Jens Norskov

List of Publications by Year in Descending Order

693 papers	155,033 citations	193 h-index	382 g-index
736 ext. papers	175,921 ext. citations	8.1 avg, IF	8.83 L-index

#	Paper	IF	Citations
693	Why ZnO is the Support for Cu in Methanol Synthesis? A Systematic Study of the Strong Metal Support Interactions. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 1722-1730	3.1	1
692	Opportunities and Challenges in Electrolytic Propylene Epoxidation.. *Journal of Physical Chemistry Letters*, **2022**, 2057-2063	1.7	2
691	Stability and Activity of Cobalt Antimonate for Oxygen Reduction in Strong Acid. *ACS Energy Letters*, **2022**, 7, 993-1000	6.8	3
690	OH Binding Energy as a Universal Descriptor of the Potential of Zero Charge on Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 5521-5528	1.2	1
689	Insights into the Hydrogen Evolution Reaction on 2D Transition-Metal Dichalcogenides. *Journal of Physical Chemistry C*, **2022**, 126, 5151-5158	1.2	6
688	Monitoring oxygen production on mass-selected iridium□tantalum oxide electrocatalysts. *Nature Energy*, **2022**, 7, 55-64	18	17
687	A spin promotion effect in catalytic ammonia synthesis.. *Nature Communications*, **2022**, 13, 2382	5	5
686	Nonaqueous Solvent Adsorption on Transition Metal Surfaces with Density Functional Theory: Interaction of N,N-Dimethylformamide (DMF), Tetrahydrofuran (THF), and Dimethyl Sulfoxide (DMSO) with Ag, Cu, Pt, Rh, and Re Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 21943-21957	1.2	2
685	Theory-Aided Discovery of Metallic Catalysts for Selective Propane Dehydrogenation to Propylene. *ACS Catalysis*, **2021**, 11, 6290-6297	4.1	6
684	Origins of the Instability of Nonprecious Hydrogen Evolution Reaction Catalysts at Open-Circuit Potential. *ACS Energy Letters*, **2021**, 6, 2268-2274	6.8	12
683	Generalizable Trends in Electrochemical Protonation Barriers. *Journal of Physical Chemistry Letters*, **2021**, 12, 5193-5200	1.7	11
682	Analysis of the limitations in the oxygen reduction activity of transition metal oxide surfaces. *Nature Catalysis*, **2021**, 4, 463-468	10.3	48
681	Probing the Effects of Acid Electrolyte Anions on Electrocatalyst Activity and Selectivity for the Oxygen Reduction Reaction. *ChemElectroChem*, **2021**, 8, 2467-2478	1.2	4
680	Electrochemical oxidation of molecular nitrogen to nitric acid - towards a molecular level understanding of the challenges. *Chemical Science*, **2021**, 12, 6442-6448	2.5	12
679	Neural Network Sampling of the Free Energy Landscape for Nitrogen Dissociation on Ruthenium. *Journal of Physical Chemistry Letters*, **2021**, 12, 2954-2962	1.7	8
678	New insights on CO and CO2 hydrogenation for methanol synthesis: The key role of adsorbate-adsorbate interactions on Cu and the highly active MgO-Cu interface. *Journal of Catalysis*, **2021**, 400, 325-331	2.3	6
677	Understanding Trends in Ethylene Epoxidation on Group IB Metals. *ACS Catalysis*, **2021**, 11, 12052-12057	4.1	3

676	Relations between Surface Oxygen Vacancies and Activity of Methanol Formation from CO2 Hydrogenation over In2O3 Surfaces. *ACS Catalysis*, **2021**, 11, 1780-1786	4.1	31
675	Tuning the electronic structure of Ag-Pd alloys to enhance performance for alkaline oxygen reduction. *Nature Communications*, **2021**, 12, 620	5	32
674	Enhancement of lithium-mediated ammonia synthesis by addition of oxygen.. *Science*, **2021**, 374, 1593-1597	19	19
673	Identifying and Tuning the In Situ Oxygen-Rich Surface of Molybdenum Nitride Electrocatalysts for Oxygen Reduction. *ACS Applied Energy Materials*, **2020**, 3, 12433-12446	2.1	8
