

David J Willock

List of Publications by Year in descending order

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331
papers

29,804
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docs citations

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times ranked

20804
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| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | The Direct Synthesis of Hydrogen Peroxide Over Supported Pd-Based Catalysts: An Investigation into the Role of the Support and Secondary Metal Modifiers. <i>Catalysis Letters</i> , 2023, 153, 32-40. | 2.6 | 6 |
| 2 | Effect of the Preparation Method of LaSrCoFeO _x Perovskites on the Activity of N ₂ O Decomposition. <i>Catalysis Letters</i> , 2022, 152, 213-226. | 2.6 | 4 |
| 3 | Intramolecular modulation of iron-based metal organic framework with energy level adjusting for efficient photocatalytic activity. <i>Applied Catalysis B: Environmental</i> , 2022, 302, 120823. | 20.2 | 45 |
| 4 | Band gap engineering of amine functionalized Ag(I)-based coordination polymers and their plasmonic Ag ₀ coupled novel visible light driven photo-redox system for selective oxidation of benzyl alcohol. <i>Applied Catalysis B: Environmental</i> , 2022, 303, 120821. | 20.2 | 6 |
| 5 | Au-ZSM-5 catalyses the selective oxidation of CH ₄ to CH ₃ OH and CH ₃ COOH using O ₂ . <i>Nature Catalysis</i> , 2022, 5, 45-54. | 34.4 | 95 |
| 6 | Iron-chromium mixed metal oxides catalyse the oxidative dehydrogenation of propane using carbon dioxide. <i>Catalysis Communications</i> , 2022, 162, 106383. | 3.3 | 4 |
| 7 | Materials and Molecular Modeling at the Exascale. <i>Computing in Science and Engineering</i> , 2022, 24, 36-45. | 1.2 | 7 |
| 8 | The oxidative degradation of phenol <i>via in situ</i> H ₂ O ₂ synthesis using Pd supported Fe-modified ZSM-5 catalysts. <i>Catalysis Science and Technology</i> , 2022, 12, 2943-2953. | 4.1 | 7 |
| 9 | Heterogeneous Trimetallic Nanoparticles as Catalysts. <i>Chemical Reviews</i> , 2022, 122, 6795-6849. | 47.7 | 61 |
| 10 | Selective oxidation of methane to methanol and methyl hydroperoxide over palladium modified MoO ₃ photocatalyst under ambient conditions. <i>Catalysis Science and Technology</i> , 2022, 12, 3727-3736. | 4.1 | 9 |
| 11 | The direct synthesis of hydrogen peroxide over Au and Pd nanoparticles: A DFT study. <i>Catalysis Today</i> , 2021, 381, 76-85. | 4.4 | 11 |
| 12 | The Influence of Reaction Conditions on the Oxidation of Cyclohexane via the In-Situ Production of H ₂ O ₂ . <i>Catalysis Letters</i> , 2021, 151, 164-171. | 2.6 | 16 |
| 13 | A combined periodic DFT and QM/MM approach to understand the radical mechanism of the catalytic production of methanol from glycerol. <i>Faraday Discussions</i> , 2021, 229, 108-130. | 3.2 | 5 |
| 14 | The interaction of CO with a copper(ii) chloride oxy-chlorination catalyst. <i>Faraday Discussions</i> , 2021, 229, 318-340. | 3.2 | 2 |
| 15 | Theory: general discussion. <i>Faraday Discussions</i> , 2021, 229, 131-160. | 3.2 | 0 |
| 16 | Controlled reduction of aromaticity of alkylated polyaromatic compounds by selective oxidation using H ₂ WO ₄ , H ₃ PO ₄ and H ₂ O ₂ : a route for upgrading heavy oil fractions. <i>New Journal of Chemistry</i> , 2021, 45, 13885-13892. | 2.8 | 1 |
| 17 | Gas Phase Glycerol Valorization over Ceria Nanostructures with Well-Defined Morphologies. <i>ACS Catalysis</i> , 2021, 11, 4893-4907. | 11.2 | 13 |
| 18 | Combination of Cu/ZnO Methanol Synthesis Catalysts and ZSM-5 Zeolites to Produce Oxygenates from CO ₂ and H ₂ . <i>Topics in Catalysis</i> , 2021, 64, 965-973. | 2.8 | 6 |

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|----|---|------|-----------|
| 19 | Methane Oxidation to Methanol in Water. <i>Accounts of Chemical Research</i> , 2021, 54, 2614-2623. | 15.6 | 69 |
| 20 | Density Functional Theory Study of the Partial Oxidation of Methane to Methanol on Au and Pd Surfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18770-18785. | 3.1 | 2 |
| 21 | A Perspective on Heterogeneous Catalysts for the Selective Oxidation of Alcohols. <i>Chemistry - A European Journal</i> , 2021, 27, 16809-16833. | 3.3 | 45 |
| 22 | Lanthanum modified Fe-ZSM-5 zeolites for selective methane oxidation with H_2O . <i>Catalysis Science and Technology</i> , 2021, 11, 8052-8064. | 4.1 | 11 |
| 23 | Direct and oxidative dehydrogenation of propane: from catalyst design to industrial application. <i>Green Chemistry</i> , 2021, 23, 9747-9799. | 9.0 | 66 |
| 24 | Low temperature selective oxidation of methane using gold-palladium colloids. <i>Catalysis Today</i> , 2020, 342, 32-38. | 4.4 | 38 |
| 25 | Low temperature solvent-free allylic oxidation of cyclohexene using graphitic oxide catalysts. <i>Catalysis Today</i> , 2020, 357, 3-7. | 4.4 | 8 |
| 26 | Sustainable production of glucaric acid from corn stover via glucose oxidation: An assessment of homogeneous and heterogeneous catalytic oxidation production routes. <i>Chemical Engineering Research and Design</i> , 2020, 153, 337-349. | 5.6 | 23 |
| 27 | Gold-palladium colloids as catalysts for hydrogen peroxide synthesis, degradation and methane oxidation: effect of the PVP stabiliser. <i>Catalysis Science and Technology</i> , 2020, 10, 5935-5944. | 4.1 | 21 |
| 28 | CO_2 Hydrogenation to CH_3OH over PdZn Catalysts, with Reduced CH_4 Production. <i>ChemCatChem</i> , 2020, 12, 6024-6032. | 3.7 | 16 |
| 29 | Probing composition distributions in nanoalloy catalysts with correlative electron microscopy. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15725-15733. | 10.3 | 4 |
| 30 | Role of the Support in Gold-Containing Nanoparticles as Heterogeneous Catalysts. <i>Chemical Reviews</i> , 2020, 120, 3890-3938. | 47.7 | 275 |
| 31 | DFT-Assisted Spectroscopic Studies on the Coordination of Small Ligands to Palladium: From Isolated Ions to Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4781-4790. | 3.1 | 4 |
| 32 | Lowering the Operating Temperature of Perovskite Catalysts for N_2O Decomposition through Control of Preparation Methods. <i>ACS Catalysis</i> , 2020, 10, 5430-5442. | 11.2 | 31 |
| 33 | The formation of methanol from glycerol bio-waste over doped ceria-based catalysts. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2020, 378, 20200059. | 3.4 | 2 |
| 34 | Electron Microscopy Informed Catalyst Design. <i>Microscopy and Microanalysis</i> , 2019, 25, 2282-2283. | 0.4 | 0 |
| 35 | Photoactive Ag(I)-Based Coordination Polymer as a Potential Semiconductor for Photocatalytic Water Splitting and Environmental Remediation: Experimental and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23940-23950. | 3.1 | 12 |
| 36 | The hydrogenation of levulinic acid to $\hat{3}$ -valerolactone over Cu-ZrO ₂ catalysts prepared by a pH-gradient methodology. <i>Journal of Energy Chemistry</i> , 2019, 36, 15-24. | 12.9 | 30 |

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|----|---|------|-----------|
| 37 | The Direct Synthesis of H ₂ O ₂ and Selective Oxidation of Methane to Methanol Using HZSM-5 Supported AuPd Catalysts. <i>Catalysis Letters</i> , 2019, 149, 3066-3075. | 2.6 | 30 |
| 38 | Investigating the Influence of Reaction Conditions and the Properties of Ceria for the Valorisation of Glycerol. <i>Energies</i> , 2019, 12, 1359. | 3.1 | 10 |
| 39 | New insights for the valorisation of glycerol over MgO catalysts in the gas-phase. <i>Catalysis Science and Technology</i> , 2019, 9, 1464-1475. | 4.1 | 12 |
