# Alexis T Bell

List of Publications by Year
in descending order

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|---|---|---|---|
| 531 papers | 59,447 citations | 1094 112 h-index | 1341 223 g-index |
| 560 all docs | 560 docs citations | 560 times ranked | 40452 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191. | 1.3 | 2,597 |
| 2 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 0.8 | 2,561 |
| 3 | The Impact of Nanoscience on Heterogeneous Catalysis. Science, 2003, 299, 1688-1691. | 6.0 | 2,263 |
| 4 | An Investigation of Thin-Film Niâ€“Fe Oxide Catalysts for the Electrochemical Evolution of Oxygen. Journal of the American Chemical Society, 2013, 135, 12329-12337. | 6.6 | 2,132 |
| 5 | Identification of Highly Active Fe Sites in (Ni,Fe)OOH for Electrocatalytic Water Splitting. Journal of the American Chemical Society, 2015, 137, 1305-1313. | 6.6 | 2,018 |
| 6 | Catalysis Research of Relevance to Carbon Management:â€‰ Progress, Challenges, and Opportunities. Chemical Reviews, 2001, 101, 953-996. | 23.0 | 1,311 |
| 7 | Enhanced Activity of Gold-Supported Cobalt Oxide for the Electrochemical Evolution of Oxygen. Journal of the American Chemical Society, 2011, 133, 5587-5593. | 6.6 | 1,264 |
| 8 | Theoretical Investigation of the Activity of Cobalt Oxides for the Electrochemical Oxidation of Water. Journal of the American Chemical Society, 2013, 135, 13521-13530. | 6.6 | 1,093 |
| 9 | Effects of Fe Electrolyte Impurities on Ni(OH)<sub>2</sub>/NiOOH Structure and Oxygen Evolution Activity. Journal of Physical Chemistry C, 2015, 119, 7243-7254. | 1.5 | 806 |
| 10 | Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method. Journal of Chemical Physics, 2005, 123, 224101. | 1.2 | 662 |
| 11 | Promoter Effects of Alkali Metal Cations on the Electrochemical Reduction of Carbon Dioxide. Journal of the American Chemical Society, 2017, 139, 11277-11287. | 6.6 | 653 |
| 12 | Hydrolysis of Electrolyte Cations Enhances the Electrochemical Reduction of CO<sub>2</sub> over Ag and Cu. Journal of the American Chemical Society, 2016, 138, 13006-13012. | 6.6 | 640 |
| 13 | In Situ Raman Study of Nickel Oxide and Gold-Supported Nickel Oxide Catalysts for the Electrochemical Evolution of Oxygen. Journal of Physical Chemistry C, 2012, 116, 8394-8400. | 1.5 | 609 |
| 14 | Mechanism of CO<sub>2</sub> Reduction at Copper Surfaces: Pathways to C<sub>2</sub> Products. ACS Catalysis, 2018, 8, 1490-1499. | 5.5 | 608 |
| 15 | Structure and Catalytic Properties of Supported Vanadium Oxides: Support Effects on Oxidative Dehydrogenation Reactions. Journal of Catalysis, 1999, 181, 205-216. | 3.1 | 573 |
| 16 | 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 |
| 17 | Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals. Journal of Physical Chemistry A, 2007, 111, 8753-8765. | 1.1 | 508 |
| 18 | Size-Dependent Activity of Co<sub>3</sub>O<sub>4</sub> Nanoparticle Anodes for Alkaline Water Electrolysis. Journal of Physical Chemistry C, 2009, 113, 15068-15072. | 1.5 | 496 |

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| 19 | Identification of Possible Pathways for Câ€“C Bond Formation during Electrochemical Reduction of CO<sub>2</sub>: New Theoretical Insights from an Improved Electrochemical Model. Journal of Physical Chemistry Letters, 2016, 7, 1471-1477. | 2.1 | 479 |
| 20 | Electrochemical CO<sub>2</sub> Reduction over Compressively Strained CuAg Surface Alloys with Enhanced Multi-Carbon Oxygenate Selectivity. Journal of the American Chemical Society, 2017, 139, 15848-15857. | 6.6 | 470 |