672	Acetonitrile Transition Metal Interfaces from First Principles. *Journal of Physical Chemistry Letters*, **2020**, 11, 9802-9811	1.7	5
671	Atomistic Insight into Cation Effects on Binding Energies in Cu-Catalyzed Carbon Dioxide Reduction. *Journal of Physical Chemistry C*, **2020**, 124, 24765-24775	1.2	12
670	Electric Field Effects in Oxygen Reduction Kinetics: Rationalizing pH Dependence at the Pt(111), Au(111), and Au(100) Electrodes. *Journal of Physical Chemistry C*, **2020**, 124, 14581-14591	1.2	44
669	The Challenge of CO Hydrogenation to Methanol: Fundamental Limitations Imposed by Linear Scaling Relations. *Topics in Catalysis*, **2020**, 63, 635-648	1.1	7
668	Active Learning Accelerated Discovery of Stable Iridium Oxide Polymorphs for the Oxygen Evolution Reaction. *Chemistry of Materials*, **2020**, 32, 5854-5863	2.7	34
667	Nitride or Oxynitride? Elucidating the Composition–Activity Relationships in Molybdenum Nitride Electrocatalysts for the Oxygen Reduction Reaction. *Chemistry of Materials*, **2020**, 32, 2946-2960	2.7	28
666	Micro-kinetic model of electrochemical carbon dioxide reduction over platinum in non-aqueous solvents. *Physical Chemistry Chemical Physics*, **2020**, 22, 9040-9045	1.1	8
665	A Combined Theory-Experiment Analysis of the Surface Species in Lithium-Mediated NH3 Electrosynthesis. *ChemElectroChem*, **2020**, 7, 1513-1513	1.2	0
664	A cyclic electrochemical strategy to produce acetylene from CO2, CH4, or alternative carbon sources. *Sustainable Energy and Fuels*, **2020**, 4, 2752-2759	2	5
663	A Combined Theory-Experiment Analysis of the Surface Species in Lithium-Mediated NH3 Electrosynthesis. *ChemElectroChem*, **2020**, 7, 1542-1549	1.2	34
662	Effect of Manganese on the Selective Catalytic Hydrogenation of COx in the Presence of Light Hydrocarbons Over Ni/Al2O3: An Experimental and Computational Study. *ACS Catalysis*, **2020**, 10, 1535-1547	4.1	9
661	Scaling Relations in Homogeneous Catalysis: Analyzing the Buchwald–Hartwig Amination Reaction. *ACS Catalysis*, **2020**, 10, 336-345	4.1	17
660	Acidic Oxygen Evolution Reaction Activity–Stability Relationships in Ru-Based Pyrochlores. *ACS Catalysis*, **2020**, 10, 12182-12196	4.1	30
659	Increasing stability, efficiency, and fundamental understanding of lithium-mediated electrochemical nitrogen reduction. *Energy and Environmental Science*, **2020**, 13, 4291-4300	10.7	50

658	Circumventing Scaling Relations in Oxygen Electrochemistry Using Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2020**, 11, 10029-10036	1.7	16
657	Analysis of Acid-Stable and Active Oxides for the Oxygen Evolution Reaction. *ACS Energy Letters*, **2020**, 5, 3778-3787	6.8	27
656	Two-Dimensional Conductive Ni-HAB as a Catalyst for the Electrochemical Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2020**, 12, 39074-39081	3.1	15
655	Predicting aqueous stability of solid with computed Pourbaix diagram using SCAN functional. *Npj Computational Materials*, **2020**, 6,	2.8	16
654	Effects of a conductive support on the bonding of oxygen containing molecules to transition metal oxide surfaces. *Physical Chemistry Chemical Physics*, **2020**, 22, 26216-26222	1.1	5
653	Scaling Relationships and Volcano Plots in Homogeneous Catalysis. *Journal of Physical Chemistry Letters*, **2020**, 11, 8518-8526	1.7	11
652	Acid-Stable Oxides for Oxygen Electrocatalysis. *ACS Energy Letters*, **2020**, 5, 2905-2908	6.8	34
651	Modeling Hydrogen Evolution Reaction Kinetics through Explicit Water–Metal Interfaces. *Journal of Physical Chemistry C*, **2020**, 124, 28083-28092	1.2	24
