C Richard A Catlow

List of Publications by Year in Descending Order

830 papers	37,295 citations	93 h-index	154 g-index
886 ext. papers	39,771 ext. citations	5.4 avg, IF	7.27 L-index

#	Paper	IF	Citations
830	Carbene-like reactivity of methoxy groups in a single crystal SAPO-34 MTO catalyst. *Catalysis Science and Technology*, **2022**, 12, 2289-2305	5.5	0
829	Cation-doping strategies for tuning of zirconia acid-base properties.. *Royal Society Open Science*, **2022**, 9, 211423	3.3	1
828	A comparative study on the stability of the furfural molecule on the low index Ni, Pd and Pt surfaces.. *Royal Society Open Science*, **2022**, 9, 211516	3.3	1
827	Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) Surfaces of TiC and ZrC: A Computational Study.. *Journal of Physical Chemistry C*, **2022**, 126, 5138-5150	3.8	1
826	A comparative analysis of the mechanisms of ammonia synthesis on various catalysts using density functional theory. *Royal Society Open Science*, **2021**, 8, 210952	3.3	1
825	Gas Phase Glycerol Valorization over Ceria Nanostructures with Well-Defined Morphologies. *ACS Catalysis*, **2021**, 11, 4893-4907	13.1	3
824	Combined Experimental and Theoretical Study of the Competitive Absorption of CO and NO by a Superbase Ionic Liquid. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 7578-7586	8.3	3
823	Methanol dynamics in H-ZSM-5 with Si/Al ratio of 25: a quasi-elastic neutron scattering (QENS) study. *Topics in Catalysis*, **2021**, 64, 699-706	2.3	4
822	A combined periodic DFT and QM/MM approach to understand the radical mechanism of the catalytic production of methanol from glycerol. *Faraday Discussions*, **2021**, 229, 108-130	3.6	0
821	Combination of theoretical and in situ experimental investigations of the role of lithium dopant in manganese nitride: a two-stage reagent for ammonia synthesis. *Faraday Discussions*, **2021**, 229, 281-296	3.6	0
820	Design, Identification, and Evolution of a Surface Ruthenium(II/III) Single Site for CO Activation. *Angewandte Chemie*, **2021**, 133, 1232-1239	3.6	
819	Design, Identification, and Evolution of a Surface Ruthenium(II/III) Single Site for CO Activation. *Angewandte Chemie - International Edition*, **2021**, 60, 1212-1219	16.4	2
818	Tuning the transition barrier of H dissociation in the hydrogenation of CO to formic acid on Ti-doped SnO clusters. *Physical Chemistry Chemical Physics*, **2021**, 23, 204-210	3.6	1
817	Electrochemical upgrading of biomass-derived 5-hydroxymethylfurfural and furfural over oxygen vacancy-rich NiCoMn-layered double hydroxides nanosheets. *Green Chemistry*, **2021**, 23, 4034-4043	10	32
816	A computational investigation of the adsorption of small copper clusters on the CeO(110) surface. *Physical Chemistry Chemical Physics*, **2021**, 23, 19329-19342	3.6	1
815	Selectivity of the Lindlar catalyst in alkyne semi-hydrogenation: a direct liquid-phase adsorption study. *Catalysis Science and Technology*, **2021**, 11, 6205-6216	5.5	3
814	QM/MM study of the reactivity of zeolite bound methoxy and carbene groups. *Physical Chemistry Chemical Physics*, **2021**, 23, 17634-17644	3.6	6

813	Catalytic decomposition of NO2 over a copper-decorated metal-organic framework by non-thermal plasma. *Cell Reports Physical Science*, **2021**, 2, 100349	6.1	3
812	Spatial Profiling of a Pd/AlO Catalyst during Selective Ammonia Oxidation. *ACS Catalysis*, **2021**, 11, 2141-2149	13	7
811	Density Functional Theory Study of the Partial Oxidation of Methane to Methanol on Au and Pd Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 18770-18785	3.8	0
810	Concluding remarks: Reaction mechanisms in catalysis: perspectives and prospects. *Faraday Discussions*, **2021**, 229, 502-513	3.6	1