| 21 | Understanding cation effects in electrochemical CO<sub>2</sub> reduction. Energy and Environmental Science, 2019, 12, 3001-3014. | 15.6 | 433 |
| 22 | Laser Raman spectroscopy of supported vanadium oxide catalysts. The Journal of Physical Chemistry, 1990, 94, 4240-4246. | 2.9 | 416 |
| 23 | Investigation of CO and CO2 Adsorption on Tetragonal and Monoclinic Zirconia. Langmuir, 2001, 17, 4297-4303. | 1.6 | 415 |
| 24 | A two-step approach for the catalytic conversion of glucose to 2,5-dimethylfuran in ionic liquids. Green Chemistry, 2010, 12, 1253. | 4.6 | 392 |
| 25 | Investigations of the State of Fe in Hâ€“ZSM-5. Journal of Catalysis, 1999, 186, 242-253. | 3.1 | 388 |
| 26 | Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. The Journal of Physical Chemistry, 1993, 97, 13742-13752. | 2.9 | 366 |
| 27 | Catalytic Synthesis of Hydrocarbons over Group VIII Metals. A Discussion of the Reaction Mechanism. Catalysis Reviews - Science and Engineering, 1981, 23, 203-232. | 5.7 | 364 |
| 28 | Etherification and reductive etherification of 5-(hydroxymethyl)furfural: 5-(alkoxymethyl)furfurals and 2,5-bis(alkoxymethyl)furans as potential bio-diesel candidates. Green Chemistry, 2012, 14, 1626. | 4.6 | 347 |
| 29 | Ambient-Pressure XPS Study of a Niâ€“Fe Electrocatalyst for the Oxygen Evolution Reaction. Journal of Physical Chemistry C, 2016, 120, 2247-2253. | 1.5 | 336 |
| 30 | 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, 18924-18936. | 1.3 | 312 |
| 31 | In-SituInfrared Study of Methanol Synthesis from H2/CO2over Cu/SiO2and Cu/ZrO2/SiO2. Journal of Catalysis, 1997, 172, 222-237. | 3.1 | 311 |
| 32 | Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. Journal of Physical Chemistry C, 2012, 116, 21077-21082. | 1.5 | 305 |
| 33 | Modeling gas-diffusion electrodes for CO<sub>2</sub> reduction. Physical Chemistry Chemical Physics, 2018, 20, 16973-16984. | 1.3 | 305 |
| 34 | Electron Paramagnetic Resonance Studies of Copper Ion-Exchanged ZSM-5. The Journal of Physical Chemistry, 1994, 98, 11533-11540. | 2.9 | 302 |
| 35 | Effect of Catalyst Structure on Oxidative Dehydrogenation of Ethane and Propane on Alumina-Supported Vanadia. Journal of Catalysis, 2002, 208, 139-149. | 3.1 | 298 |
| 36 | Isotopic Tracer and Kinetic Studies of Oxidative Dehydrogenation Pathways on Vanadium Oxide Catalysts. Journal of Catalysis, 1999, 186, 325-333. | 3.1 | 295 |

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| 37 | A growing string method for determining transition states: Comparison to the nudged elastic band and string methods. Journal of Chemical Physics, 2004, 120, 7877-7886. | 1.2 | 293 |
| 38 | 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. | 1.5 | 282 |
| 39 | Kinetics and Mechanism of Oxidative Dehydrogenation of Propane on Vanadium, Molybdenum, and Tungsten Oxides. Journal of Physical Chemistry B, 2000, 104, 1292-1299. | 1.2 | 276 |
| 40 | Towards membrane-electrode assembly systems for CO<sub>2</sub> reduction: a modeling study. Energy and Environmental Science, 2019, 12, 1950-1968. | 15.6 | 273 |
| 41 | Structure and properties of vanadium oxide-zirconia catalysts for propane oxidative dehydrogenation. Journal of Catalysis, 1998, 177, 343-351. | 3.1 | 267 |
| 42 | Structure and Properties of Oxidative Dehydrogenation Catalysts Based on MoO3/Al2O3. Journal of Catalysis, 2001, 198, 232-242. | 3.1 | 265 |
| 43 | Quantitative structural analysis of dispersed vanadia species in TiO2(anatase)-supported V2O5. Journal of Catalysis, 1992, 134, 479-491. | 3.1 | 259 |
