-quaternary Ammonium Structure-Directing Agent. *Angewandte Chemie - International Edition*, **2021**, 60, 19214-19221 | 16.4 | 4 |
| 509 | The Role of Roughening to Enhance Selectivity to C2+ Products during CO2 Electroreduction on Copper. *ACS Energy Letters*, **2021**, 6, 3252-3260 | 20.1 | 4 |
| 508 | Few-Unit-Cell MFI Zeolite Synthesized using a Simple Di-quaternary Ammonium Structure-Directing Agent. *Angewandte Chemie*, **2021**, 133, 19363-19370 | 3.6 | 1 |
| 507 | Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites. *Journal of Catalysis*, **2021**, 404, 832-832 | 7.3 | 1 |

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| 506 | Computational Modeling Predicts the Stability of Both Pd and Pd Ion-Exchanged into H-CHA. *Journal of Materials Chemistry A*, **2021**, 9, 2161-2174 | 13 | 9 |
| 505 | Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations. *Catalysis Science and Technology*, **2021**, 11, 3539-3555 | 5.5 | 1 |
| 504 | Propane Dehydrogenation Catalyzed by Isolated Pt Atoms in ?SiOZn-OH Nests in Dealuminated Zeolite Beta. *Journal of the American Chemical Society*, **2021**, | 16.4 | 19 |
| 503 | Understanding Multi-Ion Transport Mechanisms in Bipolar Membranes. *ACS Applied Materials & Interfaces*, **2020**, 12, 52509-52526 | 9.5 | 22 |
| 502 | Experimental and Computational Studies of Carbon□Carbon Bond Formation via Ketonization and Aldol Condensation over Site-Isolated Zirconium Catalysts. *ACS Catalysis*, **2020**, 10, 4566-4579 | 13.1 | 14 |
| 501 | Effects of Surface Roughness on the Electrochemical Reduction of CO2 over Cu. *ACS Energy Letters*, **2020**, 5, 1206-1214 | 20.1 | 80 |
| 500 | Production of C2/C3 Oxygenates from Planar Copper Nitride-Derived Mesoporous Copper via Electrochemical Reduction of CO2. *Chemistry of Materials*, **2020**, 32, 3304-3311 | 9.6 | 32 |
| 499 | Heterogenized Pyridine-Substituted Cobalt(II) Phthalocyanine Yields Reduction of CO by Tuning the Electron Affinity of the Co Center. *ACS Applied Materials & Interfaces*, **2020**, 12, 5251-5258 | 9.5 | 22 |
| 498 | Impact of Pulsed Electrochemical Reduction of CO2 on the Formation of C2+ Products over Cu. *ACS Catalysis*, **2020**, 10, 12403-12413 | 13.1 | 29 |
| 497 | Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. *Physical Chemistry Chemical Physics*, **2020**, 22, 781-798 | 3.6 | 15 |
| 496 | Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. *Inorganic Chemistry*, **2020**, 59, 15410-15420 | 5.1 | 8 |
| 495 | The Role of Water in Vapor-fed Proton-Exchange-Membrane Electrolysis. *Journal of the Electrochemical Society*, **2020**, 167, 104508 | 3.9 | 15 |
| 494 | Electrocatalytic CO2 Reduction to Fuels: Progress and Opportunities. *Trends in Chemistry*, **2020**, 2, 825-836 | 14.8 | 41 |
| 493 | Influence of surface Sn species and hydrogen interactions on the OH group formation over spherical silica-supported tin oxide catalysts. *Reaction Chemistry and Engineering*, **2020**, 5, 1814-1823 | 4.9 | 2 |
| 492 | Ethanol Conversion to Butadiene over Isolated Zinc and Yttrium Sites Grafted onto Dealuminated Beta Zeolite. *Journal of the American Chemical Society*, **2020**, 142, 14674-14687 | 16.4 | 25 |
| 491 | A Perspective on the Electrochemical Oxidation of Methane to Methanol in Membrane Electrode Assemblies. *ACS Energy Letters*, **2020**, 5, 2954-2963 | 20.1 | 21 |