650	Subsurface Nitrogen Dissociation Kinetics in Lithium Metal from Metadynamics. *Journal of Physical Chemistry C*, **2020**, 124, 26368-26378	1.2	6
649	Systematic Investigation of Iridium-Based Bimetallic Thin Film Catalysts for the Oxygen Evolution Reaction in Acidic Media. *ACS Applied Materials & Interfaces*, **2019**, 11, 34059-34066	3.1	34
648	Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. *Nature Communications*, **2019**, 10, 3997	5	264
647	Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO2 Reduction. *Journal of Physical Chemistry C*, **2019**, 123, 4256-4261	1.2	28
646	Progress and Perspectives of Electrochemical CO Reduction on Copper in Aqueous Electrolyte. *Chemical Reviews*, **2019**, 119, 7610-7672	16.3	1244
645	A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements. *Nature*, **2019**, 570, 504-508	16.4	617
644	Stable Two-Dimensional Materials for Oxygen Reduction and Oxygen Evolution Reactions. *ACS Energy Letters*, **2019**, 4, 1410-1411	6.8	33
643	First principles micro-kinetic model of catalytic non-oxidative dehydrogenation of ethane over close-packed metallic facets. *Journal of Catalysis*, **2019**, 374, 161-170	2.3	31
642	Predicting Chemical Reaction Barriers with a Machine Learning Model. *Catalysis Letters*, **2019**, 149, 2347-2354	2	36
641	ZnO As an Active and Selective Catalyst for Electrochemical Water Oxidation to Hydrogen Peroxide. *ACS Catalysis*, **2019**, 9, 4593-4599	4.1	95

640	Selective and Efficient Gd-Doped BiVO4 Photoanode for Two-Electron Water Oxidation to H2O2. *ACS Energy Letters*, **2019**, 4, 720-728	6.8	76
639	Insights into the Electrochemical Oxygen Evolution Reaction with ab Initio Calculations and Microkinetic Modeling: Beyond the Limiting Potential Volcano. *Journal of Physical Chemistry C*, **2019**, 123, 18960-18977	1.2	84
638	Precious Metal-Free Nickel Nitride Catalyst for the Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2019**, 11, 26863-26871	3.1	47
637	Electro-Oxidation of Methane on Platinum under Ambient Conditions. *ACS Catalysis*, **2019**, 9, 7578-7587	4.1	32
636	Strategies toward Selective Electrochemical Ammonia Synthesis. *ACS Catalysis*, **2019**, 9, 8316-8324	4.1	88
635	Improved Oxygen Reduction Reaction Activity of Nanostructured CoS2 through Electrochemical Tuning. *ACS Applied Energy Materials*, **2019**, 2, 8605-8614	2.1	21
634	Facile Electron Transfer to CO2 during Adsorption at the Metal|Solution Interface. *Journal of Physical Chemistry C*, **2019**, 123, 29278-29283	1.2	23
633	A theoretical explanation of the effect of oxygen poisoning on industrial Haber-Bosch catalysts. *Journal of Catalysis*, **2019**, 372, 33-38	2.3	20
632	Solvent–Adsorbate Interactions and Adsorbate-Specific Solvent Structure in Carbon Dioxide Reduction on a Stepped Cu Surface. *Journal of Physical Chemistry C*, **2019**, 123, 5999-6009	1.2	39
631	The Difficulty of Proving Electrochemical Ammonia Synthesis. *ACS Energy Letters*, **2019**, 4, 2986-2988	6.8	74
630	Efficient Pourbaix diagrams of many-element compounds. *Physical Chemistry Chemical Physics*, **2019**, 21, 25323-25327	1.1	20
629	Prediction of Stable and Active (Oxy-Hydro) Oxide Nanoislands on Noble-Metal Supports for Electrochemical Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2019**, 11, 2006-2013	3.1	14
628	pH effects on the electrochemical reduction of CO towards C products on stepped copper. *Nature Communications*, **2019**, 10, 32	5	207
627	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. *ACS Catalysis*, **2019**, 9, 920-931	4.1	100
626	Role of Co2C in ZnO-promoted Co Catalysts for Alcohol Synthesis from Syngas. *ChemCatChem*, **2019**, 11, 799-809	1.4	19