| 44 | Molecular dynamics study of methane and xenon in silicalite. The Journal of Physical Chemistry, 1990, 94, 8232-8240. | 2.9 | 258 |
| 45 | The Relationship between the Electronic and Redox Properties of Dispersed Metal Oxides and Their Turnover Rates in Oxidative Dehydrogenation Reactions. Journal of Catalysis, 2002, 209, 35-42. | 3.1 | 255 |
| 46 | Optimizing Câ€“C Coupling on Oxide-Derived Copper Catalysts for Electrochemical CO<sub>2</sub> Reduction. Journal of Physical Chemistry C, 2017, 121, 14191-14203. | 1.5 | 254 |
| 47 | Standards and Protocols for Data Acquisition and Reporting for Studies of the Electrochemical Reduction of Carbon Dioxide. ACS Catalysis, 2018, 8, 6560-6570. | 5.5 | 250 |
| 48 | Molecular dynamics studies of butane and hexane in silicalite. The Journal of Physical Chemistry, 1992, 96, 1051-1060. | 2.9 | 244 |
| 49 | The effects of structure on the catalytic activity and selectivity of V2O5/TiO2 for the reduction of NO by NH3. Journal of Catalysis, 1992, 134, 492-505. | 3.1 | 241 |
| 50 | Effect of alkali metal catalysts on gasification of coal char. Fuel, 1978, 57, 194-200. | 3.4 | 240 |
| 51 | A Study of the Acidâ€Catalyzed Hydrolysis of Cellulose Dissolved in Ionic Liquids and the Factors Influencing the Dehydration of Glucose and the Formation of Humins. ChemSusChem, 2011, 4, 1166-1173. | 3.6 | 232 |
| 52 | A mathematical model for spin coating of polymer resists. Journal of Applied Physics, 1984, 56, 1199-1206. | 1.1 | 225 |
| 53 | The effects of zirconia morphology on methanol synthesis from CO and H2H2 over Cu/ZrO2Cu/ZrO2 catalystsPart I. Steady-state studies. Journal of Catalysis, 2005, 233, 198-209. | 3.1 | 225 |
| 54 | A Study of the Dynamics of Pd Oxidation and PdO Reduction by H2and CH4. Journal of Catalysis, 1998, 176, 125-135. | 3.1 | 223 |

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| 55 | Mechanistic insights into electrochemical reduction of CO <sub>2</sub> 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. | 3.3 | 219 |
| 56 | Calibration of the DFT/GGA+U Method for Determination of Reduction Energies for Transition and Rare Earth Metal Oxides of Ti, V, Mo, and Ce. Journal of Chemical Theory and Computation, 2011, 7, 2218-2223. | 2.3 | 215 |
| 57 | Prediction of low occupancy sorption of alkanes in silicalite. The Journal of Physical Chemistry, 1990, 94, 1508-1516. | 2.9 | 210 |
| 58 | Comparison of Cobaltâ€based Nanoparticles as Electrocatalysts for Water Oxidation. ChemSusChem, 2011, 4, 1566-1569. | 3.6 | 209 |
| 59 | A review of theoretical models of adsorption, diffusion, desorption, and reaction of gases on metal surfaces. Surface Science Reports, 1991, 13, 3-72. | 3.8 | 208 |
| 60 | Role of Hydrogen Spillover in Methanol Synthesis over Cu/ZrO2. Journal of Catalysis, 2000, 193, 207-223. | 3.1 | 207 |
| 61 | Synthesis, Characterization, and Catalytic Performance of Single-Site Iron(III) Centers on the Surface of SBA-15 Silica. Journal of the American Chemical Society, 2002, 124, 13194-13203. | 6.6 | 207 |
| 62 | Novel Pt/Mg(In)(Al)O catalysts for ethane and propane dehydrogenation. Journal of Catalysis, 2011, 282, 165-174. | 3.1 | 206 |
| 63 | In Situ Infrared Study of Methanol Synthesis from H2/CO over Cu/SiO2and Cu/ZrO2/SiO2. Journal of Catalysis, 1998, 178, 153-173. | 3.1 | 203 |
| 64 | Ethane dehydrogenation on Pt/Mg(Al)O and PtSn/Mg(Al)O catalysts. Journal of Catalysis, 2010, 271, 209-219. | 3.1 | 199 |