809	A computational study of the properties of low- and high-index Pd, Cu and Zn surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 14649-14661	3.6	2
808	QM/MM study of the stability of dimethyl ether in zeolites H-ZSM-5 and H-Y. *Physical Chemistry Chemical Physics*, **2021**, 23, 2088-2096	3.6	2
807	How bulk and surface properties of TiSiC, VSiC, NbSiC and ZrSiC tune reactivity: a computational study. *Faraday Discussions*, **2021**, 230, 87-99	3.6	0
806	Role of Sulfation of Zirconia Catalysts in Vapor Phase Ketonization of Acetic Acid.. *Journal of Physical Chemistry C*, **2021**, 125, 27578-27595	3.8	3
805	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide.. *Frontiers in Chemistry*, **2021**, 9, 780935	5	0
804	Octane isomer dynamics in H-ZSM-5 as a function of Si/Al ratio: a quasi-elastic neutron scattering study. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2020**, 378, 20200063	3	1
803	Probing the dynamics and structure of confined benzene in MCM-41 based catalysts. *Physical Chemistry Chemical Physics*, **2020**, 22, 11485-11489	3.6	3
802	Mechanism of CO conversion to methanol over Cu(110) and Cu(100) surfaces. *Dalton Transactions*, **2020**, 49, 8478-8497	4.3	13
801	Methanol loading dependent methoxylation in zeolite H-ZSM-5. *Chemical Science*, **2020**, 11, 6805-6814	9.4	10
800	Effects of crystal size on methanol to hydrocarbon conversion over single crystals of ZSM-5 studied by synchrotron infrared microspectroscopy. *Physical Chemistry Chemical Physics*, **2020**, 22, 18849-18859	3.6	7
799	The influence of oxygen vacancy and Ce3+ ion positions on the properties of small gold clusters supported on CeO2(111). *Journal of Materials Chemistry A*, **2020**, 8, 15695-15705	13	8
798	Modelling the bulk properties of ambient pressure polymorphs of zirconia. *Physical Chemistry Chemical Physics*, **2020**, 22, 6660-6676	3.6	11
797	Synergistic ultraviolet and visible light photo-activation enables intensified low-temperature methanol synthesis over copper/zinc oxide/alumina. *Nature Communications*, **2020**, 11, 1615	17.4	37
796	Synchrotron Radiation and Catalytic Science. *Synchrotron Radiation News*, **2020**, 33, 10-14	0.6	1

795	A DFT and KMC based study on the mechanism of the water gas shift reaction on the Pd(100) surface. *Physical Chemistry Chemical Physics*, **2020**, 22, 3620-3632	3.6	18
794	DFT-Assisted Spectroscopic Studies on the Coordination of Small Ligands to Palladium: From Isolated Ions to Nanoparticles. *Journal of Physical Chemistry C*, **2020**, 124, 4781-4790	3.8	2
793	The direct synthesis of hydrogen peroxide over Au and Pd nanoparticles: A DFT study. *Catalysis Today*, **2020**, 381, 76-76	5.3	2
792	Silicon microfabricated reactor for operando XAS/DRIFTS studies of heterogeneous catalytic reactions. *Catalysis Science and Technology*, **2020**, 10, 7842-7856	5.5	1
791	Mechanistic Insight into the Framework Methylation of H-ZSM-5 for Varying Methanol Loadings and Si/Al Ratios Using First-Principles Molecular Dynamics Simulations. *ACS Catalysis*, **2020**, 10, 8904-8915	13.1	17
790	Recent developments and perspectives in CdS-based photocatalysts for water splitting. *Journal of Materials Chemistry A*, **2020**, 8, 20752-20780	13	71
789	Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (000) surfaces. *Journal of Materials Chemistry A*, **2020**, 8, 22840-22857	13	5
788	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. *Journal of Materials Chemistry A*, **2020**, 8, 14054-14061	13	5
787	Investigation of MoOx/Al2O3 under Cyclic Operation for Oxidative and Non-Oxidative Dehydrogenation of Propane. *Catalysts*, **2020**, 10, 1370	4	2