625	An electronic structure descriptor for oxygen reactivity at metal and metal-oxide surfaces. *Surface Science*, **2019**, 681, 122-129	0.7	92
624	Understanding Catalytic Activity Trends in the Oxygen Reduction Reaction. *Chemical Reviews*, **2018**, 118, 2302-2312	16.3	908
623	A theoretical study of the effect of a non-aqueous proton donor on electrochemical ammonia synthesis. *Physical Chemistry Chemical Physics*, **2018**, 20, 4982-4989	1.1	60

622	Ultrathin Cobalt Oxide Overlayer Promotes Catalytic Activity of Cobalt Nitride for the Oxygen Reduction Reaction. *Journal of Physical Chemistry C*, **2018**, 122, 4783-4791	1.2	36
621	Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO oxides. *Physical Chemistry Chemical Physics*, **2018**, 20, 3813-3818	1.1	66
620	Metal ion cycling of Cu foil for selective C□ coupling in electrochemical CO2 reduction. *Nature Catalysis*, **2018**, 1, 111-119	10.3	383
619	High-efficiency oxygen reduction to hydrogen peroxide catalysed by oxidized carbon materials. *Nature Catalysis*, **2018**, 1, 156-162	10.3	632
618	Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis. *ACS Catalysis*, **2018**, 8, 4017-4024	4.1	52
617	Selectivity of Synthesis Gas Conversion to C2+ Oxygenates on fcc(111) Transition-Metal Surfaces. *ACS Catalysis*, **2018**, 8, 3447-3453	4.1	48
616	Cation-exchanged zeolites for the selective oxidation of methane to methanol. *Catalysis Science and Technology*, **2018**, 8, 114-123	1.6	110
615	The Role of Sodium in Tuning Product Distribution in Syngas Conversion by Rh Catalysts. *Catalysis Letters*, **2018**, 148, 289-297	1	10
614	Defective Carbon-Based Materials for the Electrochemical Synthesis of Hydrogen Peroxide. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 311-317	3.1	153
613	Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 16023-16032	1.2	21
612	Electrochemical Carbon Monoxide Reduction on Polycrystalline Copper: Effects of Potential, Pressure, and pH on Selectivity toward Multicarbon and Oxygenated Products. *ACS Catalysis*, **2018**, 8, 7445-7454	4.1	175
611	Copper Silver Thin Films with Metastable Miscibility for Oxygen Reduction Electrocatalysis in Alkaline Electrolytes. *ACS Applied Energy Materials*, **2018**, 1, 1990-1999	2.1	21
610	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. *Nature Communications*, **2018**, 9, 3202	5	31
609	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO2. *Angewandte Chemie*, **2018**, 130, 15265-15270	0.7	12
608	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO. *Angewandte Chemie - International Edition*, **2018**, 57, 15045-15050	4.6	46
607	Nature of Lone-Pair-Surface Bonds and Their Scaling Relations. *Inorganic Chemistry*, **2018**, 57, 7222-7238	1.4	35
606	Rapid flame doping of Co to WS2 for efficient hydrogen evolution. *Energy and Environmental Science*, **2018**, 11, 2270-2277	10.7	45
605	Designing Boron Nitride Islands in Carbon Materials for Efficient Electrochemical Synthesis of Hydrogen Peroxide. *Journal of the American Chemical Society*, **2018**, 140, 7851-7859	4.3	184

604	Role of Subsurface Oxygen on Cu Surfaces for CO2 Electrochemical Reduction. *Journal of Physical Chemistry C*, **2018**, 122, 16209-16215	1.2	49
603	Exploring the Effect of Gold Support on the Oxygen Reduction Reaction Activity of Metal Porphycenes. *ChemCatChem*, **2018**, 10, 5505-5510	1.4	4
602	Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single-Atom Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 29307-29318	1.2	39
601	Theoretical and Experimental Studies of CoGa Catalysts for the Hydrogenation of CO2 to Methanol. *Catalysis Letters*, **2018**, 148, 3583-3591	1	9