| 65 | Tailored catalyst microenvironments for CO2 electroreduction to multicarbon products on copper using bilayer ionomer coatings. Nature Energy, 2021, 6, 1026-1034. | 19.8 | 194 |
| 66 | Quantum Mechanical Screening of Single-Atom Bimetallic Alloys for the Selective Reduction of CO<sub>2</sub> to C<sub>1</sub> Hydrocarbons. ACS Catalysis, 2016, 6, 7769-7777. | 5.5 | 190 |
| 67 | A Mechanistic Study of Methanol Decomposition over Cu/SiO2, ZrO2/SiO2, and Cu/ZrO2/SiO2. Journal of Catalysis, 1999, 184, 357-376. | 3.1 | 189 |
| 68 | An in Situ Infrared Study of Dimethyl Carbonate Synthesis from Carbon Dioxide and Methanol over Zirconia. Journal of Catalysis, 2001, 204, 339-347. | 3.1 | 188 |
| 69 | Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. Journal of Chemical Physics, 2008, 128, 184112. | 1.2 | 188 |
| 70 | Effects of Si/Al Ratio on the Distribution of Framework Al and on the Rates of Alkane Monomolecular Cracking and Dehydrogenation in H-MFI. Journal of the American Chemical Society, 2013, 135, 19193-19207. | 6.6 | 187 |
| 71 | Catalyst performance of novel Pt/Mg(Ga)(Al)O catalysts for alkane dehydrogenation. Journal of Catalysis, 2010, 274, 200-206. | 3.1 | 184 |
| 72 | Transition-state studies of xenon and sulfur hexafluoride diffusion in silicalite. The Journal of Physical Chemistry, 1991, 95, 8866-8878. | 2.9 | 180 |

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| 73 | The effects of synthesis and pretreatment conditions on the bulk structure and surface properties of zirconia. Journal of Molecular Catalysis A, 2000, 163, 27-42. | 4.8 | 180 |
| 74 | Effects of Support Composition and Pretreatment Conditions on the Structure of Vanadia Dispersed on SiO2, Al2O3, TiO2, ZrO2, and HfO2. Journal of Physical Chemistry B, 2000, 104, 1516-1528. | 1.2 | 180 |
| 75 | An efficient self-consistent field method for large systems of weakly interacting components. Journal of Chemical Physics, 2006, 124, 204105. | 1.2 | 179 |
| 76 | Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5â€. Journal of Physical Chemistry B, 2005, 109, 1857-1873. | 1.2 | 176 |
| 77 | Direct Observation of the Local Reaction Environment during the Electrochemical Reduction of CO<sub>2</sub>. Journal of the American Chemical Society, 2018, 140, 7012-7020. | 6.6 | 176 |
| 78 | 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 |
| 79 | Discovering Ce-rich oxygen evolution catalysts, from high throughput screening to water electrolysis. Energy and Environmental Science, 2014, 7, 682-688. | 15.6 | 165 |
| 80 | Effects of Anion Identity and Concentration on Electrochemical Reduction of CO<sub>2</sub>. ChemElectroChem, 2018, 5, 1064-1072. | 1.7 | 165 |
| 81 | Structure and Properties of Zirconia-Supported Molybdenum Oxide Catalysts for Oxidative Dehydrogenation of Propane. Journal of Catalysis, 2000, 189, 421-430. | 3.1 | 163 |
| 82 | Platinum-Based Catalysts for the Hydroamination of Olefins with Sulfonamides and Weakly Basic Anilines. Journal of the American Chemical Society, 2005, 127, 12640-12646. | 6.6 | 161 |
| 83 | Novel Strategies for the Production of Fuels, Lubricants, and Chemicals from Biomass. Accounts of Chemical Research, 2017, 50, 2589-2597. | 7.6 | 159 |
| 84 | Efficient exploration of reaction paths via a freezing string method. Journal of Chemical Physics, 2011, 135, 224108. | 1.2 | 154 |
| 85 | Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. ACS Catalysis, 2019, 9, 920-931. | 5.5 | 153 |
| 86 | Kinetic Isotopic Effects in Oxidative Dehydrogenation of Propane on Vanadium Oxide Catalysts. Journal of Catalysis, 2000, 192, 197-203. | 3.1 | 152 |