786	In-depth characterisation of metal-support compounds in spent Co/SiO2 Fischer-Tropsch model catalysts. *Catalysis Today*, **2020**, 342, 71-78	5.3	10
785	Synthesis, characterisation and water-gas shift activity of nano-particulate mixed-metal (Al, Ti) cobalt oxides. *Dalton Transactions*, **2019**, 48, 13858-13868	4.3	7
784	An experimental and computational IR and hybrid DFT-D3 study of the conformations of l-lactic and acrylic acid: new insight into the dehydration mechanism of lactic acid to acrylic acid. *Physical Chemistry Chemical Physics*, **2019**, 21, 22331-22343	3.6	3
783	Structural selectivity of supported Pd nanoparticles for catalytic NH3 oxidation resolved using combined operando spectroscopy. *Nature Catalysis*, **2019**, 2, 157-163	36.5	38
782	Hydrogen adsorption on transition metal carbides: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 5335-5343	3.6	25
781	Computational QM/MM investigation of the adsorption of MTH active species in H-Y and H-ZSM-5. *Physical Chemistry Chemical Physics*, **2019**, 21, 2639-2650	3.6	13
780	Extracting structural information of Au colloids at ultra-dilute concentrations: identification of growth during nanoparticle immobilization. *Nanoscale Advances*, **2019**, 1, 2546-2552	5.1	2
779	Elementary Steps in the Formation of Hydrocarbons from Surface Methoxy Groups in HZSM-5 Seen by Synchrotron Infrared Microspectroscopy. *ACS Catalysis*, **2019**, 9, 6564-6570	13.1	29
778	Carbidisation of Pd Nanoparticles by Ethene Decomposition with Methane Production. *ChemCatChem*, **2019**, 11, 4334-4339	5.2	7

777	Hydrogenated Si12Au20 cluster as a molecular sensor with high performance for NH3 and NO detection: A first-principle study. *Journal of Molecular Liquids*, **2019**, 289, 111153	6	6
776	Synchrotron science in the UK: NINA, the SRS and Diamond. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2019**, 377, 20190147	3	1
775	Carbon dioxide and water co-adsorption on the low-index surfaces of TiC, VC, ZrC and NbC: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 10750-10760	3.6	13
774	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
773	Water-Induced Formation of Cobalt-Support Compounds under Simulated High Conversion Fischer□ropsch Environment. *ACS Catalysis*, **2019**, 9, 4902-4918	13.1	19
772	Advances in Sustainable Catalysis: A Computational Perspective. *Frontiers in Chemistry*, **2019**, 7, 182	5	27
771	Combined spatially resolved operando spectroscopy: New insights into kinetic oscillations of CO oxidation on Pd/□Al2O3. *Journal of Catalysis*, **2019**, 373, 201-208	7.3	8
770	Energy materials for a low carbon future. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2019**, 377, 20190219	3	1
769	Intrinsic point defects and the n- and p-type dopability of the narrow gap semiconductors GaSb and InSb. *Physical Review B*, **2019**, 100,	3.3	8
768	Impact of Nanoparticle-Support Interactions in CoO/AlO Catalysts for the Preferential Oxidation of Carbon Monoxide. *ACS Catalysis*, **2019**, 9, 7166-7178	13.1	33
767	Pd local structure and size correlations to the activity of Pd/TiO for photocatalytic reforming of methanol. *Physical Chemistry Chemical Physics*, **2019**, 21, 16154-16160	3.6	13
766	Investigating the Effect of NO on the Capture of CO2 Using Superbase Ionic Liquids for Flue Gas Applications. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 3567-3574	8.3	20
765	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. *Journal of Physical Chemistry C*, **2019** , 123, 8133-8144	3.8	6
764	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. *Journal of Chemical Theory and Computation*, **2019**, 15, 1317-1328	6.4	17