| 490 | A systematic analysis of Cu-based membrane-electrode assemblies for CO2 reduction through multiphysics simulation. *Energy and Environmental Science*, **2020**, 13, 3592-3606 | 35.4 | 22 |
| 489 | Scanning Nanobeam Diffraction and Energy Dispersive Spectroscopy Characterization of a Model Mn-Promoted Co/Al2O3 Nanosphere Catalyst for Fischer□Tropsch Synthesis. *ACS Catalysis*, **2020**, 10, 12071-12079 | 13.1 | 4 |

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| 488 | Synthesis of Biomass-Derived Ethers for Use as Fuels and Lubricants. *ChemSusChem*, **2019**, 12, 2835-2858 | 8.3 | 24 |
| 487 | Zeolite-Catalyzed Isobutene Amination: Mechanism and Kinetics. *ACS Catalysis*, **2019**, 9, 7012-7022 | 13.1 | 8 |
| 486 | Towards membrane-electrode assembly systems for CO2 reduction: a modeling study. *Energy and Environmental Science*, **2019**, 12, 1950-1968 | 35.4 | 145 |
| 485 | Response to "Impact of Zeolite Structure on Entropic-Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study". *Chemistry - A European Journal*, **2019**, 25, 7225-7226 | 4.8 | 0 |
| 484 | Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO2 to CO. *ACS Catalysis*, **2019**, 9, 4006-4014 | 13.1 | 72 |
| 483 | Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. *Journal of the American Chemical Society*, **2019**, 141, 4191-4193 | 16.4 | 18 |
| 482 | Understanding cation effects in electrochemical CO2 reduction. *Energy and Environmental Science*, **2019**, 12, 3001-3014 | 35.4 | 231 |
| 481 | Factors and Dynamics of Cu Nanocrystal Reconstruction under CO2 Reduction. *ACS Applied Energy Materials*, **2019**, 2, 7744-7749 | 6.1 | 35 |
| 480 | Mechanism and Kinetics of Isobutene Formation from Ethanol and Acetone over ZnxZryOz. *ACS Catalysis*, **2019**, 9, 10588-10604 | 13.1 | 18 |
| 479 | Propanol Amination over Supported Nickel Catalysts: Reaction Mechanism and Role of the Support. *ACS Catalysis*, **2019**, 9, 2931-2939 | 13.1 | 32 |
| 478 | Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl. *Journal of the American Chemical Society*, **2019**, 141, 1614-1627 | 16.4 | 58 |
| 477 | Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. *ACS Catalysis*, **2019**, 9, 920-931 | 13.1 | 100 |
| 476 | Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. *ChemPhysChem*, **2018**, 19, 338-338 | 3.2 | |
| 475 | Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. *Catalysis Today*, **2018**, 312, 51-65 | 5.3 | 22 |
| 474 | Effects of Anion Identity and Concentration on Electrochemical Reduction of CO2. *ChemElectroChem*, **2018**, 5, 1064-1072 | 4.3 | 102 |
| 473 | Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO on Copper?. *Journal of Physical Chemistry Letters*, **2018**, 9, 601-606 | 6.4 | 93 |
| 472 | Mechanism of CO2 Reduction at Copper Surfaces: Pathways to C2 Products. *ACS Catalysis*, **2018**, 8, 1490-1499 | 13.1 | 377 |
| 471 | Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of n-Alkanes in Brønsted-Acid Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 9397-9410 | 3.8 | 24 |

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| 470 | Effect of Alcohol Structure on the Kinetics of Etherification and Dehydration over Tungstated Zirconia. *ChemSusChem*, **2018**, 11, 3104-3111 | 8.3 | 20 |
| 469 | The mechanism and kinetics of methyl isobutyl ketone synthesis from acetone over ion-exchanged hydroxyapatite. *Journal of Catalysis*, **2018**, 365, 174-183 | 7.3 | 15 |