| 87 | Effects of Zirconia Phase on the Synthesis of Methanol over Zirconia-Supported Copper. Catalysis Letters, 2002, 80, 63-68. | 1.4 | 152 |
| 88 | Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. ACS Catalysis, 2014, 4, 1537-1545. | 5.5 | 148 |
| 89 | Quantum Chemical Modeling of Benzene Ethylation over H-ZSM-5 Approaching Chemical Accuracy: A Hybrid MP2:DFT Study. Journal of the American Chemical Society, 2010, 132, 11525-11538. | 6.6 | 144 |
| 90 | Effects of Mn promotion on the activity and selectivity of Co/SiO2 for Fischerâ€“Tropsch Synthesis. Journal of Catalysis, 2012, 288, 104-114. | 3.1 | 143 |

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| 91 | Trace Levels of Copper in Carbon Materials Show Significant Electrochemical CO<sub>2</sub> Reduction Activity. ACS Catalysis, 2016, 6, 202-209. | 5.5 | 143 |
| 92 | CO<sub>2</sub> Electroreduction with Enhanced Ethylene and Ethanol Selectivity by Nanostructuring Polycrystalline Copper. ChemElectroChem, 2016, 3, 1012-1019. | 1.7 | 142 |
| 93 | Mechanism and Kinetics of Ethanol Coupling to Butanol over Hydroxyapatite. ACS Catalysis, 2016, 6, 939-948. | 5.5 | 139 |
| 94 | An Investigation into the Effects of Mn Promotion on the Activity and Selectivity of Co/SiO<sub>2</sub> for Fischerâ€“Tropsch Synthesis: Evidence for Enhanced CO Adsorption and Dissociation. ACS Catalysis, 2015, 5, 5888-5903. | 5.5 | 138 |
| 95 | Effects of temperature and gasâ€“liquid mass transfer on the operation of small electrochemical cells for the quantitative evaluation of CO<sub>2</sub>reduction electrocatalysts. Physical Chemistry Chemical Physics, 2016, 18, 26777-26785. | 1.3 | 138 |
| 96 | Methanol formation on Fe/Al-MFI via the oxidation of methane by nitrous oxide. Journal of Catalysis, 2004, 225, 300-306. | 3.1 | 137 |
| 97 | A Study of Oxygen Vacancy Formation and Annihilation in Submonolayer Coverages of TiO<sub>2</sub> Dispersed on MCM-48. Journal of Physical Chemistry C, 2010, 114, 16937-16945. | 1.5 | 136 |
| 98 | Electron Donation in the Waterâ€“Water Hydrogen Bond. Chemistry - A European Journal, 2009, 15, 851-855. | 1.7 | 135 |
| 99 | Effects of molybdena on the catalytic properties of vanadia domains supported on alumina for oxidative dehydrogenation of propane. Journal of Catalysis, 2004, 221, 491-499. | 3.1 | 131 |
| 100 | Density Functional Theory Study of Proton Mobility in Zeolites:Â Proton Migration and Hydrogen Exchange in ZSM-5. Journal of Physical Chemistry B, 2000, 104, 6998-7011. | 1.2 | 130 |
| 101 | Studies on the mechanism of ZSM-5 formation. Catalysis Letters, 1991, 8, 305-316. | 1.4 | 127 |
| 102 | Investigations of the Dispersion of Pd in H-ZSM-5. Journal of Catalysis, 1997, 172, 453-462. | 3.1 | 126 |
| 103 | Formation of an amorphous powder during the polymerization of ethylene in a radio-frequency discharge. Journal of Applied Polymer Science, 1973, 17, 885-892. | 1.3 | 124 |
| 104 | Raman studies of the structure of niobium oxide/titanium oxide (Nb2O5.TiO2). The Journal of Physical Chemistry, 1993, 97, 12178-12185. | 2.9 | 123 |
| 105 | p-Type Transparent Conducting Oxide/n-Type Semiconductor Heterojunctions for Efficient and Stable Solar Water Oxidation. Journal of the American Chemical Society, 2015, 137, 9595-9603. | 6.6 | 122 |
| 106 | Studies of CO desorption and reaction with H2 on alumina-supported Ru. Journal of Catalysis, 1979, 57, 397-405. | 3.1 | 121 |
| 107 | Identification of Hydroperoxy Species as Reaction Intermediates in the Electrochemical Evolution of Oxygen on Gold. ChemPhysChem, 2010, 11, 1854-1857. | 1.0 | 120 |
