William Goddard

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

749 papers	67,293 citations	119 h-index	238 g-index
786 ext. papers	75,423 ext. citations	8.5 avg, IF	8.17 L-index

#	Paper	IF	Citations
749	Complete inhibition of a polyol nucleation by a micromolar biopolymer additive.. *Cell Reports Physical Science*, **2022**, 3, 100723-100723	6.1	0
748	Au-activated N motifs in non-coherent cupric porphyrin metal organic frameworks for promoting and stabilizing ethylene production.. *Nature Communications*, **2022**, 13, 63	17.4	11
747	Programmable siRNA pro-drugs that activate RNAi activity in response to specific cellular RNA biomarkers.. *Molecular Therapy - Nucleic Acids*, **2022**, 27, 797-809	10.7	0
746	Biased Agonists Favoring Gs over Arrestin for Individualized Treatment of Obstructive Lung Disease.. *Journal of Personalized Medicine*, **2022**, 12,	3.6	1
745	Electron-catalysed molecular recognition.. *Nature*, **2022**, 603, 265-270	50.4	7
744	Performance of electrochemical immunoassays for clinical diagnostics of SARS-CoV-2 based on selective nucleocapsid N protein detection: Boron-doped diamond, gold and glassy carbon evaluation.. *Biosensors and Bioelectronics*, **2022**, 209, 114222	11.8	3
743	The mechanism for ligand activation of the GPCR-G protein complex.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2110085119	11.5	2
742	The L-G phase transition in binary Cu-Zr metallic liquids.. *Physical Chemistry Chemical Physics*, **2021**, 24, 497-506	3.6	0
741	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. *Journal of Physical Chemistry Letters*, **2021**, 11886-11893	6.4	4
740	Order-Tuned Deformability of Bismuth Telluride Semiconductors: An Energy-Dissipation Strategy for Large Fracture Strain. *ACS Applied Materials & Interfaces*, **2021**, 13, 57629-57637	9.5	
739	Reaction Mechanism and Strategy for Optimizing the Hydrogen Evolution Reaction on Single-Layer 1T' WSe and WTe Based on Grand Canonical Potential Kinetics. *ACS Applied Materials & Interfaces*, **2021**, 13, 55611-55620	9.5	2
738	Identification and characterization of an atypical G-biased AR agonist that fails to evoke airway smooth muscle cell tachyphylaxis. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	4
737	Structure, Energetics, and Spectra for the Oxygen Vacancy in Rutile: Prominence of the Ti-H-Ti Bond. *Journal of Physical Chemistry Letters*, **2021**, 12, 10175-10181	6.4	1
736	Reaction Mechanism and Energetics of Decomposition of Tetrakis(1,3-dimethyltetrazol-5-imidoperchloratomanganese(II)) from Quantum-Mechanics-based Reactive Dynamics. *Journal of the American Chemical Society*, **2021**, 143, 16960-16975	16.4	1
735	Synergic Effects in the Activation of the Sweet Receptor GPCR Heterodimer for Various Sweeteners Predicted Using Molecular Metadynamics Simulations. *Journal of Agricultural and Food Chemistry*, **2021**, 69, 12250-12261	5.7	1
734	Electrochemical Performance and Structures of Chromium and Molybdenum-Doped LixVOPO4 Predicted as Promising Cathodes for Next Generation Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2021**, 125, 275-282	3.8	1
733	Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis. *ACS Nano*, **2021**, 15, 1675-1684	16.7	3

732	Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation. *Journal of the American Chemical Society*, **2021**, 143, 5355-5363	16.4	7
731	Selective Activation of Propane Using Intermediates Generated during Water Oxidation. *Journal of the American Chemical Society*, **2021**, 143, 3967-3974	16.4	8
730	Self-assembly mechanism of PEG-b-PCL and PEG-b-PBO-b-PCL amphiphilic copolymer micelles in aqueous solution from coarse grain modeling. *Journal of Polymer Science*, **2021**, 59, 614-626	2.4	0