600	Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes. *ACS Catalysis*, **2018**, 8, 10555-10563	4.1	6
599	Tuning Methane Activation Chemistry on Alkaline Earth Metal Oxides by Doping. *Journal of Physical Chemistry C*, **2018**, 122, 22544-22548	1.2	13
598	Mechanistic Insights into the Synthesis of Higher Alcohols from Syngas on CuCo Alloys. *ACS Catalysis*, **2018**, 8, 10148-10155	4.1	39
597	Resolving Hysteresis in Perovskite Solar Cells with Rapid Flame-Processed Cobalt-Doped TiO2. *Advanced Energy Materials*, **2018**, 8, 1801717	7.1	54
596	Direct Methane to Methanol: The Selectivity Conversion Limit and Design Strategies. *ACS Catalysis*, **2018**, 8, 6894-6907	4.1	116
595	Mechanistic insights into heterogeneous methane activation. *Physical Chemistry Chemical Physics*, **2017**, 19, 3575-3581	1.1	72
594	Combining theory and experiment in electrocatalysis: Insights into materials design. *Science*, **2017**, 355,	10	5239
593	Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. *ACS Catalysis*, **2017**, 7, 2528-2534	4.1	30
592	One- or Two-Electron Water Oxidation, Hydroxyl Radical, or HO Evolution. *Journal of Physical Chemistry Letters*, **2017**, 8, 1157-1160	1.7	142
591	Development of a reactor with carbon catalysts for modular-scale, low-cost electrochemical generation of H2O2. *Reaction Chemistry and Engineering*, **2017**, 2, 239-245	1.4	100
590	To address surface reaction network complexity using scaling relations machine learning and DFT calculations. *Nature Communications*, **2017**, 8, 14621	5	268
589	Catalysis in real time using X-ray lasers. *Chemical Physics Letters*, **2017**, 675, 145-173	1	35
588	Scaling-Relation-Based Analysis of Bifunctional Catalysis: The Case for Homogeneous Bimetallic Alloys. *ACS Catalysis*, **2017**, 7, 3960-3967	4.1	55
587	Electrochemical generation of sulfur vacancies in the basal plane of MoS for hydrogen evolution. *Nature Communications*, **2017**, 8, 15113	5	396

586	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. *Nano Research*, **2017**, 10, 1163-1177	3.1	50
585	Solvation Effects for Oxygen Evolution Reaction Catalysis on IrO2(110). *Journal of Physical Chemistry C*, **2017**, 121, 11455-11463	1.2	123
584	Understanding Selectivity for the Electrochemical Reduction of Carbon Dioxide to Formic Acid and Carbon Monoxide on Metal Electrodes. *ACS Catalysis*, **2017**, 7, 4822-4827	4.1	402
583	Electrochemical CO reduction on Au surfaces: mechanistic aspects regarding the formation of major and minor products. *Physical Chemistry Chemical Physics*, **2017**, 19, 15856-15863	1.1	89
582	Understanding trends in electrochemical carbon dioxide reduction rates. *Nature Communications*, **2017**, 8, 15438	5	369
581	A Theoretical Study of Methanol Oxidation on RuO2(110): Bridging the Pressure Gap. *ACS Catalysis*, **2017**, 7, 4527-4534	4.1	5
580	Electrochemical Activation of CO through Atomic Ordering Transformations of AuCu Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 8329-8336	4.3	392
579	Electrochemical Ammonia Synthesis□he Selectivity Challenge. *ACS Catalysis*, **2017**, 7, 706-709	4.1	442
578	Trends in Adsorption Energies of the Oxygenated Species on Single Platinum Atom Embedded in Carbon Nanotubes. *Catalysis Letters*, **2017**, 147, 2689-2696	1	10
577	Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. *Nature Communications*, **2017**, 8, 701	5	193
576	Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO2. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 11080-11085	3.1	68
575	Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. *CheM*, **2017**, 3, 950-960	4.6	249