| 108 | Band-Gap Energy as a Descriptor of Catalytic Activity for Propene Oxidation over Mixed Metal Oxide Catalysts. Journal of the American Chemical Society, 2014, 136, 13684-13697. | 6.6 | 120 |

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| 109 | 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. | 16.1 | 120 |
| 110 | Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO<sub>2</sub> to CO. ACS Catalysis, 2019, 9, 4006-4014. | 5.5 | 119 |
| 111 | Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO<sub>2</sub> on Copper?. Journal of Physical Chemistry Letters, 2018, 9, 601-606. | 2.1 | 118 |
| 112 | Structural Characterization of Molybdenum Oxide Supported on Zirconia. Journal of Physical Chemistry B, 2000, 104, 10059-10068. | 1.2 | 116 |
| 113 | An in situ infrared study of NO reduction by C3H8 over Feâ€ZSMâ€5. Catalysis Letters, 1999, 63, 233-240. | 1.4 | 115 |
| 114 | Effects of Temperature on the Raman Spectra and Dispersed Oxides. Journal of Physical Chemistry B, 2001, 105, 5144-5152. | 1.2 | 115 |
| 115 | Ethane Oxidative Dehydrogenation Pathways on Vanadium Oxide Catalysts. Journal of Physical Chemistry B, 2002, 106, 5421-5427. | 1.2 | 114 |
| 116 | Role of Catalyst Preparation on the Electrocatalytic Activity of Ni<sub>1â€“x</sub>Fe<sub>x</sub>OOH for the Oxygen Evolution Reaction. Journal of Physical Chemistry C, 2015, 119, 18303-18316. | 1.5 | 114 |
| 117 | Water-Assisted Tetragonal-to-Monoclinic Phase Transformation of ZrO2at Low Temperatures. Chemistry of Materials, 2000, 12, 2442-2447. | 3.2 | 112 |
| 118 | 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. | 1.5 | 110 |
| 119 | Effects of composition and metal particle size on ethane dehydrogenation over PtxSn100â^'x/Mg(Al)O (70â©½xâ©½100). Journal of Catalysis, 2014, 311, 161-168. | 3.1 | 109 |
| 120 | Oxidative Dehydrogenation of Propane over Vanadiaâ€“Magnesia Catalysts Prepared by Thermolysis of OV(OtBu)3 in the Presence of Nanocrystalline MgO. Journal of Catalysis, 2002, 206, 49-59. | 3.1 | 108 |
| 121 | Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl<sub>3</sub>. Journal of the American Chemical Society, 2019, 141, 1614-1627. | 6.6 | 107 |
| 122 | Nitrous oxide decomposition and surface oxygen formation on Fe-ZSM-5. Journal of Catalysis, 2004, 224, 148-155. | 3.1 | 106 |
| 123 | Mechanistic Studies of the Hydroamination of Norbornene with Electrophilic Platinum Complexes: The Role of Proton Transfer. Journal of the American Chemical Society, 2008, 130, 16562-16571. | 6.6 | 106 |
| 124 | Are pressure fluctuation-based equilibrium methods really worse than nonequilibrium methods for calculating viscosities?. Journal of Chemical Physics, 2009, 131, 246101. | 1.2 | 105 |
| 125 | Highly Selective Condensation of Biomassâ€Derived Methyl Ketones as a Source of Aviation Fuel. ChemSusChem, 2015, 8, 1726-1736. | 3.6 | 105 |
| 126 | Mechanism and Site Requirements for Ethanol Oxidation on Vanadium Oxide Domains. Journal of Physical Chemistry C, 2009, 113, 2830-2836. | 1.5 | 104 |

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| 127 | Electrocatalytic CO2 Reduction to Fuels: Progress and Opportunities. Trends in Chemistry, 2020, 2, 825-836. | 4.4 | 104 |
| 128 | The effects of local structural relaxation on aluminum siting within H-ZSM-5. Catalysis Letters, 1991, 11, 209-217. | 1.4 | 103 |
| 129 | Local Spin Density Functional Theory Study of Copper Ion-Exchanged ZSM-5. The Journal of Physical Chemistry, 1996, 100, 4173-4179. | 2.9 | 103 |