| 40 | The Direct Synthesis of H ₂ O ₂ Using TS-1 Supported Catalysts. <i>ChemCatChem</i> , 2019, 11, 1673-1680. | 3.7 | 42 |
| 41 | The Key Role of Nanocasting in Gold-based Fe ₂ O ₃ Nanocasted Catalysts for Oxygen Activation at the Metal-support Interface. <i>ChemCatChem</i> , 2019, 11, 1915-1927. | 3.7 | 13 |
| 42 | The Effects of Dopants on the Cu-ZrO ₂ Catalyzed Hydrogenation of Levulinic Acid. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7879-7888. | 3.1 | 21 |
| 43 | Recent Advances in the Direct Synthesis of H ₂ O ₂ . <i>ChemCatChem</i> , 2019, 11, 298-308. | 3.7 | 156 |
| 44 | Solvent-free aerobic epoxidation of 1-decene using supported cobalt catalysts. <i>Catalysis Today</i> , 2019, 333, 154-160. | 4.4 | 11 |
| 45 | Low-Temperature Catalytic Selective Oxidation of Methane to Methanol. <i>Green Chemistry and Sustainable Technology</i> , 2019, , 37-59. | 0.7 | 3 |
| 46 | Ni-Cu-ZrO ₂ catalysts for the hydrogenation of levulinic acid to gamma valorlactone. <i>Journal of Lithic Studies</i> , 2018, 4, 12-23. | 0.5 | 9 |
| 47 | The Role of Mg(OH) ₂ in the So-called "Base-Free" Oxidation of Glycerol with AuPd Catalysts. <i>Chemistry - A European Journal</i> , 2018, 24, 2396-2402. | 3.3 | 23 |
| 48 | Structural behaviour of copper chloride catalysts during the chlorination of CO to phosgene. <i>Faraday Discussions</i> , 2018, 208, 67-85. | 3.2 | 3 |
| 49 | Selective Hydrogenation of Levulinic Acid Using Ru/C Catalysts Prepared by Sol-Immobilisation. <i>Topics in Catalysis</i> , 2018, 61, 833-843. | 2.8 | 21 |
| 50 | Selective Oxidation of Methane to Methanol Using Supported AuPd Catalysts Prepared by Stabilizer-Free Sol-Immobilization. <i>ACS Catalysis</i> , 2018, 8, 2567-2576. | 11.2 | 99 |
| 51 | The electronic properties of Au clusters on CeO ₂ (110) surface with and without O-defects. <i>Faraday Discussions</i> , 2018, 208, 123-145. | 3.2 | 12 |
| 52 | A Kinetic Study of Methane Partial Oxidation over Fe-ZSM-5 Using N ₂ O as an Oxidant. <i>ChemPhysChem</i> , 2018, 19, 402-411. | 2.1 | 31 |
| 53 | Homocoupling of Phenylboronic Acid using Atomically Dispersed Gold on Carbon Catalysts: Catalyst Evolution Before Reaction. <i>ChemCatChem</i> , 2018, 10, 1853-1859. | 3.7 | 15 |
| 54 | Elucidating the Role of CO ₂ in the Soft Oxidative Dehydrogenation of Propane over Ceria-Based Catalysts. <i>ACS Catalysis</i> , 2018, 8, 3454-3468. | 11.2 | 80 |

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|----|--|------|-----------|
| 55 | Investigating the influence of acid sites in continuous methane oxidation with N ₂ O over Fe/MFI zeolites. <i>Catalysis Science and Technology</i> , 2018, 8, 154-163. | 4.1 | 32 |
| 56 | The Role of Copper Speciation in the Low Temperature Oxidative Upgrading of Short Chain Alkanes over Cu/ZSM-5 Catalysts. <i>ChemPhysChem</i> , 2018, 19, 469-478. | 2.1 | 22 |
| 57 | Oxidation of Polynuclear Aromatic Hydrocarbons using Ruthenium-Catalyzed Oxidation: The Role of Aromatic Ring Number in Reaction Kinetics and Product Distribution. <i>Chemistry - A European Journal</i> , 2018, 24, 655-662. | 3.3 | 9 |
| 58 | Recent Advances in the Gold-Catalysed Low-Temperature Water-Gas Shift Reaction. <i>Catalysts</i> , 2018, 8, 627. | 3.5 | 28 |
| 59 | Zinc promoted alumina catalysts for the fluorination of chlorofluorocarbons. <i>Journal of Catalysis</i> , 2018, 364, 102-111. | 6.2 | 12 |
| 60 | A DFT mechanistic study of the ODH of n-hexane over isolated H ₃ VO ₄ . <i>Molecular Catalysis</i> , 2018, 452, 83-92. | 2.0 | 4 |
| 61 | Mechanistic Insights into Selective Oxidation of Polyaromatic Compounds using RICO Chemistry. <i>Chemistry - A European Journal</i> , 2018, 24, 12359-12369. | 3.3 | 7 |
| 62 | Gold as a Catalyst for the Ring Opening of 2,5-Dimethylfuran. <i>Catalysis Letters</i> , 2018, 148, 2109-2116. | 2.6 | 3 |
| 63 | Investigating the Influence of Fe Speciation on N ₂ O Decomposition Over Fe-ZSM-5 Catalysts. <i>Topics in Catalysis</i> , 2018, 61, 1983-1992. | 2.8 | 18 |
| 64 | Theory as a driving force to understand reactions on nanoparticles: general discussion. <i>Faraday Discussions</i> , 2018, 208, 147-185. | 3.2 | 3 |
| 65 | Application of new nanoparticle structures as catalysts: general discussion. <i>Faraday Discussions</i> , 2018, 208, 575-593. | 3.2 | 1 |
| 66 | The challenges of characterising nanoparticulate catalysts: general discussion. <i>Faraday Discussions</i> , 2018, 208, 339-394. | 3.2 | 5 |
| 67 | The effect of ring size on the selective carboxylation of cycloalkene oxides. <i>Catalysis Science and Technology</i> , 2017, 7, 1433-1439. | 4.1 | 2 |
| 68 | Addressing stability challenges of using bimetallic electrocatalysts: the case of gold-palladium nanoalloys. <i>Catalysis Science and Technology</i> , 2017, 7, 1848-1856. | 4.1 | 35 |
| 69 | Highly Active Gold and Gold-Palladium Catalysts Prepared by Colloidal Methods in the Absence of Polymer Stabilizers. <i>ChemCatChem</i> , 2017, 9, 2914-2918. | 3.7 | 17 |
| 70 | Identification of single-site gold catalysis in acetylene hydrochlorination. <i>Science</i> , 2017, 355, 1399-1403. | 12.6 | 380 |
| 71 | The adsorption of Cu on the CeO ₂ (110) surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27191-27203. | 2.8 | 17 |
| 72 | Aqueous Au-Pd colloids catalyze selective CH ₄ oxidation to CH ₃ OH with O ₂ under mild conditions. <i>Science</i> , 2017, 358, 223-227. | 12.6 | 478 |

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|----|---|------|-----------|
| 73 | The controlled catalytic oxidation of furfural to furoic acid using AuPd/Mg(OH) ₂ . Catalysis Science and Technology, 2017, 7, 5284-5293. | 4.1 | 87 |
| 74 | Identification of the catalytically active component of Cuâ€Zrâ€O catalyst for the hydrogenation of levulinic acid to Î³-valerolactone. Green Chemistry, 2017, 19, 225-236. | 9.0 | 68 |
| 75 | The Lowâ€Temperature Oxidation of Propane by using H ₂ O ₂ and Fe/ZSMâ€5 Catalysts: Insights into the Active Site and Enhancement of Catalytic Turnover Frequencies. ChemCatChem, 2017, 9, 642-650. | 3.7 | 16 |
| 76 | Density functional theory studies of the uncatalysed gas-phase oxidative dehydrogenation conversion of n-hexane to hexenes. Computational and Theoretical Chemistry, 2017, 1114, 153-164. | 2.5 | 10 |
| 77 | An Overview of Recent Advances of the Catalytic Selective Oxidation of Ethane to Oxygenates. Catalysts, 2016, 6, 71. | 3.5 | 24 |
| 78 | Explicit Detection of the Mechanism of Platinum Nanoparticle Shape Control by Polyvinylpyrrolidone. Journal of Physical Chemistry C, 2016, 120, 7532-7542. | 3.1 | 36 |
| 79 | Methane Activation by Selective Oxidation. Topics in Catalysis, 2016, 59, 658-662. | 2.8 | 43 |
| 80 | The conversion of levulinic acid into Î³-valerolactone using Cuâ€ZrO ₂ catalysts. Catalysis Science and Technology, 2016, 6, 6022-6030. | 4.1 | 40 |
| 81 | The partial oxidation of propane under mild aqueous conditions with H ₂ O ₂ and ZSM-5 catalysts. Catalysis Science and Technology, 2016, 6, 7521-7531. | 4.1 | 12 |
| 82 | Gas phase stabiliser-free production of hydrogen peroxide using supported goldâ€palladium catalysts. Chemical Science, 2016, 7, 5833-5837. | 7.4 | 16 |
| 83 | Tuning graphitic oxide for initiator- and metal-free aerobic epoxidation of linear alkenes. Nature Communications, 2016, 7, 12855. | 12.8 | 18 |