| 468 | Nonempirical Meta-Generalized Gradient Approximations for Modeling Chemisorption at Metal Surfaces. *Journal of Chemical Theory and Computation*, **2018**, 14, 3083-3090 | 6.4 | 13 |
| 467 | Modeling gas-diffusion electrodes for CO reduction. *Physical Chemistry Chemical Physics*, **2018**, 20, 16973-16984 | 3.6 | 66 |
| 466 | Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. *ChemPhysChem*, **2018**, 19, 341-358 | 3.2 | 18 |
| 465 | Chapter 3:Understanding the Effects of Composition and Structure on the Oxygen Evolution Reaction (OER) Occurring on NiFeOx Catalysts. *RSC Energy and Environment Series*, **2018**, 79-116 | 0.6 | 1 |
| 464 | Reaction mechanism of the selective reduction of CO to CO by a tetraaza [CoNH] complex in the presence of protons. *Physical Chemistry Chemical Physics*, **2018**, 20, 24058-24064 | 3.6 | 11 |
| 463 | Characterization of Isolated Ga3+Cations in Ga/H-MFI Prepared by Vapor-Phase Exchange of H-MFI Zeolite with GaCl3. *ACS Catalysis*, **2018**, 8, 6106-6126 | 13.1 | 48 |
| 462 | Continuous pervaporation-assisted furfural production catalyzed by CrCl3. *Green Chemistry*, **2018**, 20, 2903-2912 | 10 | 17 |
| 461 | Standards and Protocols for Data Acquisition and Reporting for Studies of the Electrochemical Reduction of Carbon Dioxide. *ACS Catalysis*, **2018**, 8, 6560-6570 | 13.1 | 160 |
| 460 | Direct Observation of the Local Reaction Environment during the Electrochemical Reduction of CO. *Journal of the American Chemical Society*, **2018**, 140, 7012-7020 | 16.4 | 114 |
| 459 | Computational Modeling of the Nature and Role of Ga Species for Light Alkane Dehydrogenation Catalyzed by Ga/H-MFI. *ACS Catalysis*, **2018**, 8, 6146-6162 | 13.1 | 53 |
| 458 | Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation of n-Butane in Brønsted Acidic Zeolites. *ACS Catalysis*, **2017**, 7, 2685-2697 | 13.1 | 33 |
| 457 | Production of Biomass-Based Automotive Lubricants by Reductive Etherification. *ChemSusChem*, **2017**, 10, 2527-2533 | 8.3 | 25 |
| 456 | Optimizing C□□ Coupling on Oxide-Derived Copper Catalysts for Electrochemical CO2 Reduction. *Journal of Physical Chemistry C*, **2017**, 121, 14191-14203 | 3.8 | 187 |
| 455 | Artificial neural network based predictions of cetane number for furanic biofuel additives. *Fuel*, **2017**, 206, 171-179 | 7.1 | 44 |
| 454 | Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature. *Journal of Physical Chemistry C*, **2017**, 121, 1618-1638 | 3.8 | 12 |
| 453 | Mechanistic insights into electrochemical reduction of CO over Ag using density functional theory and transport models. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8812-E8821 | 11.5 | 163 |

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| 452 | Mechanism and kinetics of 1-dodecanol etherification over tungstated zirconia. *Journal of Catalysis*, **2017**, 354, 13-23 | 7.3 | 18 |
| 451 | Nanoporous gold assemblies of calixarene-phosphine-capped colloids. *Chemical Communications*, **2017**, 53, 10870-10873 | 5.8 | 4 |
| 450 | Integrated catalytic sequences for catalytic upgrading of bio-derived carboxylic acids to fuels, lubricants and chemical feedstocks. *Sustainable Energy and Fuels*, **2017**, 1, 1805-1809 | 5.8 | 14 |
| 449 | Novel Strategies for the Production of Fuels, Lubricants, and Chemicals from Biomass. *Accounts of Chemical Research*, **2017**, 50, 2589-2597 | 24.3 | 115 |