763	Investigation of ZSM-5 catalysts for dimethylether conversion using inelastic neutron scattering. *Applied Catalysis A: General*, **2019**, 569, 1-7	5.1	14
762	Bulk and surface properties of metal carbides: implications for catalysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 6905-6916	3.6	53
761	Computational investigation of CO adsorbed on Aux, Agx and (AuAg)x nanoclusters (x = 1 □5, 147) and monometallic Au and Ag low-energy surfaces. *European Physical Journal B*, **2018**, 91, 1	1.2	1
760	The electronic properties of Au clusters on CeO (110) surface with and without O-defects. *Faraday Discussions*, **2018**, 208, 123-145	3.6	9

759	Low-T Mechanisms of Ammonia Synthesis on Co3Mo3N. *Journal of Physical Chemistry C*, **2018**, 122, 6078-6082	3.6	54
758	Thermodynamically accessible titanium clusters Ti, N = 2-32. *Physical Chemistry Chemical Physics*, **2018**, 20, 13962-13973	3.6	10
757	Comparing ammonia diffusion in NH-SCR zeolite catalysts: a quasielastic neutron scattering and molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2018**, 20, 11976-11986	3.6	17
756	Supported metal nanoparticles with tailored catalytic properties through sol-immobilisation: applications for the hydrogenation of nitrophenols. *Faraday Discussions*, **2018**, 208, 443-454	3.6	8
755	The potential of manganese nitride based materials as nitrogen transfer reagents for nitrogen chemical looping. *Applied Catalysis B: Environmental*, **2018**, 223, 60-66	21.8	41
754	The integration of experiment and computational modelling in heterogeneously catalysed ammonia synthesis over metal nitrides. *Physical Chemistry Chemical Physics*, **2018**, 20, 21803-21808	3.6	15
753	Directed aqueous-phase reforming of glycerol through tailored platinum nanoparticles. *Applied Catalysis B: Environmental*, **2018**, 238, 618-628	21.8	40
752	Molecular dynamics study of tridymite. *IUCrJ*, **2018**, 5, 325-334	4.7	7
751	The effects of MTG catalysis on methanol mobility in ZSM-5. *Catalysis Science and Technology*, **2018**, 8, 3304-3312	5.5	15
750	Deep vs shallow nature of oxygen vacancies and consequent n-type carrier concentrations in transparent conducting oxides. *Physical Review Materials*, **2018**, 2,	3.2	46
749	Defect formation in In2O3 and SnO2: a new atomistic approach based on accurate lattice energies. *Journal of Materials Chemistry C*, **2018**, 6, 12386-12395	7.1	28
748	Room temperature methoxylation in zeolite H-ZSM-5: an operando DRIFTS/mass spectrometric study. *Chemical Communications*, **2018**, 54, 12875-12878	5.8	17
747	Interatomic potential parameters for Li-Cl-Ti interaction. *IOP Conference Series: Materials Science and Engineering*, **2018**, 430, 012016	0.4	
746	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
745	Modeling Hydrocarbon Oxidation Mechanisms Catalyzed by Microporous Materials **2018**, 265-295		
744	Bandgap Engineering of Organic Semiconductors for Highly Efficient Photocatalytic Water Splitting. *Advanced Energy Materials*, **2018**, 8, 1801084	21.8	90
743	Tandem Site- and Size-Controlled Pd Nanoparticles for the Directed Hydrogenation of Furfural. *ACS Catalysis*, **2017**, 7, 2266-2274	13.1	86
742	On the synthesis and performance of hierarchical nanoporous TS-1 catalysts. *Microporous and Mesoporous Materials*, **2017**, 244, 83-92	5.3	22

741	A DFT+U investigation of hydrogen adsorption on the LaFeO(010) surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 7399-7409	3.6	22
740	Heterostructures of GaN with SiC and ZnO enhance carrier stability and separation in framework semiconductors. *Physica Status Solidi (A) Applications and Materials Science*, **2017**, 214, 1600440	1.6	6
739	An assessment of hydrocarbon species in the methanol-to-hydrocarbon reaction over a ZSM-5 catalyst. *Faraday Discussions*, **2017**, 197, 447-471	3.6	27