729	The first order L-G phase transition in liquid Ag and Ag-Cu alloys is driven by deviatoric strain. *Scripta Materialia*, **2021**, 194, 113695	5.6	4
728	Effects of High and Low Salt Concentrations in Electrolytes at Lithium-Metal Anode Surfaces Using DFT-ReaxFF Hybrid Molecular Dynamics Method. *Journal of Physical Chemistry Letters*, **2021**, 12, 2922-2929	6.4	12
727	Stabilizing Highly Active Ru Sites by Suppressing Lattice Oxygen Participation in Acidic Water Oxidation. *Journal of the American Chemical Society*, **2021**, 143, 6482-6490	16.4	38
726	Fracture toughness of thermoelectric materials. *Materials Science and Engineering Reports*, **2021**, 144, 100607	30.9	7
725	Mechanistic Studies of Styrene Production from Benzene and Ethylene Using [(□-C2H4)2Rh(□OAc)]2 as Catalyst Precursor: Identification of a Bis-RhI Mono-CuII Complex As the Catalyst. *ACS Catalysis*, **2021**, 11, 5688-5702	13.1	3
724	Functionalization of RhIII□Me Bonds: Use of □Capping Arene□Ligands to Facilitate Me□X Reductive Elimination. *Organometallics*, **2021**, 40, 1889-1906	3.8	2
723	Real-time control of dendritic propagation in rechargeable batteries using adaptive pulse relaxation. *Journal of Chemical Physics*, **2021**, 154, 194702	3.9	1
722	Double-Exchange-Induced in situ Conductivity in Nickel-Based Oxyhydroxides: An Effective Descriptor for Electrocatalytic Oxygen Evolution. *Angewandte Chemie - International Edition*, **2021**, 60, 16448-16456	16.4	15
721	Electrocatalytic Water Oxidation by a Trinuclear Copper(II) Complex. *ACS Catalysis*, **2021**, 11, 7223-7240	13.1	8
720	Predicted Operando Polymerization at Lithium Anode via Boron Insertion. *ACS Energy Letters*, **2021**, 6, 2320-2327	20.1	7
719	CO reduction on pure Cu produces only H after subsurface O is depleted: Theory and experiment. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	11
718	Predictions of Chemical Shifts for Reactive Intermediates in CO Reduction under Conditions. *ACS Applied Materials & Interfaces*, **2021**, 13, 31554-31560	9.5	3
717	Double-Exchange-Induced in situ Conductivity in Nickel-Based Oxyhydroxides: An Effective Descriptor for Electrocatalytic Oxygen Evolution. *Angewandte Chemie*, **2021**, 133, 16584-16592	3.6	0
716	Sulfur-doped graphene anchoring of ultrafine Au25 nanoclusters for electrocatalysis. *Nano Research*, **2021**, 14, 3509-3513	10	11
715	Understanding Reaction Networks through Controlled Approach to Equilibrium Experiments Using Transient Methods. *Journal of the American Chemical Society*, **2021**, 143, 10998-11006	16.4	0

714	Shear induced deformation twinning evolution in thermoelectric InSb. *Npj Computational Materials*, **2021**, 7,	10.9	4
713	Approaching 100% Selectivity at Low Potential on Ag for Electrochemical CO2 Reduction to CO Using a Surface Additive. *ACS Catalysis*, **2021**, 11, 9034-9042	13.1	5
712	Sulfated glycans engage the Ang-Tie pathway to regulate vascular development. *Nature Chemical Biology*, **2021**, 17, 178-186	11.7	11
711	A Novel Method for Estimating the Charge Equilibrium within the Dendrites of Rechargeable Batteries. *Computational Materials Science*, **2021**, 187, 110059	3.2	4
710	Artificial Intelligence and QM/MM with a Polarizable Reactive Force Field for Next-Generation Electrocatalysts. *Matter*, **2021**, 4, 195-216	12.7	16
709	London Dispersion Corrections to Density Functional Theory for Transition Metals Based on Fitting to Experimental Temperature-Programmed Desorption of Benzene Monolayers. *Journal of Physical Chemistry Letters*, **2021**, 12, 73-79	6.4	
708	Oxygen evolution reaction over catalytic single-site Co in a well-defined brookite TiO2 nanorod surface. *Nature Catalysis*, **2021**, 4, 36-45	36.5	88