| 448 | Promoter Effects of Alkali Metal Cations on the Electrochemical Reduction of Carbon Dioxide. *Journal of the American Chemical Society*, **2017**, 139, 11277-11287 | 16.4 | 381 |
| 447 | Electrochemical CO Reduction over Compressively Strained CuAg Surface Alloys with Enhanced Multi-Carbon Oxygenate Selectivity. *Journal of the American Chemical Society*, **2017**, 139, 15848-15857 | 16.4 | 331 |
| 446 | A DFT Investigation of the Mechanism of Propene Ammoxidation over □Bismuth Molybdate. *ACS Catalysis*, **2017**, 7, 161-176 | 13.1 | 19 |
| 445 | Kinetics of hydrogenation and hydrogenolysis of 2,5-dimethylfuran over noble metals catalysts under mild conditions. *Applied Catalysis B: Environmental*, **2017**, 202, 557-568 | 21.8 | 33 |
| 444 | Effects of catalyst crystal structure on the oxidation of propene to acrolein. *Catalysis Today*, **2016**, 261, 146-153 | 5.3 | 16 |
| 443 | Hydrolysis of Electrolyte Cations Enhances the Electrochemical Reduction of CO over Ag and Cu. *Journal of the American Chemical Society*, **2016**, 138, 13006-13012 | 16.4 | 412 |
| 442 | Operando Analyses of Solar Fuels Light Absorbers and Catalysts. *Electrochimica Acta*, **2016**, 211, 711-719 | 6.7 | 20 |
| 441 | Delignification of miscanthus using ethylenediamine (EDA) with or without ammonia and subsequent enzymatic hydrolysis to sugars. *3 Biotech*, **2016**, 6, 23 | 2.8 | 8 |
| 440 | Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. *Journal of the American Chemical Society*, **2016**, 138, 4739-56 | 16.4 | 53 |
| 439 | A systematic study on Pt based, subnanometer-sized alloy cluster catalysts for alkane dehydrogenation: effects of intermetallic interaction. *Physical Chemistry Chemical Physics*, **2016**, 18, 10906-17 | 3.6 | 26 |
| 438 | Production of renewable lubricants via self-condensation of methyl ketones. *Green Chemistry*, **2016** , 18, 3577-3581 | 10 | 25 |
| 437 | The role of hydrogen during Pt-Ga nanocatalyst formation. *Physical Chemistry Chemical Physics*, **2016**, 18, 3234-43 | 3.6 | 23 |
| 436 | Ambient-Pressure XPS Study of a Ni□Fe Electrocatalyst for the Oxygen Evolution Reaction. *Journal of Physical Chemistry C*, **2016**, 120, 2247-2253 | 3.8 | 253 |
| 435 | Mechanism and Kinetics of Ethanol Coupling to Butanol over Hydroxyapatite. *ACS Catalysis*, **2016**, 6, 939-948 | 13.1 | 111 |

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| 434 | Trace Levels of Copper in Carbon Materials Show Significant Electrochemical CO2 Reduction Activity. *ACS Catalysis*, **2016**, 6, 202-209 | 13.1 | 118 |
| 433 | Role of ZrO2 in Promoting the Activity and Selectivity of Co-Based Fischer□ropsch Synthesis Catalysts. *ACS Catalysis*, **2016**, 6, 100-114 | 13.1 | 45 |
| 432 | Design of an artificial photosynthetic system for production of alcohols in high concentration from CO2. *Energy and Environmental Science*, **2016**, 9, 193-199 | 35.4 | 41 |
| 431 | Ga[OSi(O(t)Bu)3]3□THF, a thermolytic molecular precursor for high surface area gallium-containing silica materials of controlled dispersion and stoichiometry. *Dalton Transactions*, **2016**, 45, 11025-34 | 4.3 | 17 |
| 430 | From Sugars to Wheels: The Conversion of Ethanol to 1,3-Butadiene over Metal-Promoted Magnesia-Silicate Catalysts. *ChemSusChem*, **2016**, 9, 1462-72 | 8.3 | 61 |