574	Theoretical Insights into Methane C□H Bond Activation on Alkaline Metal Oxides. *Journal of Physical Chemistry C*, **2017**, 121, 16440-16446	1.2	34
573	Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO2 Reduction. *ACS Catalysis*, **2017**, 7, 6600-6608	4.1	224
572	A Theoretical Investigation into the Role of Surface Defects for Oxygen Evolution on RuO2. *Journal of Physical Chemistry C*, **2017**, 121, 18516-18524	1.2	66
571	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2017**, 121, 19807-19815	1.2	67
570	Formic Acid Dissociative Adsorption on NiO(111): Energetics and Structure of Adsorbed Formate. *Journal of Physical Chemistry C*, **2017**, 121, 28001-28006	1.2	8
569	Understanding the Influence of [EMIM]Cl on the Suppression of the Hydrogen Evolution Reaction on Transition Metal Electrodes. *Langmuir*, **2017**, 33, 9464-9471	1.3	36

568	Rh-MnO Interface Sites Formed by Atomic Layer Deposition Promote Syngas Conversion to Higher Oxygenates. *ACS Catalysis*, **2017**, 7, 5746-5757	4.1	49
567	Ammonia synthesis from N2 and H2O using a lithium cycling electrification strategy at atmospheric pressure. *Energy and Environmental Science*, **2017**, 10, 1621-1630	10.7	236
566	Understanding trends in C-H bond activation in heterogeneous catalysis. *Nature Materials*, **2017**, 16, 225-229	8.6	276
565	Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. *ACS Central Science*, **2017**, 3, 1286-1293	5.3	41
564	Materials for solar fuels and chemicals. *Nature Materials*, **2016**, 16, 70-81	8.6	846
563	Two-Dimensional Materials as Catalysts for Energy Conversion. *Catalysis Letters*, **2016**, 146, 1917-1921	1	39
562	A highly active and stable IrOx/SrIrO3 catalyst for the oxygen evolution reaction. *Science*, **2016**, 353, 1011-1014	10	1094
561	Chemical Bond Activation Observed with an X-ray Laser. *Journal of Physical Chemistry Letters*, **2016**, 7, 3647-51	1.7	15
560	Automated Discovery and Construction of Surface Phase Diagrams Using Machine Learning. *Journal of Physical Chemistry Letters*, **2016**, 7, 3931-3935	1.7	56
559	Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. *ACS Catalysis* , **2016**, 6, 6531-6536	4.1	136
558	Direct and continuous strain control of catalysts with tunable battery electrode materials. *Science*, **2016**, 354, 1031-1036	10	369
557	Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface. *ACS Catalysis*, **2016**, 6, 7377-7384	4.1	46
556	Barriers of Electrochemical CO2 Reduction on Transition Metals. *Organic Process Research and Development*, **2016**, 20, 1424-1430	1	98
555	Methanol Partial Oxidation on Ag(1 1 1) from First Principles. *ChemCatChem*, **2016**, 8, 3621-3625	1.4	10
554	Functional Independent Scaling Relation for ORR/OER Catalysts. *Journal of Physical Chemistry C*, **2016**, 120, 24910-24916	1.2	86
553	Analyzing the Case for Bifunctional Catalysis. *Angewandte Chemie*, **2016**, 128, 5296-5300	0.7	15
552	Exploring Scaling Relations for Chemisorption Energies on Transition-Metal-Exchanged Zeolites ZSM-22 and ZSM-5. *ChemCatChem*, **2016**, 8, 767-772	1.4	16
551	How Doped MoS2 Breaks Transition-Metal Scaling Relations for CO2 Electrochemical Reduction. *ACS Catalysis*, **2016**, 6, 4428-4437	4.1	193

550	Analyzing the Case for Bifunctional Catalysis. *Angewandte Chemie - International Edition*, **2016**, 55, 5210-4	4.6	54
549	Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening. *Catalysis Letters*, **2016**, 146, 718-724	1	11
548	Intrinsic Selectivity and Structure Sensitivity of Rhodium Catalysts for C(2+) Oxygenate Production. *Journal of the American Chemical Society*, **2016**, 138, 3705-14	4.3	137