707	Pulse Reverse Protocol for efficient suppression of dendritic micro-structures in rechargeable batteries. *Electrochimica Acta*, **2021**, 367, 137469	6.7	2
706	Morphometry of Dendritic Materials in Rechargeable Batteries. *Journal of Power Sources*, **2021**, 481, 228914	8.9	6
705	Quantum mechanics based mechanisms for selective activation of hydrocarbons by mixed metal oxide heterogeneous catalysts A tribute to Robert Grasselli. *Catalysis Today*, **2021**, 363, 3-9	5.3	
704	Coarse-grained force-field for large scale molecular dynamics simulations of polyacrylamide and polyacrylamide-gels based on quantum mechanics. *Physical Chemistry Chemical Physics*, **2021**, 23, 10909-10918	3.6	1
703	Predicted structure of fully activated human bitter taste receptor TAS2R4 complexed with G protein and agonists. *QRB Discovery*, **2021**, 2,	2.7	4
702	Design of robust 2,2'-bipyridine ligand linkers for the stable immobilization of molecular catalysts on silicon(111) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 9921-9929	3.6	1
701	The G protein-first activation mechanism of opioid receptors by Gi protein and agonists. *QRB Discovery*, **2021**, 2,	2.7	3
700	Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphere-Water Systems. *ACS Nano*, **2021**, 15, 6276-6288	16.7	3
699	Reduction of N to Ammonia by Phosphate Molten Salt and Li Electrode: Proof of Concept Using Quantum Mechanics. *Journal of Physical Chemistry Letters*, **2021**, 12, 1696-1701	6.4	1
698	Hedgehog proteins create a dynamic cholesterol interface. *PLoS ONE*, **2021**, 16, e0246814	3.7	4
697	Operando Electrochemical Spectroscopy for CO on Cu(100) at pH 1 to 13: Validation of Grand Canonical Potential Predictions. *ACS Catalysis*, **2021**, 11, 3173-3181	13.1	3

696	Selective CO Electrochemical Reduction Enabled by a Tricomponent Copolymer Modifier on a Copper Surface. *Journal of the American Chemical Society*, **2021**, 143, 2857-2865	16.4	31
695	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. *ACS Nano*, **2021**, 15, 6369-6385	16.7	2
694	Role of Ferryl Ion Intermediates in Fast Fenton Chemistry on Aqueous Microdroplets. *Environmental Science & Technology*, **2021**, 55, 14370-14377	10.3	5
693	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
692	Rhodium and Iridium Complexes Bearing Capping Arene Ligands: Synthesis and Characterization. *Organometallics*, **2021**, 40, 2808-2825	3.8	3
691	Identifying the Imperative Role of Metal-Olefin Interactions in Catalytic C-O Reductive Elimination from Nickel(II).. *ACS Catalysis*, **2021**, 11, 10208-10222	13.1	3
690	Development of the ReaxFF Reactive Force Field for Cu/Si Systems with Application to Copper Cluster Formation during Cu Diffusion Inside Silicon. *Journal of Physical Chemistry C*, **2021**, 125, 19455-19466	3.8	1
689	Temperature-dependent anharmonic effects on shear deformability of Bi2Te3 semiconductor. *Scripta Materialia*, **2021**, 202, 114016	5.6	2
688	Dramatic Change in the Step Edges of the Cu(100) Electrocatalyst upon Exposure to CO: Operando Observations by Electrochemical STM and Explanation Using Quantum Mechanical Calculations. *ACS Catalysis*, **2021**, 11, 12068-12074	13.1	0
687	Entropic Stabilization of Water at Graphitic Interfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 9162-9168	6.4	0
686	Predicted Structure of Fully Activated Tas1R3/1R3' Homodimer Bound to G Protein and Natural Sugars: Structural Insights into G Protein Activation by a Class C Sweet Taste Homodimer with Natural Sugars. *Journal of the American Chemical Society*, **2021**, 143, 16824-16838	16.4	2
685	Structures and Agonist Binding Sites of Bitter Taste Receptor TAS2R5 Complexed with Gi Protein and Validated against Experiment. *Journal of Physical Chemistry Letters*, **2021**, 12, 9293-9300	6.4	2