| 84 | Population and hierarchy of active species in gold iron oxide catalysts for carbon monoxide oxidation. Nature Communications, 2016, 7, 12905. | 12.8 | 62 |
| 85 | Designing new catalysts: synthesis of new active structures: general discussion. Faraday Discussions, 2016, 188, 131-159. | 3.2 | 4 |
| 86 | Catalyst design from theory to practice: general discussion. Faraday Discussions, 2016, 188, 279-307. | 3.2 | 2 |
| 87 | Bridging model and real catalysts: general discussion. Faraday Discussions, 2016, 188, 565-589. | 3.2 | 3 |
| 88 | Characterisation of gold catalysts. Chemical Society Reviews, 2016, 45, 4953-4994. | 38.1 | 140 |
| 89 | Stable amorphous georgeite as a precursor to a high-activity catalyst. Nature, 2016, 531, 83-87. | 27.8 | 128 |
| 90 | Structure Sensitivity in Catalytic Hydrogenation at Platinum Surfaces Measured by Shell-Isolated Nanoparticle Enhanced Raman Spectroscopy (SHINERS). ACS Catalysis, 2016, 6, 1822-1832. | 11.2 | 60 |

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|-----|--|------|-----------|
| 91 | Depressing the hydrogenation and decomposition reaction in H ₂ O ₂ synthesis by supporting AuPd on oxygen functionalized carbon nanofibers. <i>Catalysis Science and Technology</i> , 2016, 6, 694-697. | 4.1 | 20 |
| 92 | Low temperature selective oxidation of methane to methanol using titania supported gold palladium copper catalysts. <i>Catalysis Science and Technology</i> , 2016, 6, 3410-3418. | 4.1 | 64 |
| 93 | Continuous selective oxidation of methane to methanol over Cu- and Fe-modified ZSM-5 catalysts in a flow reactor. <i>Catalysis Today</i> , 2016, 270, 93-100. | 4.4 | 113 |
| 94 | Base-free oxidation of glucose to gluconic acid using supported gold catalysts. <i>Catalysis Science and Technology</i> , 2016, 6, 107-117. | 4.1 | 53 |
| 95 | CO adsorption over Pd nanoparticles: A general framework for IR simulations on nanoparticles. <i>Surface Science</i> , 2016, 646, 210-220. | 1.9 | 65 |
| 96 | Co-oxidation of octane and benzaldehyde using molecular oxygen with Au-Pd/carbon prepared by sol-immobilisation. <i>Catalysis Science and Technology</i> , 2015, 5, 3953-3959. | 4.1 | 3 |
| 97 | Selective Oxidation of Alkyl-Substituted Polyaromatics Using Ruthenium-Ion-Catalyzed Oxidation. <i>Chemistry - A European Journal</i> , 2015, 21, 4285-4293. | 3.3 | 8 |
| 98 | Selective Oxidation of Alkyl-Substituted Polyaromatics Using Ruthenium-Ion-Catalyzed Oxidation. <i>Chemistry - A European Journal</i> , 2015, 21, 4169-4169. | 3.3 | 0 |
| 99 | Discovery, Development, and Commercialization of Gold Catalysts for Acetylene Hydrochlorination. <i>Journal of the American Chemical Society</i> , 2015, 137, 14548-14557. | 13.7 | 283 |
| 100 | Solvent-free oxidation of dec-1-ene using gold/graphite catalyst using an in situ generated oxidant. <i>Catalysis Science and Technology</i> , 2015, 5, 1307-1313. | 4.1 | 3 |
| 101 | The functionalisation of graphite surfaces with nitric acid: Identification of functional groups and their effects on gold deposition. <i>Journal of Catalysis</i> , 2015, 323, 10-18. | 6.2 | 59 |
| 102 | Solvent-Free Aerobic Epoxidation of Dec-1-ene Using Gold/Graphite as a Catalyst. <i>Catalysis Letters</i> , 2015, 145, 689-696. | 2.6 | 16 |
| 103 | Ruthenium Nanoparticles Supported on Carbon: An Active Catalyst for the Hydrogenation of Lactic Acid to 1,2-Propanediol. <i>ACS Catalysis</i> , 2015, 5, 5047-5059. | 11.2 | 91 |
| 104 | Low temperature catalytic partial oxidation of ethane to oxygenates by Fe and Cu-ZSM-5 in a continuous flow reactor. <i>Journal of Catalysis</i> , 2015, 330, 84-92. | 6.2 | 24 |
| 105 | Liquid phase oxidation of cyclohexane using bimetallic Au-Pd/MgO catalysts. <i>Applied Catalysis A: General</i> , 2015, 504, 373-380. | 4.3 | 45 |
| 106 | A density functional study of oxygen vacancy formation on $\hat{\Gamma}$ -Fe ₂ O ₃ (0001) surface and the effect of supported Au nanoparticles. <i>Research on Chemical Intermediates</i> , 2015, 41, 9587-9601. | 2.7 | 20 |
| 107 | Efficient green methanol synthesis from glycerol. <i>Nature Chemistry</i> , 2015, 7, 1028-1032. | 13.6 | 106 |
| 108 | Epoxidation of Propene with Graphite AuPd-Supported Nanoparticles. <i>Catalysis Letters</i> , 2015, 145, 697-701. | 2.6 | 4 |

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|-----|---|------|-----------|
| 109 | Gold Catalysis: A Reflection on Where We are Now. <i>Catalysis Letters</i> , 2015, 145, 71-79. | 2.6 | 56 |
| 110 | Advances in the direct synthesis of hydrogen peroxide from hydrogen and oxygen. <i>Catalysis Today</i> , 2015, 248, 3-9. | 4.4 | 189 |
| 111 | Tailoring the selectivity of glycerol oxidation by tuning the acid-base properties of Au catalysts. <i>Catalysis Science and Technology</i> , 2015, 5, 1126-1132. | 4.1 | 78 |
| 112 | Modelling analysis of the structure and porosity of covalent triazine-based frameworks. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 817-823. | 2.8 | 15 |
| 113 | The adsorption of ethene on Fe(111) and surface carbide formation. <i>Catalysis Today</i> , 2015, 244, 122-129. | 4.4 | 9 |
| 114 | Base-free glucose oxidation using air with supported gold catalysts. <i>Green Chemistry</i> , 2014, 16, 3132-3141. | 9.0 | 71 |
| 115 | Novel radical tandem 1,6-enynes thioacylation/cyclization: Au-Pd nanoparticles catalysis versus thermal activation as a function of the substrate specificity. <i>Tetrahedron</i> , 2014, 70, 9635-9643. | 1.9 | 7 |
| 116 | Spectroscopic and atomic force studies of the functionalisation of carbon surfaces: new insights into the role of the surface topography and specific chemical states. <i>Faraday Discussions</i> , 2014, 173, 257-272. | 3.2 | 18 |
| 117 | Gold-Based Nanoparticulate Catalysts for the Oxidative Esterification of 1,4-Butanediol to Dimethyl Succinate. <i>Topics in Catalysis</i> , 2014, 57, 723-729. | 2.8 | 5 |
| 118 | The adsorption and dissociation of CO on Fe(111). <i>Surface Science</i> , 2014, 625, 69-83. | 1.9 | 10 |
| 119 | The Effect of Grafting Zirconia and Ceria onto Alumina as a Support for Silicotungstic Acid for the Catalytic Dehydration of Glycerol to Acrolein. <i>Chemistry - A European Journal</i> , 2014, 20, 1743-1752. | 3.3 | 36 |
| 120 | Strategies for Designing Supported Gold-Palladium Bimetallic Catalysts for the Direct Synthesis of Hydrogen Peroxide. <i>Accounts of Chemical Research</i> , 2014, 47, 845-854. | 15.6 | 179 |
| 121 | High Activity Redox Catalysts Synthesized by Chemical Vapor Impregnation. <i>ACS Nano</i> , 2014, 8, 957-969. | 14.6 | 25 |
| 122 | Initiator-free hydrocarbon oxidation using supported gold nanoparticles. <i>Catalysis Science and Technology</i> , 2014, 4, 908-911. | 4.1 | 24 |
| 123 | Deactivation studies of a carbon supported AuPt nanoparticulate catalyst in the liquid-phase aerobic oxidation of 1,2-propanediol. <i>Catalysis Science and Technology</i> , 2014, 4, 1313-1322. | 4.1 | 34 |
| 124 | All-atom molecular dynamics simulation of HPMA polymers. <i>RSC Advances</i> , 2014, 4, 7003. | 3.6 | 3 |
| 125 | Light alkane oxidation using catalysts prepared by chemical vapour impregnation: tuning alcohol selectivity through catalyst pre-treatment. <i>Chemical Science</i> , 2014, 5, 3603-3616. | 7.4 | 45 |
| 126 | Catalysis using colloidal-supported gold-based nanoparticles. <i>Applied Petrochemical Research</i> , 2014, 4, 85-94. | 1.3 | 13 |

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|-----|---|------|-----------|