547	Bifunctional alloys for the electroreduction of CO2 and CO. *Physical Chemistry Chemical Physics*, **2016**, 18, 9194-201	1.1	101
546	Scaling Relationships for Binding Energies of Transition Metal Complexes. *Catalysis Letters*, **2016**, 146, 304-308	1	18
545	Activating and optimizing MoS2 basal planes for hydrogen evolution through the formation of strained sulphur vacancies. *Nature Materials*, **2016**, 15, 48-53	8.6	1563
544	Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid. *ChemSusChem*, **2016**, 9, 358-63	2.4	225
543	Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper. *Angewandte Chemie*, **2016**, 128, 1472-1476	0.7	31
542	Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper. *Angewandte Chemie - International Edition*, **2016**, 55, 1450-4	4.6	134
541	Potential Dependence of Electrochemical Barriers from ab Initio Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 1686-90	1.7	138
540	Opportunities and challenges in the electrocatalysis of CO2 and CO reduction using bifunctional surfaces: A theoretical and experimental study of Au□d alloys. *Journal of Catalysis*, **2016**, 343, 215-231	2.3	96
539	Theoretical Insights into the Selective Oxidation of Methane to Methanol in Copper-Exchanged Mordenite. *ACS Catalysis*, **2016**, 6, 3760-3766	4.1	110
538	CO-CO coupling on Cu facets: Coverage, strain and field effects. *Surface Science*, **2016**, 654, 56-62	0.7	142
537	Electric Field Effects in Electrochemical CO2 Reduction. *ACS Catalysis*, **2016**, 6, 7133-7139	4.1	275
536	Identification of highly active Fe sites in (Ni,Fe)OOH for electrocatalytic water splitting. *Journal of the American Chemical Society*, **2015**, 137, 1305-13	4.3	1553
535	The Mechanism of CO and CO2 Hydrogenation to Methanol over Cu-Based Catalysts. *ChemCatChem* , **2015**, 7, 1105-1111	1.4	336
534	Screened Hybrid Exact Exchange Correction Scheme for Adsorption Energies on Perovskite Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 17662-17666	1.2	7
533	Theoretical Limits to the Anode Potential in Aqueous Mg□Air Batteries. *Journal of Physical Chemistry C*, **2015**, 119, 19660-19667	1.2	36

532	Electrochemical Barriers Made Simple. *Journal of Physical Chemistry Letters*, **2015**, 6, 2663-8	1.7	211
531	Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics on Ru(0001) Probed by Ultrafast X-Ray Spectroscopy and Ab□nitio Simulations. *Physical Review Letters*, **2015**, 114, 156101	1.9	22
530	A systematic study of metal-supported boron nitride materials for the oxygen reduction reaction. *Physical Chemistry Chemical Physics*, **2015**, 17, 12722-7	1.1	58
529	Theoretical Insights into a CO Dimerization Mechanism in CO2 Electroreduction. *Journal of Physical Chemistry Letters*, **2015**, 6, 2032-7	1.7	419
528	A benchmark database for adsorption bond energies to transition metal surfaces and comparison to selected DFT functionals. *Surface Science*, **2015**, 640, 36-44	0.7	288
527	Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation. *Journal of Physical Chemistry Letters*, **2015**, 6, 4224-8	1.7	96
526	Effect of Boron Modifications of Palladium Catalysts for the Production of Hydrogen from Formic Acid. *ACS Catalysis*, **2015**, 5, 6579-6586	4.1	68
525	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. *Physical Chemistry Chemical Physics*, **2015**, 17, 29541-7	1.1	62
524	Surface Tension Effects on the Reactivity of Metal Nanoparticles. *Journal of Physical Chemistry Letters*, **2015**, 6, 3797-801	1.7	52