738	Why Are Polar Surfaces of ZnO Stable?. *Chemistry of Materials*, **2017**, 29, 5306-5320	9.6	94
737	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
736	DFT-D3 study of H and N chemisorption over cobalt promoted TaN-(100), (010) and (001) surfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 11968-11974	3.6	18
735	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM. *Physica Status Solidi (A) Applications and Materials Science*, **2017**, 214, 1600445	1.6	9
734	Probing the Role of a Non-Thermal Plasma (NTP) in the Hybrid NTP Catalytic Oxidation of Methane. *Angewandte Chemie - International Edition*, **2017**, 56, 9351-9355	16.4	40
733	Quantum and Statistical Mechanical Simulations for Porous Catalyst Modelling **2017**, 253-288		1
732	Identification of single-site gold catalysis in acetylene hydrochlorination. *Science*, **2017**, 355, 1399-1403	33.3	285
731	Understanding the Role of Molecular Diffusion and Catalytic Selectivity in Liquid-Phase Beckmann Rearrangement. *ACS Catalysis*, **2017**, 7, 2926-2934	13.1	24
730	Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study. *Applied Surface Science*, **2017**, 400, 293-303	6.7	8
729	Neutron spectroscopy as a tool in catalytic science. *Chemical Communications*, **2017**, 53, 12164-12176	5.8	33
728	Screening Divalent Metals for A- and B-Site Dopants in LaFeO3. *Chemistry of Materials*, **2017**, 29, 8147-8157	9.6	37
727	Magnetic coupling constants for MnO as calculated using hybrid density functional theory. *Chemical Physics Letters*, **2017**, 690, 47-53	2.5	4
726	Sorbate Dynamics in Zeolite Catalysts. *Experimental Methods in the Physical Sciences*, **2017**, 49, 349-401	0.4	6
725	The adsorption of Cu on the CeO(110) surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 27191-27203	3.6	14
724	Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches **2017**, 647-680		3

723	Probing the Role of a Non-Thermal Plasma (NTP) in the Hybrid NTP Catalytic Oxidation of Methane. *Angewandte Chemie*, **2017**, 129, 9479-9483	3.6	3
722	A Computational Study of the Heterogeneous Synthesis of Hydrazine on CoMoN. *Catalysis Letters*, **2017**, 147, 1820-1826	2.8	2
721	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. *Journal of Physical Chemistry C*, **2017**, 121, 16831-16844	3.8	17
720	CO activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 19478-19486	3.6	9
719	Nitrogen transfer properties in tantalum nitride based materials. *Catalysis Today*, **2017**, 286, 147-154	5.3	17
718	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
717	Efficient and accurate approach to modeling the microstructure and defect properties of LaCoO3. *Physical Review B*, **2016**, 93,	3.3	13
716	Controlling Structural Transitions in AuAg Nanoparticles through Precise Compositional Design. *Journal of Physical Chemistry Letters*, **2016**, 7, 4414-4419	6.4	15
715	Defects and Oxide Ion Migration in the Solid Oxide Fuel Cell Cathode Material LaFeO3. *Chemistry of Materials*, **2016**, 28, 8210-8220	9.6	79
714	Towards microfluidic reactors for in situ synchrotron infrared studies. *Review of Scientific Instruments*, **2016**, 87, 024101	1.7	6
713	The sphere-in-contact model of carbon materials. *Journal of Molecular Modeling*, **2016**, 22, 40	2	6
712	Adsorption of formate species on Cu(h,k,l) low index surfaces. *Surface Science*, **2016**, 653, 45-54	1.8	19
711	Molecular dynamics study of liquid silica under high pressure. *Journal of Non-Crystalline Solids*, **2016** , 451, 124-130	3.9	5
710	Ammonia mobility in chabazite: insight into the diffusion component of the NH3-SCR process. *Physical Chemistry Chemical Physics*, **2016**, 18, 17159-68	3.6	23