| 127 | Base-Free Oxidation of Glycerol Using Titania-Supported Trimetallic Au-Pd-Pt Nanoparticles. <i>ChemSusChem</i> , 2014, 7, 1326-1334. | 6.8 | 73 |
| 128 | Impact of co-adsorbed oxygen on crotonaldehyde adsorption over gold nanoclusters: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11202-11210. | 2.8 | 3 |
| 129 | Heterogeneously catalyzed oxidation of butanediols in base free aqueous media. <i>Tetrahedron</i> , 2014, 70, 6055-6058. | 1.9 | 14 |
| 130 | Gas Diffusion in a Porous Organic Cage: Analysis of Dynamic Pore Connectivity Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12734-12743. | 3.1 | 43 |
| 131 | Strategies for the Synthesis of Supported Gold Palladium Nanoparticles with Controlled Morphology and Composition. <i>Accounts of Chemical Research</i> , 2013, 46, 1759-1772. | 15.6 | 167 |
| 132 | Partial Oxidation of Ethane to Oxygenates Using Fe- and Cu-Containing ZSM-5. <i>Journal of the American Chemical Society</i> , 2013, 135, 11087-11099. | 13.7 | 83 |
| 133 | Systematic Study of the Oxidation of Methane Using Supported Gold Palladium Nanoparticles Under Mild Aqueous Conditions. <i>Topics in Catalysis</i> , 2013, 56, 1843-1857. | 2.8 | 35 |
| 134 | Selective catalytic oxidation using supported gold-platinum and palladium-platinum nanoalloys prepared by sol-immobilisation. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10636. | 2.8 | 37 |
| 135 | In situ spectroscopic investigation of oxidative dehydrogenation and disproportionation of benzyl alcohol. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12147. | 2.8 | 43 |
| 136 | Aqua regia activated Au/C catalysts for the hydrochlorination of acetylene. <i>Journal of Catalysis</i> , 2013, 297, 128-136. | 6.2 | 139 |
| 137 | Effect of heat treatment on Au-Pd catalysts synthesized by sol immobilisation for the direct synthesis of hydrogen peroxide and benzyl alcohol oxidation. <i>Catalysis Science and Technology</i> , 2013, 3, 308-317. | 4.1 | 64 |
| 138 | Oxidation of Methane to Methanol with Hydrogen Peroxide Using Supported Gold-Palladium Alloy Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 1280-1284. | 13.8 | 239 |
| 139 | Elucidation and Evolution of the Active Component within Cu/Fe/ZSM-5 for Catalytic Methane Oxidation: From Synthesis to Catalysis. <i>ACS Catalysis</i> , 2013, 3, 689-699. | 11.2 | 117 |
| 140 | The selective oxidation of 1,2-propanediol to lactic acid using mild conditions and gold-based nanoparticulate catalysts. <i>Catalysis Today</i> , 2013, 203, 139-145. | 4.4 | 58 |
| 141 | Effect of Reaction Conditions on the Direct Synthesis of Hydrogen Peroxide with a AuPd/TiO ₂ Catalyst in a Flow Reactor. <i>ACS Catalysis</i> , 2013, 3, 487-501. | 11.2 | 93 |
| 142 | The effect of ring size on the selective oxidation of cycloalkenes using supported metal catalysts. <i>Catalysis Science and Technology</i> , 2013, 3, 1531. | 4.1 | 18 |
| 143 | Switching-off toluene formation in the solvent-free oxidation of benzyl alcohol using supported trimetallic Au-Pd-Pt nanoparticles. <i>Faraday Discussions</i> , 2013, 162, 365. | 3.2 | 65 |
| 144 | Towards heterogeneous organocatalysis: chiral iminium cations supported on porous materials for enantioselective alkene epoxidation. <i>Catalysis Science and Technology</i> , 2013, 3, 2330. | 4.1 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 145 | Aqueous-Phase Methane Oxidation over Fe-MFI Zeolites; Promotion through Isomorphous Framework Substitution. <i>ACS Catalysis</i> , 2013, 3, 1835-1844. | 11.2 | 99 |
| 146 | Solvent Effect and Reactivity Trend in the Aerobic Oxidation of 1,3-Propanediols over Gold Supported on Titania: NMR Diffusion and Relaxation Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 11725-11732. | 3.3 | 46 |
| 147 | The Selective Oxidation of 1,2-Propanediol by Supported Gold-Based Nanoparticulate Catalysts. <i>Topics in Catalysis</i> , 2012, 55, 1283-1288. | 2.8 | 33 |
| 148 | Catalytic and Mechanistic Insights of the Low-Temperature Selective Oxidation of Methane over Cu-Promoted Fe-ZSM-5. <i>Chemistry - A European Journal</i> , 2012, 18, 15735-15745. | 3.3 | 102 |
| 149 | Oxidative Esterification of Homologous 1,3-Propanediols. <i>Catalysis Letters</i> , 2012, 142, 1114-1120. | 2.6 | 15 |
| 150 | Oxidative esterification of 1,2-propanediol using gold and gold-palladium supported nanoparticles. <i>Catalysis Science and Technology</i> , 2012, 2, 97-104. | 4.1 | 32 |
| 151 | Physical mixing of metal acetates: a simple, scalable method to produce active chloride free bimetallic catalysts. <i>Chemical Science</i> , 2012, 3, 2965. | 7.4 | 38 |
| 152 | Gold, palladium and gold-palladium supported nanoparticles for the synthesis of glycerol carbonate from glycerol and urea. <i>Catalysis Science and Technology</i> , 2012, 2, 1914. | 4.1 | 52 |
| 153 | The effect of intermolecular hydrogen bonding on the planarity of amides. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11944. | 2.8 | 22 |
| 154 | Influence of counterions on the structure of bis(oxazoline)copper(ii) complexes; an EPR and ENDOR investigation. <i>Dalton Transactions</i> , 2012, 41, 11085. | 3.3 | 14 |
| 155 | Selective liquid phase oxidation with supported metal nanoparticles. <i>Chemical Science</i> , 2012, 3, 20-44. | 7.4 | 224 |
| 156 | Influence of reaction conditions on the direct synthesis of hydrogen peroxide over AuPd/carbon catalysts. <i>Catalysis Science and Technology</i> , 2012, 2, 1908. | 4.1 | 23 |
| 157 | Bespoke Force Field for Simulating the Molecular Dynamics of Porous Organic Cages. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16639-16651. | 3.1 | 40 |
| 158 | Direct Catalytic Conversion of Methane to Methanol in an Aqueous Medium by using Copper-Promoted Fe-ZSM-5. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5129-5133. | 13.8 | 492 |
| 159 | Involvement of Surface-Bound Radicals in the Oxidation of Toluene Using Supported Au-Pd Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5981-5985. | 13.8 | 89 |
| 160 | Rubidium- and caesium-doped silicotungstic acid catalysts supported on alumina for the catalytic dehydration of glycerol to acrolein. <i>Journal of Catalysis</i> , 2012, 286, 206-213. | 6.2 | 106 |
| 161 | A periodic DFT study of the activation of O ₂ by Au nanoparticles on γ -Fe ₂ O ₃ . <i>Faraday Discussions</i> , 2011, 152, 135. | 3.2 | 30 |
| 162 | Visualizing Diastereomeric Interactions of Chiral Amine-Chiral Copper Salen Adducts by EPR Spectroscopy and DFT. <i>Inorganic Chemistry</i> , 2011, 50, 6944-6955. | 4.0 | 20 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 163 | Solvent-free selective epoxidation of cyclooctene using supported gold catalysts: an investigation of catalyst re-use. <i>Green Chemistry</i> , 2011, 13, 127-134. | 9.0 | 55 |
| 164 | On the enantioselectivity of aziridination of styrene catalysed by copper triflate and copper-exchanged zeolite Y: consequences of the phase behaviour of enantiomeric mixtures of N-arene-sulfonyl-2-phenylaziridines. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 1079-1084. | 2.8 | 16 |
| 165 | Pulsed-Field Gradient NMR Spectroscopic Studies of Alcohols in Supported Gold Catalysts. <i>Journal of Physical Chemistry C</i> , 2011, 115, 1073-1079. | 3.1 | 35 |
| 166 | Selective oxidation of alkenes using graphite-supported gold-palladium catalysts. <i>Catalysis Science and Technology</i> , 2011, 1, 747. | 4.1 | 28 |