684	The DFT-ReaxFF Hybrid Reactive Dynamics Method with Application to the Reductive Decomposition Reaction of the TFSI and DOL Electrolyte at a Lithium-Metal Anode Surface. *Journal of Physical Chemistry Letters*, **2021**, 12, 1300-1306	6.4	18
683	Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N2 Reduction to NH3 on Fe Surfaces via Density Functional Theory. *Journal of Physical Chemistry C*, **2021**, 125, 27919-27930	3.8	0
682	Novel interaction between neurotrophic factor-1/carboxypeptidase E and serotonin receptor, 5-HTR1E, protects human neurons against oxidative/neuroexcitotoxic stress via arrestin/ERK signaling.. *Cellular and Molecular Life Sciences*, **2021**, 79, 1	10.3	3
681	Preface to Advances in Heterogeneous Catalysis and Electrocatalysis Including New Insights from Surface Science and Quantum Mechanics, Published in Honor of Professor Robert K. Grasselli, Irsee VIII Symposium Kloster Irsee, Germany 23–26 May 2019 (Irsee VIII) *Topics in Catalysis*, **2020**, 63, 1645-1646	2.3	
680	Use of Ligand Steric Properties to Control the Thermodynamics and Kinetics of Oxidative Addition and Reductive Elimination with Pincer-Ligated Rh Complexes. *Organometallics*, **2020**, 39, 1917-1933	3.8	5
679	Reaction mechanism and kinetics for CO reduction on nickel single atom catalysts from quantum mechanics. *Nature Communications*, **2020**, 11, 2256	17.4	59

678	Synergy between a Silver-Copper Surface Alloy Composition and Carbon Dioxide Adsorption and Activation. *ACS Applied Materials & Interfaces*, **2020**, 12, 25374-25382	9.5	7
677	Formation of two glass phases in binary Cu-Ag liquid. *Acta Materialia*, **2020**, 195, 274-281	8.4	15
676	Electrochemical Switching of a Fluorescent Molecular Rotor Embedded within a Bistable Rotaxane. *Journal of the American Chemical Society*, **2020**, 142, 11835-11846	16.4	19
675	Design of a Graphene Nitrene Two-Dimensional Catalyst Heterostructure Providing a Well-Defined Site Accommodating One to Three Metals, with Application to CO Reduction Electrocatalysis for the Two-Metal Case. *Journal of Physical Chemistry Letters*, **2020**, 11, 2541-2549	6.4	25
674	The atomistic level structure for the activated human □opioid receptor bound to the full Gi protein and the MP1104 agonist. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 5836-5843	11.5	19
673	Effects of Surface Roughness on the Electrochemical Reduction of CO2 over Cu. *ACS Energy Letters*, **2020**, 5, 1206-1214	20.1	80
672	Highly Stable Organic Bisradicals Protected by Mechanical Bonds. *Journal of the American Chemical Society*, **2020**, 142, 7190-7197	16.4	10
671	Mechanism of □arrestin recruitment by the □opioid G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 16346-16355	11.5	18
670	Reaction Mechanism, Origins of Enantioselectivity, and Reactivity Trends in Asymmetric Allylic Alkylation: A Comprehensive Quantum Mechanics Investigation of a C(sp)-C(sp) Cross-Coupling. *Journal of the American Chemical Society*, **2020**, 142, 13917-13933	16.4	20
669	Structural failure of layered thermoelectric In4Se3-□semiconductors is dominated by shear slippage. *Acta Materialia*, **2020**, 187, 84-90	8.4	1
668	Group Vibrational Mode Assignments as a Broadly Applicable Tool for Characterizing Ionomer Membrane Structure as a Function of Degree of Hydration. *Chemistry of Materials*, **2020**, 32, 1828-1843	9.6	2
667	Synergetic Evolution of Sacrificial Bonds and Strain-Induced Defects Facilitating Large Deformation of the Bi2Te3 Semiconductor. *ACS Applied Energy Materials*, **2020**, 3, 3042-3048	6.1	2