| 429 | CO2 Electroreduction with Enhanced Ethylene and Ethanol Selectivity by Nanostructuring Polycrystalline Copper. *ChemElectroChem*, **2016**, 3, 1012-1019 | 4.3 | 110 |
| 428 | Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA. *ACS Catalysis*, **2016**, 6, 5052-5061 | 13.1 | 11 |
| 427 | Identifying the Unique Properties of □Bi2Mo3O12 for the Activation of Propene. *Journal of Physical Chemistry C*, **2016**, 120, 29233-29247 | 3.8 | 8 |
| 426 | Growth of encapsulating carbon on supported Pt nanoparticles studied by in situ TEM. *Journal of Catalysis*, **2016**, 338, 295-304 | 7.3 | 33 |
| 425 | Effects of Lewis acidity of metal oxide promoters on the activity and selectivity of Co-based Fischer□ropsch synthesis catalysts. *Journal of Catalysis*, **2016**, 338, 250-264 | 7.3 | 57 |
| 424 | The mechanism and kinetics of propene ammoxidation over □bismuth molybdate. *Journal of Catalysis*, **2016**, 339, 228-241 | 7.3 | 18 |
| 423 | Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2861-70 | 6.4 | 22 |
| 422 | Identification of Possible Pathways for C-C Bond Formation during Electrochemical Reduction of CO2: New Theoretical Insights from an Improved Electrochemical Model. *Journal of Physical Chemistry Letters*, **2016**, 7, 1471-7 | 6.4 | 313 |
| 421 | Experimental and Computational Evidence of Highly Active Fe Impurity Sites on the Surface of Oxidized Au for the Electrocatalytic Oxidation of Water in Basic Media. *ChemElectroChem*, **2016**, 3, 66-73 | 4.3 | 34 |
| 420 | Pervaporation-assisted catalytic conversion of xylose to furfural. *Green Chemistry*, **2016**, 18, 4073-4085 | 10 | 23 |
| 419 | Effects of temperature and gas-liquid mass transfer on the operation of small electrochemical cells for the quantitative evaluation of CO reduction electrocatalysts. *Physical Chemistry Chemical Physics*, **2016**, 18, 26777-26785 | 3.6 | 93 |
| 418 | Production of Hydroxyl□ich Acids from Xylose and Glucose Using Sn-BEA Zeolite. *ChemistrySelect*, **2016**, 1, 4167-4172 | 1.8 | 25 |
| 417 | Effects of Composition and Structure of Mg/Al Oxides on Their Activity and Selectivity for the Condensation of Methyl Ketones. *Industrial & Engineering Chemistry Research*, **2016**, 55, 10635-10644 | 3.9 | 29 |

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| 416 | Propene Metathesis over Supported Tungsten Oxide Catalysts: A Study of Active Site Formation. *ACS Catalysis*, **2016**, 6, 7728-7738 | 13.1 | 44 |
| 415 | Quantum Mechanical Screening of Single-Atom Bimetallic Alloys for the Selective Reduction of CO2 to C1 Hydrocarbons. *ACS Catalysis*, **2016**, 6, 7769-7777 | 13.1 | 136 |
| 414 | Identification of highly active Fe sites in (Ni,Fe)OOH for electrocatalytic water splitting. *Journal of the American Chemical Society*, **2015**, 137, 1305-13 | 16.4 | 1553 |
| 413 | p-Type Transparent Conducting Oxide/n-Type Semiconductor Heterojunctions for Efficient and Stable Solar Water Oxidation. *Journal of the American Chemical Society*, **2015**, 137, 9595-603 | 16.4 | 98 |
| 412 | Role of Catalyst Preparation on the Electrocatalytic Activity of Ni1−xFexOOH for the Oxygen Evolution Reaction. *Journal of Physical Chemistry C*, **2015**, 119, 18303-18316 | 3.8 | 100 |
| 411 | Effects of electrolyte, catalyst, and membrane composition and operating conditions on the performance of solar-driven electrochemical reduction of carbon dioxide. *Physical Chemistry Chemical Physics*, **2015**, 17, 18924-36 | 3.6 | 230 |