| 167 | Enantioselective Hydrogenation of α -Ketoesters: An in Situ Surface-Enhanced Raman Spectroscopy (SERS) Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 21363-21372. | 3.1 | 9 |
| 168 | Facile removal of stabilizer-ligands from supported gold nanoparticles. <i>Nature Chemistry</i> , 2011, 3, 551-556. | 13.6 | 517 |
| 169 | Solvent-Free Oxidation of Primary Carbon-Hydrogen Bonds in Toluene Using Au-Pd Alloy Nanoparticles. <i>Science</i> , 2011, 331, 195-199. | 12.6 | 708 |
| 170 | CO bond cleavage on supported nano-gold during low temperature oxidation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2528-2538. | 2.8 | 28 |
| 171 | On-Off Porosity Switching in a Molecular Organic Solid. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 749-753. | 13.8 | 176 |
| 172 | Cover Picture: On-Off Porosity Switching in a Molecular Organic Solid (<i>Angew. Chem. Int. Ed.</i> 3/2011). <i>Angewandte Chemie - International Edition</i> , 2011, 50, 555-555. | 13.8 | 0 |
| 173 | Selective Oxidation of Glycerol by Highly Active Bimetallic Catalysts at Ambient Temperature under Base-Free Conditions. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10136-10139. | 13.8 | 212 |
| 174 | Controlling the Duality of the Mechanism in Liquid-Phase Oxidation of Benzyl Alcohol Catalysed by Supported Au-Pd Nanoparticles. <i>Chemistry - A European Journal</i> , 2011, 17, 6524-6532. | 3.3 | 100 |
| 175 | Oxidation of benzyl alcohol using supported gold-palladium nanoparticles. <i>Catalysis Today</i> , 2011, 163, 47-54. | 4.4 | 73 |
| 176 | The decomposition of H_2O_2 over the components of Au/TiO ₂ catalysts. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 1885-1899. | 2.1 | 35 |
| 177 | Probing the role of weak outer sphere interactions (H-bonds) in VO(3,5-tBu ₂ -salophen) epoxide adducts by EPR, ENDOR and HYSCORE. <i>Chemical Physics Letters</i> , 2010, 486, 74-79. | 2.6 | 9 |
| 178 | Explaining the phase behaviour of the pharmaceutically relevant polymers poly(ethylene glycol) and poly(vinyl pyrrolidone) in semi-fluorinated liquids. <i>Journal of Pharmacy and Pharmacology</i> , 2010, 57, 973-980. | 2.4 | 13 |
| 179 | Direct Synthesis of Hydrogen Peroxide and Benzyl Alcohol Oxidation Using Au-Pd Catalysts Prepared by Sol Immobilization. <i>Langmuir</i> , 2010, 26, 16568-16577. | 3.5 | 201 |
| 180 | The effect of catalyst preparation method on the performance of supported Au-Pd catalysts for the direct synthesis of hydrogen peroxide. <i>Green Chemistry</i> , 2010, 12, 915. | 9.0 | 63 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 181 | Effect of the reaction conditions on the performance of Au@Pd/TiO ₂ catalyst for the direct synthesis of hydrogen peroxide. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2488. | 2.8 | 58 |
| 182 | Effect of Halide and Acid Additives on the Direct Synthesis of Hydrogen Peroxide using Supported Gold@Palladium Catalysts. <i>ChemSusChem</i> , 2009, 2, 575-580. | 6.8 | 68 |
| 183 | Direct Synthesis of H ₂ O ₂ from H ₂ and O ₂ over Gold, Palladium, and Gold@Palladium Catalysts Supported on Acid-Pre-treated TiO ₂ . <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8512-8515. | 13.8 | 210 |
| 184 | In situ X-ray studies of crotyl alcohol selective oxidation over Au/Pd(111) surface alloys. <i>Catalysis Today</i> , 2009, 145, 251-257. | 4.4 | 38 |
| 185 | Switching Off Hydrogen Peroxide Hydrogenation in the Direct Synthesis Process. <i>Science</i> , 2009, 323, 1037-1041. | 12.6 | 759 |
| 186 | Solvent-free oxidation of benzyl alcohol using Au@Pd catalysts prepared by sol immobilisation. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5142. | 2.8 | 138 |
| 187 | Selective formation of lactate by oxidation of 1,2-propanediol using gold palladium alloy supported nanocrystals. <i>Green Chemistry</i> , 2009, 11, 1209. | 9.0 | 97 |
| 188 | Oxidation of glycerol using gold@palladium alloy-supported nanocrystals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4952. | 2.8 | 144 |
| 189 | Solvent-free selective epoxidation of cyclooctene using supported gold catalysts. <i>Green Chemistry</i> , 2009, 11, 1037. | 9.0 | 61 |
| 190 | Enantioselective binding of structural epoxide isomers by a chiral vanadyl salen complex: a pulsed EPR, cw-ENDOR and DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6757. | 2.8 | 10 |
| 191 | Discrimination of Geometrical Epoxide Isomers by ENDOR Spectroscopy and DFT Calculations: The Role of Hydrogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 1414-1416. | 13.8 | 13 |
| 192 | Palladium and Gold@Palladium Catalysts for the Direct Synthesis of Hydrogen Peroxide. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 9192-9198. | 13.8 | 316 |
| 193 | Nanocrystalline gold and gold@palladium alloy oxidation catalysts: a personal reflection on the nature of the active sites. <i>Dalton Transactions</i> , 2008, , 5523. | 3.3 | 68 |
| 194 | Direct synthesis of hydrogen peroxide from H ₂ and O ₂ using supported Au@Pd catalysts. <i>Faraday Discussions</i> , 2008, 138, 225-239. | 3.2 | 207 |
| 195 | Theory and simulation in heterogeneous gold catalysis. <i>Chemical Society Reviews</i> , 2008, 37, 2046. | 38.1 | 136 |
| 196 | The role of the support in achieving high selectivity in the direct formation of hydrogen peroxide. <i>Green Chemistry</i> , 2008, 10, 1162. | 9.0 | 89 |
| 197 | Atomistic Simulation of Micropore Structure, Surface Area, and Gas Sorption Properties for Amorphous Microporous Polymer Networks. <i>Journal of Physical Chemistry C</i> , 2008, 112, 20549-20559. | 3.1 | 59 |
| 198 | Gold@an introductory perspective. <i>Chemical Society Reviews</i> , 2008, 37, 1759. | 38.1 | 384 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 199 | Identification of Active Gold Nanoclusters on Iron Oxide Supports for CO Oxidation. <i>Science</i> , 2008, 321, 1331-1335. | 12.6 | 1,448 |
| 200 | Au-Pd supported nanocrystals prepared by a sol immobilisation technique as catalysts for selective chemical synthesis. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1921. | 2.8 | 136 |
| 201 | Au-Pd supported nanocrystals as catalysts for the direct synthesis of hydrogen peroxide from H ₂ and O ₂ . <i>Green Chemistry</i> , 2008, 10, 388-394. | 9.0 | 131 |
| 202 | A Group 13/Group 17 Analogue of CO and N ₂ : Coordinative Trapping of the Gal Molecule. <i>Journal of the American Chemical Society</i> , 2008, 130, 5449-5451. | 13.7 | 60 |
| 203 | Cationic Terminal Gallylene Complexes by Halide Abstraction: Coordination Chemistry of a Valence Isoelectronic Analogue of CO and N ₂ . <i>Journal of the American Chemical Society</i> , 2008, 130, 16111-16124. | 13.7 | 49 |
| 204 | The role of organic templates in controlling zeolite crystal morphology. <i>Studies in Surface Science and Catalysis</i> , 2007, , 1685-1692. | 1.5 | 12 |
| 205 | Comparison of supports for the direct synthesis of hydrogen peroxide from H ₂ and O ₂ using Au-Pd catalysts. <i>Catalysis Today</i> , 2007, 122, 397-402. | 4.4 | 103 |
| 206 | Catalytic aziridination and epoxidation of alkenes using modified microporous and mesoporous materials. <i>Special Publication - Royal Society of Chemistry</i> , 2007, , 94-103. | 0.0 | 1 |
| 207 | Catalysis: experimental and computational. <i>Annual Reports on the Progress of Chemistry Section B</i> , 2007, 103, 294. | 0.9 | 2 |
| 208 | Insertion reactions of dicyclohexylcarbodiimide with aminoboranes, -boryls and -borylenes. <i>Dalton Transactions</i> , 2007, , 4405. | 3.3 | 33 |