666	Permeation of CO2 and N2 through glassy poly(dimethyl phenylene) oxide under steady- and presteady-state conditions. *Journal of Polymer Science*, **2020**, 58, 1207-1228	2.4	5
665	Li-diffusion at the interface between Li-metal and [Pyr][TFSI]-ionic liquid: Ab initio molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 152, 031101	3.9	7
664	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. *Journal of the American Chemical Society*, **2020**, 142, 8223-8232	16.4	14
663	Atomistic Explanation of the Dramatically Improved Oxygen Reduction Reaction of Jagged Platinum Nanowires, 50 Times Better than Pt. *Journal of the American Chemical Society*, **2020**, 142, 8625-8632	16.4	32
662	Extracellular interaction between Neurotrophic factor-□ and HTR1E serotonin receptor promotes cell survival. *FASEB Journal*, **2020**, 34, 1-1	0.9	
661	Photochemically deposited Ir-doped NiCo oxyhydroxide nanosheets provide highly efficient and stable electrocatalysts for the oxygen evolution reaction. *Nano Energy*, **2020**, 75, 104885	17.1	18

660	Compressed Intermetallic PdCu for Enhanced Electrocatalysis. *ACS Energy Letters*, **2020**, 5, 3672-3680	20.1	19
659	Intrinsic mechanical behavior of MgAgSb thermoelectric material: An ab initio study. *Journal of Materiomics*, **2020**, 6, 24-32	6.7	1
658	Predicted Optimal Bifunctional Electrocatalysts for the Hydrogen Evolution Reaction and the Oxygen Evolution Reaction Using Chalcogenide Heterostructures Based on Machine Learning Analysis of in Silico Quantum Mechanics Based High Throughput Screening. *Journal of Physical Chemistry Letters*, **2020**, 11, 869-876	6.4	23
657	First-Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase. *Journal of Physical Chemistry Letters*, **2020**, 11, 632-645	6.4	15
656	The Mechanism of Deformation and Failure of In4Se3 Based Thermoelectric Materials. *ACS Applied Energy Materials*, **2020**, 3, 1054-1062	6.1	1
655	Comparing the oxygen reduction reaction on selectively edge halogen doped graphene from quantum mechanics. *Journal of Catalysis*, **2020**, 381, 295-307	7.3	2
654	A coarse-grain force field based on quantum mechanics (CGq FF) for molecular dynamics simulation of poly(ethylene glycol)-block-poly(ε-caprolactone) (PEG-b-PCL) micelles. *Physical Chemistry Chemical Physics*, **2020**, 22, 24028-24040	3.6	3
653	New Quantum Mechanics Based Methods for Multiscale Simulations with Applications to Reaction Mechanisms for Electrocatalysis. *Topics in Catalysis*, **2020**, 63, 1658-1666	2.3	1
652	Toward Concurrent Engineering of the M1-Based Catalytic Systems for Oxidative Dehydrogenation (ODH) of Alkanes. *Topics in Catalysis*, **2020**, 63, 1667-1681	2.3	3
651	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. *Chemistry of Materials*, **2020**, 32, 9914-9924	9.6	3
650	Highly Selective Electrocatalytic Reduction of CO into Methane on Cu-Bi Nanoalloys. *Journal of Physical Chemistry Letters*, **2020**, 11, 7261-7266	6.4	20
649	Oxygen induced promotion of electrochemical reduction of CO via co-electrolysis. *Nature Communications*, **2020**, 11, 3844	17.4	35
648	Inertial dynamics of an interface with interfacial mass flux: Stability and flow fields□structure, inertial stabilization mechanism, degeneracy of Landau□ solution, effect of energy fluctuations, and chemistry-induced instabilities. *Physics of Fluids*, **2020**, 32, 082105	4.4	4
647	The Transition Metal Catalyzed [□s + □s + □s + □s] Pericyclic Reaction: Woodward-Hoffmann Rules, Aromaticity, and Electron Flow. *Journal of the American Chemical Society*, **2020**, 142, 19033-19039	16.4	4
646	Highly active and stable stepped Cu surface for enhanced electrochemical CO2 reduction to C2H4. *Nature Catalysis*, **2020**, 3, 804-812	36.5	118