| 410 | SnCl4-catalyzed isomerization/dehydration of xylose and glucose to furanics in water. *Catalysis Science and Technology*, **2015**, 5, 2839-2847 | 5.5 | 76 |
| 409 | Highly selective condensation of biomass-derived methyl ketones as a source of aviation fuel. *ChemSusChem*, **2015**, 8, 1726-36 | 8.3 | 90 |
| 408 | Nitric-acid hydrolysis of Miscanthus giganteus to sugars fermented to bioethanol. *Biotechnology and Bioprocess Engineering*, **2015**, 20, 304-314 | 3.1 | 16 |
| 407 | An Atomic-Scale View of the Nucleation and Growth of Graphene Islands on Pt Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 7124-7129 | 3.8 | 20 |
| 406 | Effects of Fe Electrolyte Impurities on Ni(OH)2/NiOOH Structure and Oxygen Evolution Activity. *Journal of Physical Chemistry C*, **2015**, 119, 7243-7254 | 3.8 | 572 |
| 405 | Tailoring Metal-Porphyrin-Like Active Sites on Graphene to Improve the Efficiency and Selectivity of Electrochemical CO2 Reduction. *Journal of Physical Chemistry C*, **2015**, 119, 21345-21352 | 3.8 | 67 |
| 404 | Thermodynamic and achievable efficiencies for solar-driven electrochemical reduction of carbon dioxide to transportation fuels. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E6111-8 | 11.5 | 89 |
| 403 | Differential Electrochemical Mass Spectrometer Cell Design for Online Quantification of Products Produced during Electrochemical Reduction of CO. *Analytical Chemistry*, **2015**, 87, 8013-20 | 7.8 | 53 |
| 402 | Wavefunction stability analysis without analytical electronic Hessians: application to orbital-optimised second-order Møller–Plesset theory and VV10-containing density functionals. *Molecular Physics*, **2015**, 113, 1802-1808 | 1.7 | 20 |
| 401 | Electrochemical Study of the Energetics of the Oxygen Evolution Reaction at Nickel Iron (Oxy)Hydroxide Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 19022-19029 | 3.8 | 213 |
| 400 | Ethane and propane dehydrogenation over PtIr/Mg(Al)O. *Applied Catalysis A: General*, **2015**, 506, 25-32 | 5.1 | 50 |
| 399 | An Investigation into the Effects of Mn Promotion on the Activity and Selectivity of Co/SiO2 for Fischer–Tropsch Synthesis: Evidence for Enhanced CO Adsorption and Dissociation. *ACS Catalysis*, **2015**, 5, 5888-5903 | 13.1 | 107 |

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| 398 | The role of hydroxyl group acidity on the activity of silica-supported secondary amines for the self-condensation of n-butanal. *ChemSusChem*, **2015**, 8, 466-72 | 8.3 | 22 |
| 397 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215 | 1.7 | 2068 |
| 396 | Non-Oxidative Dehydrogenation Pathways for the Conversion of C2□4 Alcohols to Carbonyl Compounds. *ChemSusChem*, **2015**, 8, 3917-3917 | 8.3 | |
| 395 | Catalytic Upgrading of Biomass-Derived Methyl Ketones to Liquid Transportation Fuel Precursors by an Organocatalytic Approach. *Angewandte Chemie*, **2015**, 127, 4756-4760 | 3.6 | 9 |
| 394 | Upgrading Lignocellulosic Products to Drop-In Biofuels via Dehydrogenative Cross-Coupling and Hydrodeoxygenation Sequence. *ChemSusChem*, **2015**, 8, 2609-14 | 8.3 | 26 |
| 393 | Non-Oxidative Dehydrogenation Pathways for the Conversion of C2 -C4 Alcohols to Carbonyl Compounds. *ChemSusChem*, **2015**, 8, 3959-62 | 8.3 | 10 |