709	Room temperature methoxylation in zeolites: insight into a key step of the methanol-to-hydrocarbons process. *Chemical Communications*, **2016**, 52, 2897-900	5.8	46
708	Design and control of Lewis acid sites in Sn-substituted microporous architectures. *Journal of Materials Chemistry A*, **2016**, 4, 5706-5712	13	5
707	A density functional theory study of arsenic immobilization by the Al(III)-modified zeolite clinoptilolite. *Physical Chemistry Chemical Physics*, **2016**, 18, 11297-305	3.6	7
706	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. *Faraday Discussions*, **2016**, 188, 235-55	3.6	26

705	Catalysis making the world a better place: satellite meeting. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	5
704	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. *Physical Review B*, **2016**, 93,	3.3	33
703	Evidence for a surface gold hydride on a nanostructured gold catalyst. *Chemical Communications*, **2016**, 52, 533-6	5.8	35
702	Challenges in the structural science of materials. *IUCrJ*, **2016**, 3, 226-7	4.7	
701	Prediction of Rate Constants for Catalytic Reactions with Chemical Accuracy. *Angewandte Chemie - International Edition*, **2016**, 55, 9132-3	16.4	5
700	Vorhersage von Geschwindigkeitskonstanten katalytischer Reaktionen mit chemischer Genauigkeit. *Angewandte Chemie*, **2016**, 128, 9278-9279	3.6	
699	Nonstoichiometry and Weyl fermionic behavior in TaAs. *Physical Review B*, **2016**, 94,	3.3	16
698	Band gap reduction in InNxSb1-x alloys: Optical absorption, k □P modeling, and density functional theory. *Applied Physics Letters*, **2016**, 109, 132104	3.4	9
697	The adsorbed state of a thiol on palladium nanoparticles. *Physical Chemistry Chemical Physics*, **2016**, 18, 17265-71	3.6	5
696	Methanol diffusion in zeolite HY: a combined quasielastic neutron scattering and molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2016**, 18, 17294-302	3.6	29
695	The reaction of formic acid with Raney copper. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2016**, 472, 20160126	2.4	2
694	Phase control during the synthesis of nickel sulfide nanoparticles from dithiocarbamate precursors. *Nanoscale*, **2016**, 8, 11067-75	7.7	52
693	Optimised hydrogen production by aqueous phase reforming of glycerol on Pt/Al2O3. *International Journal of Hydrogen Energy*, **2016**, 41, 18441-18450	6.7	34
692	DFT-D3 Study of Molecular N2 and H2 Activation on Co3Mo3N Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 21390-21398	3.8	42
691	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 28648-28660	3.6	7
690	Compressive straining of bilayer phosphorene leads to extraordinary electron mobility at a new conduction band edge. *Nano Letters*, **2015**, 15, 2006-10	11.5	37
689	Tailoring Gold Nanoparticle Characteristics and the Impact on Aqueous-Phase Oxidation of Glycerol. *ACS Catalysis*, **2015**, 5, 4377-4384	13.1	44
688	Restructuring of AuPd Nanoparticles Studied by a Combined XAFS/DRIFTS Approach. *Chemistry of Materials*, **2015**, 27, 3714-3720	9.6	44

687	Advances in theory and their application within the field of zeolite chemistry. *Chemical Society Reviews*, **2015**, 44, 7044-111	58.5	319
686	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92
685	Bio-inspired CO2 conversion by iron sulfide catalysts under sustainable conditions. *Chemical Communications*, **2015**, 51, 7501-4	5.8	149
684	Applying a new interatomic potential for the modelling of hexagonal and orthorhombic YMnO3. *Journal of Materials Chemistry C*, **2015**, 3, 4787-4793	7.1	17
683	Influence of Composition and Chemical Arrangement on the Kinetic Stability of 147-Atom Au Ag Bimetallic Nanoclusters. *Journal of Physical Chemistry C*, **2015**, 119, 23685-23697	3.8	24