| 209 | Cationic Terminal Aminoborylene Complexes: Controlled Stepwise Insertion into M π $\frac{3}{4}$ B and B π $\frac{3}{4}$ N Double Bonds. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 2043-2046. | 13.8 | 47 |
| 210 | Solvent free liquid phase oxidation of benzyl alcohol using Au supported catalysts prepared using a sol immobilization technique. <i>Catalysis Today</i> , 2007, 122, 317-324. | 4.4 | 150 |
| 211 | Solvent-free oxidation of benzyl alcohol using titania-supported gold-palladium catalysts: Effect of Au-Pd ratio on catalytic performance. <i>Catalysis Today</i> , 2007, 122, 407-411. | 4.4 | 104 |
| 212 | Hydrochlorination of acetylene using a supported gold catalyst: A study of the reaction mechanism. <i>Journal of Catalysis</i> , 2007, 250, 231-239. | 6.2 | 219 |
| 213 | Keto-enol isomerism on transition metal surfaces, a density functional theory study. <i>Special Publication - Royal Society of Chemistry</i> , 2007, , 247-252. | 0.0 | 0 |
| 214 | Complexes of a gallium heterocycle with transition metal dicyclopentadienyl and cyclopentadienylcarbonyl fragments, and with a dialkylmanganese compound. <i>Dalton Transactions</i> , 2006, , 3313. | 3.3 | 66 |
| 215 | Selective oxidation of CO in the presence of H ₂ , H ₂ O and CO ₂ utilising Au/Fe ₂ O ₃ catalysts for use in fuel cells. <i>Journal of Materials Chemistry</i> , 2006, 16, 199-208. | 6.7 | 92 |
| 216 | Simulation of the structure of organosilane film coatings. <i>Molecular Simulation</i> , 2006, 32, 1095-1101. | 2.0 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 217 | Catalysis: experimental and computational. Annual Reports on the Progress of Chemistry Section B, 2006, 102, 325. | 0.9 | 2 |
| 218 | Calculations on the adsorption of Au to MgO surfaces using SIESTA. Journal of Materials Chemistry, 2006, 16, 1978. | 6.7 | 33 |
| 219 | Solvent-Free Oxidation of Primary Alcohols to Aldehydes Using Au-Pd/TiO ₂ Catalysts. Science, 2006, 311, 362-365. | 12.6 | 1,976 |
| 220 | Direct Synthesis of Hydrogen Peroxide from H ₂ and O ₂ Using Al ₂ O ₃ Supported Au-Pd Catalysts. Chemistry of Materials, 2006, 18, 2689-2695. | 6.7 | 183 |
| 221 | Supported gold catalysts for the total oxidation of alkanes and carbon monoxide. Applied Catalysis A: General, 2006, 312, 67-76. | 4.3 | 134 |
| 222 | Unexpected inversion of enantioselectivity during the hydrogenation of ethyl pyruvate using hydroquinine and hydroquinidine modified Pt/Al ₂ O ₃ . Catalysis Letters, 2006, 110, 135-138. | 2.6 | 9 |
| 223 | Role of gold cations in the oxidation of carbon monoxide catalyzed by iron oxide-supported gold. Journal of Catalysis, 2006, 242, 71-81. | 6.2 | 322 |
| 224 | Inversion of enantioselectivity for the hydrogenation of ethyl pyruvate in the gas-phase over Pt/SiO ₂ modified with derivatives of hydroquinidine. Journal of Catalysis, 2006, 243, 165-170. | 6.2 | 13 |
| 225 | Enantioselective hydrogenation of N-acetyl dehydrophenylalanine methyl ester using cinchonine-modified Pd/Al ₂ O ₃ catalysts. Journal of Catalysis, 2006, 243, 360-367. | 6.2 | 10 |
| 226 | Novel Properties from Experimental Charge Densities: An Application to the Zwitterionic Neurotransmitter Taurine. Chemistry - A European Journal, 2006, 12, 7603-7614. | 3.3 | 19 |
| 227 | Cationic Terminal Borylene Complexes: Structure/Bonding Analysis and [4+1] Cycloaddition Reactivity of a BN Vinylidene Analogue. Angewandte Chemie - International Edition, 2006, 45, 6118-6122. | 13.8 | 75 |
| 228 | Gold Catalysis. Angewandte Chemie - International Edition, 2006, 45, 7896-7936. | 13.8 | 3,254 |
| 229 | A density functional theory study of the adsorption of acetone to the (111) surface of Pt: Implications for hydrogenation catalysis. Catalysis Today, 2005, 105, 85-92. | 4.4 | 43 |
| 230 | Diastereoselective Dimerisation of Alkenylthiazolines: A Combined Synthetic and Computational Study. European Journal of Organic Chemistry, 2005, 2005, 3791-3800. | 2.4 | 6 |
| 231 | Continuous stable enantioselective hydrogenation of alkyl pyruvate esters using pre-modified cinchonidine platinum catalysts. Catalysis Letters, 2005, 100, 255-258. | 2.6 | 10 |
| 232 | Solvent-free Oxidation of Primary Alcohols to Aldehydes using Supported Gold Catalysts. Catalysis Letters, 2005, 103, 43-52. | 2.6 | 194 |
| 233 | High Surface Area MgO as a Highly Effective Heterogeneous Base Catalyst for Michael Addition and Knoevenagel Condensation Reactions. Synthesis, 2005, 2005, 3468-3476. | 2.3 | 11 |
| 234 | Tunable gold catalysts for selective hydrocarbon oxidation under mild conditions. Nature, 2005, 437, 1132-1135. | 27.8 | 955 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 235 | Selective oxidation of CO in the presence of H ₂ , H ₂ O and CO ₂ via gold for use in fuel cells. <i>Chemical Communications</i> , 2005, , 3385. | 4.1 | 146 |
| 236 | Halide Abstraction as a Route to Cationic Transition-Metal Complexes Containing Two-Coordinate Gallium and Indium Ligand Systems. <i>Organometallics</i> , 2005, 24, 5891-5900. | 2.3 | 53 |
| 237 | Direct synthesis of hydrogen peroxide from H ₂ and O ₂ using Au/Pd/Fe ₂ O ₃ catalysts. <i>Journal of Materials Chemistry</i> , 2005, 15, 4595. | 6.7 | 180 |
| 238 | The (010) surface of α -MoO ₃ , a DFT + U study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3819. | 2.8 | 146 |
| 239 | HETEROGENEOUS ASYMMETRIC CATALYSTS: Strategies for Achieving High Enantioselection. <i>Annual Review of Materials Research</i> , 2005, 35, 143-166. | 9.3 | 55 |
| 240 | 13C NMR Catalysis: Experimental and computational. <i>Annual Reports on the Progress of Chemistry Section B</i> , 2005, 101, 333. | 0.9 | 3 |
| 241 | Enantioselective Hydrogenation Using Cinchona-Modified Pt/Al ₂ O ₃ Catalysts: Comparison of the Reaction of Ethyl Pyruvate and Buta-2,3-dione. <i>Catalysis Letters</i> , 2004, 96, 147-151. | 2.6 | 16 |
| 242 | The Structure of Metallomicelles. <i>Chemistry - A European Journal</i> , 2004, 10, 2022-2028. | 3.3 | 55 |
| 243 | Long range superhyperfine interactions in polycrystalline vanadium doped SnO ₂ investigated by CW and pulsed ENDOR spectroscopy. <i>Chemical Physics Letters</i> , 2004, 391, 1-8. | 2.6 | 6 |
| 244 | Fe-Ga multiple bonding? Synthesis, spectroscopic and structural characterization of a transition metal complex containing a cationic two-coordinate gallium centre. <i>Chemical Communications</i> , 2004, , 1732-1733. | 4.1 | 50 |
| 245 | Carbonyl analogues? Analysis of Fe-E (E = B, Al, Ga) bonding in cationic terminal diyl complexes by density functional theory. <i>Dalton Transactions</i> , 2004, , 2649-2654. | 3.3 | 65 |
| 246 | Reactivity of the bis(pentafluorophenyl)boranes ClB(C ₆ F ₅) ₂ and [HB(C ₆ F ₅) ₂] _n towards late transition metal reagents. <i>Dalton Transactions</i> , 2004, , 4030. | 3.3 | 25 |
| 247 | Improvement of the catalytic performance of CuMnOx catalysts for CO oxidation by the addition of Au. <i>New Journal of Chemistry</i> , 2004, 28, 708. | 2.8 | 40 |
| 248 | Vanadium phosphate: a new look at the active components of catalysts for the oxidation of butane to maleic anhydride. <i>Journal of Materials Chemistry</i> , 2004, 14, 3385. | 6.7 | 120 |
| 249 | FeB Double Bonds: Synthetic, Structural, and Reaction Chemistry of Cationic Terminal Borylene Complexes. <i>Organometallics</i> , 2004, 23, 2911-2926. | 2.3 | 119 |