| 130 | The effects of zirconia morphology on methanol synthesis from CO and H2 over Cu/ZrO2 catalystsPart II. Transient-response infrared studies. Journal of Catalysis, 2005, 233, 210-220. | 3.1 | 103 |
| 131 | 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. | 3.3 | 103 |
| 132 | Effects of Hydration and Dehydration on the Structure of Silica-Supported Vanadia Species. Langmuir, 2000, 16, 7162-7167. | 1.6 | 101 |
| 133 | Ptâ^'Ag Catalyst System for Hydroarylations with Unactivated Arenes and Olefins. Organometallics, 2004, 23, 4169-4171. | 1.1 | 101 |
| 134 | Biomass conversion to diesel via the etherification of furanyl alcohols catalyzed by Amberlyst-15. Journal of Catalysis, 2014, 313, 70-79. | 3.1 | 101 |
| 135 | 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, 7645-7649. | 3.3 | 101 |
| 136 | An infrared study of NO and CO adsorption on a silica-supported Ru catalyst. Journal of Catalysis, 1977, 49, 332-344. | 3.1 | 100 |
| 137 | Influence of ethylene on the hydrogenation of carbon monoxide over ruthenium. The Journal of Physical Chemistry, 1986, 90, 4797-4805. | 2.9 | 100 |
| 138 | NO Reduction by CH4in the Presence of O2over Pd-H-ZSM-5. Journal of Catalysis, 1999, 181, 189-204. | 3.1 | 100 |
| 139 | Density Functional Theory Study of Nitrous Oxide Decomposition over Fe- and Co-ZSM-5. Journal of Physical Chemistry B, 2002, 106, 7059-7064. | 1.2 | 100 |
| 140 | Alkali Effects on Molybdenum Oxide Catalysts for the Oxidative Dehydrogenation of Propane. Journal of Catalysis, 2000, 195, 244-252. | 3.1 | 98 |
| 141 | A Density Functional Theory Study of the Oxidation of Methanol to Formaldehyde over Vanadia Supported on Silica, Titania, and Zirconia. Journal of Physical Chemistry B, 2002, 106, 7832-7838. | 1.2 | 98 |
| 142 | Surface behaviour of reduced LaCoO3 as studied by TPD of CO, CO2 and H2 probes and by XPS. Applied Surface Science, 1988, 31, 301-316. | 3.1 | 97 |
| 143 | Al Next Nearest Neighbor, Ring Occupation, and Proximity Statistics in ZSM-5. Journal of Catalysis, 1999, 186, 222-227. | 3.1 | 97 |
| 144 | Synthesis and characterization of a new catalyst Pt/Mg(Ga)(Al)O for alkane dehydrogenation. Journal of Catalysis, 2010, 274, 192-199. | 3.1 | 97 |

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| 145 | High-resolution in situ and ex situ TEM studies on graphene formation and growth on Pt nanoparticles. Journal of Catalysis, 2012, 286, 22-29. | 3.1 | 97 |
| 146 | Oxidative Dehydrogenation of Propane over V2O5/MoO3/Al2O3and V2O5/Cr2O3/Al2O3:Â Structural Characterization and Catalytic Function. Journal of Physical Chemistry B, 2005, 109, 8987-9000. | 1.2 | 94 |
| 147 | Investigation of the dynamics of benzene in silicalite using Transition-State Theory. The Journal of Physical Chemistry, 1994, 98, 11948-11961. | 2.9 | 93 |
| 148 | A Study of the Mechanism and Kinetics of Cyclooctene Epoxidation Catalyzed by Iron(III) Tetrakispentafluorophenyl Porphyrin. Journal of the American Chemical Society, 2005, 127, 8635-8643. | 6.6 | 93 |
| 149 | Synthesis of dimethyl carbonate and dimethoxy methane over Cu-ZSM-5. Journal of Catalysis, 2006, 244, 219-229. | 3.1 | 93 |
| 150 | Decomposition and reduction of NO on transition metal surfaces: bond order conservation Morse potential analysis. Surface Science, 1993, 289, 127-138. | 0.8 | 92 |
| 151 | Isotopic Studies of Methane Oxidation Pathways on PdO Catalysts. Journal of Catalysis, 1999, 188, 132-139. | 3.1 | 92 |
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