645	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. *Journal of Physical Chemistry C*, **2020**, 124, 9787-9794	3.8	4
644	Finite-pulse waves for efficient suppression of evolving mesoscale dendrites in rechargeable batteries. *Physical Review E*, **2019**, 100, 042801	2.4	9
643	CO Coupling Chemistry of a Terminal Mo Carbide: Sequential Addition of Proton, Hydride, and CO Releases Ethenone. *Journal of the American Chemical Society*, **2019**, 141, 15664-15674	16.4	20

642	Reply to Head-Gordon and Paesani: Liquid water, a branched polymer with ~100-fs short-lived heterogeneous hydrogen bonds. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 20257-20258	11.5	1
641	Anomalies in Supercooled Water at ~230 K Arise from a 1D Polymer to 2D Network Topological Transformation. *Journal of Physical Chemistry Letters*, **2019**, 10, 6267-6273	6.4	7
640	Design of a One-Dimensional Stacked Spin Peierls System with Room-Temperature Switching from Quantum Mechanical Predictions. *Journal of Physical Chemistry Letters*, **2019**, 10, 6432-6437	6.4	1
639	Interfaces and mixing: Nonequilibrium transport across the scales. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18171-18174	11.5	7
638	The chemical reactions in electrosprays of water do not always correspond to those at the pristine air-water interface. *Chemical Science*, **2019**, 10, 2566-2577	9.4	32
637	Csp-Csp Bond-Forming Reductive Elimination from Well-Defined Copper(III) Complexes. *Journal of the American Chemical Society*, **2019**, 141, 3153-3159	16.4	56
636	Liquid water is a dynamic polydisperse branched polymer. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 1998-2003	11.5	33
635	Effect of Co doping on mechanism and kinetics of ammonia synthesis on Fe(1 1 1) surface. *Journal of Catalysis*, **2019**, 370, 364-371	7.3	12
634	Identifying Active Sites for CO Reduction on Dealloyed Gold Surfaces by Combining Machine Learning with Multiscale Simulations. *Journal of the American Chemical Society*, **2019**, 141, 11651-11657	16.4	59
633	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. *Journal of Physical Chemistry C*, **2019**, 123, 17375-17383	3.8	9
632	DFT Mechanistic Study of Methane Mono-Esterification by Hypervalent Iodine Alkane Oxidation Process. *Journal of Physical Chemistry C*, **2019**, 123, 15674-15684	3.8	9
631	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. *Nature Catalysis*, **2019**, 2, 495-503	36.5	258
630	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 11444-11454	3.6	17
629	Effectively Increased Efficiency for Electroreduction of Carbon Monoxide Using Supported Polycrystalline Copper Powder Electrocatalysts. *ACS Catalysis*, **2019**, 9, 4709-4718	13.1	47
628	Dramatic differences in carbon dioxide adsorption and initial steps of reduction between silver and copper. *Nature Communications*, **2019**, 10, 1875	17.4	40
627	Dramatically reduced lattice thermal conductivity of Mg2Si thermoelectric material from nanotwinning. *Acta Materialia*, **2019**, 169, 9-14	8.4	17
626	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of β-HMX to δ-HMX. *Journal of Physical Chemistry C*, **2019**, 123, 9231-9236	3.8	21
625	Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 7718-7722	11.5	40

624	Light irradiation induced brittle-to-ductile and ductile-to-brittle transition in inorganic semiconductors. *Physical Review B*, **2019**, 99,	3.3	12
623	Electrocatalysis at Organic-Metal Interfaces: Identification of Structure-Reactivity Relationships for CO Reduction at Modified Cu Surfaces. *Journal of the American Chemical Society*, **2019**, 141, 7355-7364	16.4	76
622	Initial Steps in Forming the Electrode-Electrolyte Interface: HO Adsorption and Complex Formation on the Ag(111) Surface from Combining Quantum Mechanics Calculations and Ambient Pressure X-ray Photoelectron Spectroscopy. *Journal of the American Chemical Society*, **2019**, 141, 6946-6954	16.4	12