| 250 | Direct Observation of Enantiomer Discrimination of Epoxides by Chiral Salen Complexes Using ENDOR. <i>Journal of the American Chemical Society</i> , 2004, 126, 15660-15661. | 18.7 | 30 |
| 251 | Catalytic Asymmetric Heterogeneous Aziridination Using CuHY/bis(oxazoline): Effect of Reaction Conditions on Enantioselectivity. <i>Topics in Catalysis</i> , 2003, 25, 81-88. | 2.8 | 25 |
| 252 | Computer Simulation of Structural Aspects of Enantioselective Heterogeneous Catalysis and the Prospects for Direct Calculation of Selectivity. <i>Topics in Catalysis</i> , 2003, 25, 89-102. | 2.8 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 253 | Title is missing!. Catalysis Letters, 2003, 87, 103-108. | 2.6 | 19 |
| 254 | A study of methane activation by modified gallium- and zinc-based catalysts. Research on Chemical Intermediates, 2003, 29, 911-920. | 2.7 | 2 |
| 255 | An ENDOR and DFT analysis of λ^6 -solvatochromic TM effects in an oxovanadium (IV) complex. Chemical Physics Letters, 2003, 380, 758-766. | 2.6 | 9 |
| 256 | Observation of High Enantioselectivity for the Gas Phase Hydrogenation of Methyl Pyruvate Using Supported Pt Catalysts Pre-Modified with Cinchonidine.. ChemInform, 2003, 34, no. | 0.0 | 1 |
| 257 | Cationic Terminal Borylenes by Halide Abstraction: A Synthesis and Spectroscopic and Structural Characterization of an FeB Double Bond. Journal of the American Chemical Society, 2003, 125, 6356-6357. | 13.7 | 148 |
| 258 | Direct synthesis of hydrogen peroxide from H ₂ and O ₂ using Pd and Au catalysts. Physical Chemistry Chemical Physics, 2003, 5, 1917-1923. | 2.8 | 336 |
| 259 | Observation of high enantioselectivity for the gas phase hydrogenation of methyl pyruvate using supported Pt catalysts pre-modified with cinchonidineElectronic supplementary information (ESI) available: use of the Kelvin equation and reactant partial pressure to estimate the effective partial pressure for condensation as a function of pore radius. See http://www.rsc.org/suppldata/2003/200304761/ . Chemical Communications, 2003, , 1026 | 4.1 | 24 |
| 260 | An IMDA Approach to Tigliane and Daphnane Diterpenoids: Generation of Rings A, B and C Incorporating C-18. Synlett, 2002, 2002, 0583-0587. | 1.8 | 16 |
| 261 | Analysis of Bonding in Cyclopentadienyl Transition-Metal Boryl Complexes. Organometallics, 2002, 21, 1146-1157. | 2.3 | 77 |
| 262 | Direct formation of hydrogen peroxide from H ₂ /O ₂ using a gold catalyst. Chemical Communications, 2002, , 2058-2059. | 4.1 | 476 |
| 263 | Co-precipitated copper zinc oxide catalysts for ambient temperature carbon monoxide oxidation: effect of precipitate ageing on catalyst activity. Physical Chemistry Chemical Physics, 2002, 4, 5915-5920. | 2.8 | 79 |
| 264 | Conformational changes of an oxovanadium complex probed by ENDOR spectroscopy and DFT calculations. Physical Chemistry Chemical Physics, 2002, 4, 4937-4943. | 2.8 | 14 |
| 265 | Linking of metal centres through boryl ligands: synthesis, spectroscopic and structural characterisation of symmetrically bridged boryl complexes. Dalton Transactions RSC, 2002, , 2020-2026. | 2.3 | 22 |
| 266 | Selective oxidation of glycerol to glyceric acid using a gold catalyst in aqueous sodium hydroxide. Chemical Communications, 2002, , 696-697. | 4.1 | 498 |
| 267 | Low-temperature redox activity in co-precipitated catalysts: a comparison between gold and platinum-group metals. Catalysis Today, 2002, 72, 107-113. | 4.4 | 91 |
| 268 | Sulfonylation of substituted benzenes using Zn-exchanged zeolites. Journal of Molecular Catalysis A, 2002, 178, 205-209. | 4.8 | 18 |
| 269 | Heterogeneous aziridination of styrene using [N-(p-nitrophenylsulfonyl)imino]phenyliodinane as nitrene donor: influence of the reaction parameters on yield and enantioselectivity. Journal of Molecular Catalysis A, 2002, 182-183, 571-575. | 4.8 | 10 |
| 270 | Title is missing!. Catalysis Letters, 2002, 78, 369-372. | 2.6 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 271 | Enantioselective Reactions Using Modified Microporous and Mesoporous Materials. <i>Fundamental and Applied Catalysis</i> , 2002, , 241-274. | 0.9 | 5 |
| 272 | A Comparison of the Adsorption and Diffusion of Hydrogen on the {111} Surfaces of Ni, Pd, and Pt from Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4889-4894. | 2.6 | 184 |
| 273 | Geometrical preferences of complexes of terpyridine N-oxide ligands: synthesis and crystal structures of nickel(II) with terpyridine 1,1'-di- π -trioxide, terpyridine 1,1'- π -dioxide and terpyridine 1-oxide. <i>Dalton Transactions RSC</i> , 2001, , 225-227. | 2.3 | 10 |
| 274 | Perfluoroaryl boryl complexes: synthesis, spectroscopic and structural characterisation of a complex containing the bis(pentafluorophenyl)boryl ligand. <i>Chemical Communications</i> , 2001, , 1846-1847. | 4.1 | 15 |
| 275 | The enumeration of structures for γ -alumina based on a defective spinel structure. <i>Chemical Communications</i> , 2001, , 1076-1077. | 4.1 | 8 |
| 276 | Asymmetric hetero-Diels-Alder reactions. Reactions of oxazolo[3,2-c]pyrimidines. <i>Tetrahedron</i> , 2001, 57, 10139-10146. | 1.9 | 21 |
| 277 | Highly diastereoselective dimerisation of alkenylthiazolines. <i>Tetrahedron Letters</i> , 2001, 42, 4937-4939. | 1.4 | 7 |
| 278 | Oxidation of crotyl alcohol using Ti^{IV} and Ti-MCM-41 catalysts. <i>Journal of Molecular Catalysis A</i> , 2001, 165, 243-247. | 4.8 | 48 |
| 279 | A combined experimental and theoretical approach to the study of methane activation over oxide catalysts. <i>Catalysis Today</i> , 2001, 71, 3-10. | 4.4 | 6 |
| 280 | The role of gallium oxide in methane partial oxidation catalysts: An experimental and theoretical study. <i>Studies in Surface Science and Catalysis</i> , 2001, 136, 319-324. | 1.5 | 2 |
| 281 | Calculation of the energy profile for the fluorination of dichloromethane over an γ -alumina catalyst. <i>Applied Catalysis A: General</i> , 2000, 200, 263-274. | 4.3 | 10 |
| 282 | The effect of pre-sulfiding of catalysts for the vapour phase catalytic synthesis of thiophenes. <i>Catalysis Letters</i> , 2000, 68, 75-77. | 2.6 | 4 |
| 283 | H_2 adsorption of ethene on to the {111} surface of copper. <i>Surface Science</i> , 2000, 459, 93-103. | 1.9 | 18 |
| 284 | Ab initio simulation of the interaction of hydrogen with the {111} surfaces of platinum, palladium and nickel. A possible explanation for their difference in hydrogenation activity. <i>Chemical Communications</i> , 2000, , 705-706. | 4.1 | 33 |
| 285 | Oxidation of thioethers and sulfoxides with hydrogen peroxide using TS-1 as catalyst. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1523-1529. | 2.8 | 36 |
| 286 | Linking of metal centres through boryl ligands: synthesis, spectroscopic and structural characterisation of a symmetrically bridged boryl complex $\text{CpFe}(\text{CO})_2\text{B}(\text{O}^i\text{Pr})_2\text{C}_6\text{H}_2\text{O}_2\text{BFe}(\text{CO})_2\text{Cp}$. <i>Chemical Communications</i> , 2000, , 1377-1378. | 4.1 | 7 |
| 287 | Density Functional Theory Calculations on the Interaction of Ethene with the {111} Surface of Platinum. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6439-6446. | 2.6 | 49 |
| 288 | Dehydration of butan-2-ol using modified zeolite crystals. <i>Applied Catalysis A: General</i> , 1999, 182, 75-84. | 4.3 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 289 | Heterogeneous aziridination of alkenes using Cu ²⁺ exchanged zeolites. <i>Applied Catalysis A: General</i> , 1999, 182, 85-89. | 4.3 | 28 |