| 392 | Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on Br□sted Acid Sites in Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 10427-10438 | 3.8 | 42 |
| 391 | Novel pathways for fuels and lubricants from biomass optimized using life-cycle greenhouse gas assessment. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 7645-9 | 11.5 | 90 |
| 390 | Investigations of element spatial correlation in Mn-promoted Co-based Fischer□ropsch synthesis catalysts. *Journal of Catalysis*, **2015**, 328, 111-122 | 7.3 | 25 |
| 389 | Catalytic upgrading of biomass-derived methyl ketones to liquid transportation fuel precursors by an organocatalytic approach. *Angewandte Chemie - International Edition*, **2015**, 54, 4673-7 | 16.4 | 52 |
| 388 | Selective oxidation and oxidative dehydrogenation of hydrocarbons on bismuth vanadium molybdenum oxide. *Journal of Catalysis*, **2015**, 325, 87-100 | 7.3 | 33 |
| 387 | Pretreatment of Miscanthus giganteus with Lime and Oxidants for Biofuels. *Energy & Fuels*, **2015**, 29, 1743-1750 | 4.1 | 8 |
| 386 | Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. *Journal of Physical Chemistry C*, **2015**, 119, 1840-1850 | 3.8 | 59 |
| 385 | Synthesis of biomass-derived methylcyclopentane as a gasoline additive via aldol condensation/hydrodeoxygenation of 2,5-hexanedione. *Green Chemistry*, **2015**, 17, 2393-2397 | 10 | 49 |
| 384 | The Role of Metal Halides in Enhancing the Dehydration of Xylose to Furfural. *ChemCatChem*, **2015**, 7, 479-489 | 5.2 | 54 |
| 383 | Effects of composition and metal particle size on ethane dehydrogenation over PtxSn100□/Mg(Al)O (70?x?100). *Journal of Catalysis*, **2014**, 311, 161-168 | 7.3 | 83 |
| 382 | n-Butane dehydrogenation over Pt/Mg(In)(Al)O. *Applied Catalysis A: General*, **2014**, 470, 208-214 | 5.1 | 34 |
| 381 | Biomass conversion to diesel via the etherification of furanyl alcohols catalyzed by Amberlyst-15. *Journal of Catalysis*, **2014**, 313, 70-79 | 7.3 | 70 |

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| 380 | Hydrogenation of butanal over silica-supported Shvoš catalyst and its use for the gas-phase conversion of propene to butanol via tandem hydroformylation and hydrogenation. *Journal of Catalysis*, **2014**, 311, 52-58 | 7.3 | 19 |
| 379 | Tailoring the Cooperative Acid–Base Effects in Silica-Supported Amine Catalysts: Applications in the Continuous Gas-Phase Self-Condensation of n-Butanal. *ChemCatChem*, **2014**, 6, n/a-n/a | 5.2 | 17 |
| 378 | Syntheses of biodiesel precursors: sulfonic acid catalysts for condensation of biomass-derived platform molecules. *ChemSusChem*, **2014**, 7, 1078-85 | 8.3 | 49 |
| 377 | Propene Oligomerization using Alkali Metal- and Nickel-Exchanged Mesoporous Aluminosilicate Catalysts. *ACS Catalysis*, **2014**, 4, 337-343 | 13.1 | 34 |
| 376 | Selective Propene Oligomerization with Nickel(II)-Based Metal–Organic Frameworks. *ACS Catalysis*, **2014**, 4, 717-721 | 13.1 | 79 |
| 375 | Reaction Dynamics of Zeolite-Catalyzed Alkene Methylation by Methanol. *Journal of Physical Chemistry C*, **2014**, 118, 21409-21419 | 3.8 | 25 |
| 374 | Two-Step Delignification of Miscanthus To Enhance Enzymatic Hydrolysis: Aqueous Ammonia Followed by Sodium Hydroxide and Oxidants. *Energy & Fuels*, **2014**, 28, 542-548 | 4.1 | 10 |
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