621	Density functional theory based neural network force fields from energy decompositions. *Physical Review B*, **2019**, 99,	3.3	40
620	Effects of Lewis Acidic Metal Ions (M) on Oxygen-Atom Transfer Reactivity of Heterometallic MnMO Cubane and FeMO(OH) and MnMO(OH) Clusters. *Inorganic Chemistry*, **2019**, 58, 2336-2345	5.1	10
619	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18193-18201	11.5	6
618	Interface dynamics: Mechanisms of stabilization and destabilization and structure of flow fields. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18218-18226	11.5	9
617	Reply to the 'Comment on "The chemical reactions in electrosprays of water do not always correspond to those at the pristine air-water interface"' by A. J. Colussi and S. Enami, , 2019, , DOI: 10.1039/c9sc00991d. *Chemical Science*, **2019**, 10, 8256-8261	9.4	9
616	Formation of carbon-nitrogen bonds in carbon monoxide electrolysis. *Nature Chemistry*, **2019**, 11, 846-851	17.6	82
615	Mechanism and kinetics for both thermal and electrochemical reduction of N catalysed by Ru(0001) based on quantum mechanics. *Physical Chemistry Chemical Physics*, **2019**, 21, 17605-17612	3.6	9
614	Interface Structure in Li-Metal/[Pyr][TFSI]-Ionic Liquid System from ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2019**, 10, 4577-4586	6.4	19
613	Computational and experimental demonstrations of one-pot tandem catalysis for electrochemical carbon dioxide reduction to methane. *Nature Communications*, **2019**, 10, 3340	17.4	81
612	Role of solvent-anion charge transfer in oxidative degradation of battery electrolytes. *Nature Communications*, **2019**, 10, 3360	17.4	26
611	Discovery of Novel Biased Opioid Receptor Ligands through Structure-Based Pharmacophore Virtual Screening and Experiment. *ChemMedChem*, **2019**, 14, 1783-1794	3.7	3
610	Accurate non-bonded potentials based on periodic quantum mechanics calculations for use in molecular simulations of materials and systems. *Journal of Chemical Physics*, **2019**, 151, 154111	3.9	16
609	First principles predicting enhanced ductility of boride carbide through magnesium microalloying. *Journal of the American Ceramic Society*, **2019**, 102, 5514-5523	3.8	5
608	Electronic Structural Origin of the Catalytic Activity Trend of Transition Metals for Electrochemical Nitrogen Reduction. *Journal of Physical Chemistry C*, **2019**, 123, 31026-31031	3.8	10
607	The PX Motif of DNA Binds Specifically to Escherichia coli DNA Polymerase I. *Biochemistry*, **2019**, 58, 575-581	3.2	4

606	Growth and Isolation of Large Area Boron-Doped Nanocrystalline Diamond Sheets: A Route toward Diamond-on-Graphene Heterojunction. *Advanced Functional Materials*, **2019**, 29, 1805242	15.6	9
605	Discrete Dimers of Redox-Active and Fluorescent Perylene Diimide-Based Rigid Isosceles Triangles in the Solid State. *Journal of the American Chemical Society*, **2019**, 141, 1290-1303	16.4	54
604	A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials. *Advanced Materials*, **2019**, 31, e1805405	24	72
603	First-principles-based reaction kinetics from reactive molecular dynamics simulations: Application to hydrogen peroxide decomposition. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18202-18208	11.5	18
602	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. *Computing in Science and Engineering*, **2019**, 21, 64-75	1.5	3
601	pH-Dependent Conformations for Hyperbranched Poly(ethylenimine) from All-Atom Molecular Dynamics. *Macromolecules*, **2018**, 51, 2187-2194	5.5	11
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