682	Nitrogen Activation in a Mars van Krevelen Mechanism for Ammonia Synthesis on Co3Mo3N. *Journal of Physical Chemistry C*, **2015**, 119, 28368-28376	3.8	98
681	Structural, energetic and electronic properties of (100) surfaces for alkaline earth metal oxides as calculated with hybrid density functional theory. *Surface Science*, **2015**, 642, 58-65	1.8	16
680	Understanding the Thermal Stability of Silver Nanoparticles Embedded in a-Si. *Journal of Physical Chemistry C*, **2015**, 119, 23767-23773	3.8	12
679	Recent developments in the structural science of materials. *IUCrJ*, **2015**, 2, 384-6	4.7	
678	Diffusion of Isobutane in Silicalite: A Neutron Spin Echo and Molecular Dynamics Simulation Study. *Journal of Physical Chemistry C*, **2015**, 119, 26999-27006	3.8	19
677	Molecular dynamics simulations of longer n-alkanes in silicalite: state-of-the-art models achieving close agreement with experiment. *Physical Chemistry Chemical Physics*, **2015**, 17, 1943-8	3.6	24
676	Buckeridge et al. Reply. *Physical Review Letters*, **2015**, 115, 029702	7.4	5
675	Iridicycle-Catalysed Imine Reduction: An Experimental and Computational Study of the Mechanism. *Chemistry - A European Journal*, **2015**, 21, 16564-77	4.8	39
674	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. *Journal of Physical Chemistry C*, **2015**, 119, 11598-11611	3.8	27
673	Modelling and Predicting Crystal Structures. *Interdisciplinary Science Reviews*, **2015**, 40, 294-307	0.7	7
672	Synchrotron radiation techniques in materials and environmental science. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2015**, 373,	3	5
671	Adsorption of Water on Yttria-Stabilized Zirconia. *Journal of Physical Chemistry C*, **2015**, 119, 22526-22533	3.8	17
670	Oxidative methane activation over yttrium stabilised zirconia. *Chemical Communications*, **2015**, 51, 5856-9	6.8	6

669	Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals. *Physical Review Letters*, **2015**, 114, 016405	7.4	58
668	Crystal electron binding energy and surface work function control of tin dioxide. *Physical Review B*, **2014**, 89,	3.3	42
667	Designer titania-supported Au-Pd nanoparticles for efficient photocatalytic hydrogen production. *ACS Nano*, **2014**, 8, 3490-7	16.7	249
666	N incorporation and associated localized vibrational modes in GaSb. *Physical Review B*, **2014**, 89,	3.3	12
665	The Nature of the Molybdenum Surface in Iron Molybdate. The Active Phase in Selective Methanol Oxidation. *Journal of Physical Chemistry C*, **2014**, 118, 26155-26161	3.8	49
664	Active Nature of Primary Amines during Thermal Decomposition of Nickel Dithiocarbamates to Nickel Sulfide Nanoparticles. *Chemistry of Materials*, **2014**, 26, 6281-6292	9.6	70
663	Double bubbles: a new structural motif for enhanced electron-hole separation in solids. *Physical Chemistry Chemical Physics*, **2014**, 16, 21098-105	3.6	10
662	Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe. *Journal of Materials Chemistry C*, **2014**, 2, 3429-3438	7.1	45
661	The reactivity of CO□and H□at trapped electron sites at an oxide surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 21153-6	3.6	7
660	The reactivity of CO2 on the MgO(100) surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 184-95	3.6	27
659	Segregation effects on the properties of (AuAg)□*Physical Chemistry Chemical Physics*, **2014**, 16, 21049-61	3.6	28
658	Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides. *Physical Review B*, **2014**, 90,	3.3	28
657	Interlayer cation exchange stabilizes polar perovskite surfaces. *Advanced Materials*, **2014**, 26, 7252-6	24	34
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