| 290 | Methanol conversion to hydrocarbons over zeolite catalysts: comments on the reaction mechanism for the formation of the first carbon-carbon bond. <i>Microporous and Mesoporous Materials</i> , 1999, 29, 67-77. | 4.4 | 42 |
| 291 | Designing oxidation catalysts. <i>Catalysis Today</i> , 1999, 49, 105-113. | 4.4 | 46 |
| 292 | Promotion by sulfur of gold catalysts for crotyl alcohol formation from crotonaldehyde hydrogenation. <i>Chemical Communications</i> , 1999, , 2151-2152. | 4.1 | 208 |
| 293 | Polarizability anisotropies of cyano-substituted azulene, biphenyl, 2,2'-bipyridyl and naphthalene. <i>Molecular Physics</i> , 1999, 97, 913-918. | 1.7 | 7 |
| 294 | Catalytic asymmetric heterogeneous aziridination of alkenes using zeolite CuHY with [N-(<i>p</i> -tolylsulfonyl)imino]phenyliodinane as nitrene donor. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1043. | 0.9 | 47 |
| 295 | Title is missing!. <i>Topics in Catalysis</i> , 1998, 5, 177-185. | 2.8 | 14 |
| 296 | Asymmetric hetero-Diels-Alder reactions. Mechanism of the reaction of alkenyloxazolines with isocyanates. <i>Tetrahedron Letters</i> , 1998, 39, 8911-8914. | 1.4 | 16 |
| 297 | The partial oxidation of methane to methanol: An approach to catalyst design. <i>Catalysis Today</i> , 1998, 42, 217-224. | 4.4 | 55 |
| 298 | Catalytic heterogeneous aziridination of alkenes using microporous materials. <i>Chemical Communications</i> , 1998, , 1601-1602. | 4.1 | 53 |
| 299 | Metabolism-Dependent Neutrophil Cytotoxicity of Amodiaquine: A Comparison with Pyronaridine and Related Antimalarial Drugs. <i>Chemical Research in Toxicology</i> , 1998, 11, 1586-1595. | 3.3 | 79 |
| 300 | High-activity Au/CuO-ZnO catalysts for the oxidation of carbon monoxide at ambient temperature. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 187-188. | 1.7 | 70 |
| 301 | Synthesis, Antimalarial Activity, and Molecular Modeling of Tebuquine Analogues. <i>Journal of Medicinal Chemistry</i> , 1997, 40, 437-448. | 6.4 | 105 |
| 302 | Enantioselective Dehydration of Butan-2-ol Using Zeolite Y Modified with Dithiane Oxides. <i>Journal of Catalysis</i> , 1997, 167, 533-542. | 6.2 | 30 |
| 303 | Title is missing!. <i>Catalysis Letters</i> , 1997, 46, 249-254. | 2.6 | 2 |
| 304 | Designing templates for the synthesis of microporous solids using de novo molecular design methods. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 415-424. | 4.8 | 38 |
| 305 | Synthesis of a Small-Pore Microporous Material Using a Computationally Designed Template. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 2675-2677. | 4.4 | 85 |
| 306 | Synthese eines kleinporigen mikroporösen Materials unter Verwendung eines computer-gestützten entworfenen Templats. <i>Angewandte Chemie</i> , 1997, 109, 2791-2793. | 2.0 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 307 | Role of Electrostatic Interactions in Determining the Crystal Structures of Polar Organic Molecules. A Distributed Multipole Study. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7352-7360. | 2.9 | 280 |
| 308 | Heterogeneous enantioselective dehydration of butan-2-ol. <i>Studies in Surface Science and Catalysis</i> , 1996, 101, 211-219. | 1.5 | 12 |
| 309 | Creating chiral centres in zeolite Y by the introduction of R-1,3-dithiane 1-oxide as a modifier: Computer simulation of the modifier stability. <i>Topics in Catalysis</i> , 1996, 3, 77-89. | 2.8 | 9 |
| 310 | Epoxidation of allyl alcohol to glycidol using titanium silicalite TS-1: effect of the reaction conditions and catalyst acidity. <i>Catalysis Letters</i> , 1996, 39, 83-90. | 2.6 | 48 |
| 311 | Enantioselection using modified zeolite catalysts. <i>Journal of Molecular Catalysis A</i> , 1996, 107, 291-295. | 4.8 | 11 |
| 312 | De novo design of structure-directing agents for the synthesis of microporous solids. <i>Nature</i> , 1996, 382, 604-606. | 27.8 | 302 |
| 313 | Gradient-based fitting of empirical potentials in the presence of a distributed-multipole electrostatic model. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1996, 73, 127-138. | 0.6 | 1 |
| 314 | The relaxation of molecular crystal structures using a distributed multipole electrostatic model. <i>Journal of Computational Chemistry</i> , 1995, 16, 628-647. | 3.3 | 154 |
| 315 | Selective conversion of allyl alcohol to oxygenates and hydrocarbons using ion exchanged zeolite Y. <i>Catalysis Letters</i> , 1995, 34, 115-127. | 2.6 | 6 |
| 316 | Epoxidation of allyl alcohol to glycidol using titanium silicalite TS-1: effect of the method of preparation. <i>Catalysis Letters</i> , 1995, 33, 369-385. | 2.6 | 51 |
| 317 | Gas-phase catalytic asymmetric reaction using chirally modified microporous catalysts. <i>Journal of the Chemical Society Chemical Communications</i> , 1995, , 2409. | 2.0 | 20 |
| 318 | The Effect of Sulfoxide Loadings on the Selectivity and Activity of Zeolite Y for Dehydration Reactions: Stability and Structure of Dithiane oxide in Zeolite Y. <i>Studies in Surface Science and Catalysis</i> , 1994, , 1611-1616. | 1.5 | 1 |
| 319 | The effects of oxygen on charge transport in PDATS. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 2533-2542. | 1.8 | 4 |
| 320 | Transit currents in a one-dimensional polymer single crystal. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 2517-2532. | 1.8 | 15 |
| 321 | Temperature dependence of transit currents in a one-dimensional polymer single crystal. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 6613-6628. | 1.8 | 4 |
| 322 | Studies of the Mechanism of the Oxidative Coupling of Methane Using Oxide Catalysts. , 1992, , 200-258. | | 9 |
| 323 | Carrier recombination in polydiacetylenes the scaling with sample size. <i>Synthetic Metals</i> , 1991, 41, 243. | 3.9 | 0 |
| 324 | Control of product selectivity in the partial oxidation of methane. <i>Nature</i> , 1990, 348, 428-429. | 27.8 | 87 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 325 | Hydrocarbon formation from methanol and dimethyl ether: a review of the experimental observations concerning the mechanism of formation of the primary products. <i>Catalysis Today</i> , 1990, 6, 279-306. | 4.4 | 125 |
| 326 | The role of gas phase reaction in the selective oxidation of methane. <i>Journal of the Chemical Society Chemical Communications</i> , 1988, , 253. | 2.0 | 28 |
| 327 | Hydrocarbon formation from methylating agents over the zeolite catalyst ZSM-5. Comments on the mechanism of carbon-carbon bond and methane formation. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1987, 83, 571. | 1.0 | 90 |
| 328 | LiAl(OPri) ₄ as a model compound for the conjugate base of the zeolite catalyst H-ZSM-5 and its reaction with various methylating agents. <i>Journal of the Chemical Society Chemical Communications</i> , 1985, , 886. | 2.0 | 6 |
| 329 | Hydrocarbon formation from methylating agents over the zeolite catalyst H-ZSM-5 and its conjugate base: evidence against the trimethyloxonium ion-ylide mechanism. <i>Journal of the Chemical Society Chemical Communications</i> , 1985, , 1643-1645. | 2.0 | 15 |
| 330 | Theory: Periodic Electronic Structure Calculations. , 0, , 323-389. | | 1 |
| 331 | Investigating the Effects of Surface Adsorbates on Gold and Palladium Deposition on Carbon. <i>Topics in Catalysis</i> , 0, , 1. | 2.8 | 1 |