523	Designing an improved transition metal phosphide catalyst for hydrogen evolution using experimental and theoretical trends. *Energy and Environmental Science*, **2015**, 8, 3022-3029	10.7	671
522	Al-Air Batteries: Fundamental Thermodynamic Limitations from First-Principles Theory. *Journal of Physical Chemistry Letters*, **2015**, 6, 175-9	1.7	46
521	Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting. *Physical Chemistry Chemical Physics*, **2015**, 17, 2634-40	1.1	49
520	Rational design of MoS2 catalysts: tuning the structure and activity via transition metal doping. *Catalysis Science and Technology*, **2015**, 5, 246-253	1.6	128
519	Surface energetics of alkaline-earth metal oxides: Trends in stability and adsorption of small molecules. *Physical Review B*, **2015**, 91,	1	34
518	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. *ChemSusChem*, **2015**, 8, 2180-6	2.4	666
517	New design paradigm for heterogeneous catalysts. *National Science Review*, **2015**, 2, 140-143	3.6	191
516	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. *Journal of Catalysis*, **2015**, 328, 36-42	2.3	715
515	Optical laser-induced CO desorption from Ru(0001) monitored with a free-electron X-ray laser: DFT prediction and X-ray confirmation of a precursor state. *Surface Science*, **2015**, 640, 80-88	0.7	10

514	Toward Controlled Growth of Helicity-Specific Carbon Nanotubes. *Journal of Physical Chemistry Letters*, **2015**, 6, 2232-7	1.7	6
513	Mechanistic Pathway in the Electrochemical Reduction of CO2 on RuO2. *ACS Catalysis*, **2015**, 5, 4075-4084	4.1	95
512	Theoretical Study of EMIM+ Adsorption on Silver Electrode Surfaces. *Journal of Physical Chemistry C* , **2015**, 119, 20023-20029	1.2	33
511	On the role of the surface oxygen species during A-H (A = C, N, O) bond activation: a density functional theory study. *Chemical Communications*, **2015**, 51, 2621-4	1.5	38
510	CatMAP: A Software Package for Descriptor-Based Microkinetic Mapping of Catalytic Trends. *Catalysis Letters*, **2015**, 145, 794-807	1	217
509	Surface chemistry. Probing the transition state region in catalytic CO oxidation on Ru. *Science*, **2015** , 347, 978-82	10	150
508	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. *Surface Science*, **2015**, 640, 133-140	0.7	256
507	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. *Nano Research*, **2015**, 8, 566-575	3.1	478
506	Insights into carbon nanotube nucleation: cap formation governed by catalyst interfacial step flow. *Scientific Reports*, **2014**, 4, 6510	1.5	35
505	Tuning the MoS□edge-site activity for hydrogen evolution via support interactions. *Nano Letters*, **2014**, 14, 1381-7	3.2	533
504	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. *Nature Chemistry*, **2014**, 6, 320-4	4.4	689
503	Methanol-to-hydrocarbons conversion: The alkene methylation pathway. *Journal of Catalysis*, **2014**, 314, 159-169	2.3	108
502	Effects of d-band shape on the surface reactivity of transition-metal alloys. *Physical Review B*, **2014**, 89,	1	236
501	Activity and Selectivity Trends in Synthesis Gas Conversion to Higher Alcohols. *Topics in Catalysis*, **2014**, 57, 135-142	1.1	144
500	Thermochemistry and micro-kinetic analysis of methanol synthesis on ZnO (0 0 0 1). *Journal of Catalysis*, **2014**, 309, 397-407	2.3	46
499	Understanding the Reactivity of Layered Transition-Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption. *Journal of Physical Chemistry Letters*, **2014**, 5, 3884-9	1.7	57
498	Hydrogen adsorption on bimetallic PdAu(111) surface alloys: minimum adsorption ensemble, ligand and ensemble effects, and ensemble confinement. *Physical Chemistry Chemical Physics*, **2014**, 16, 23930-43	11	32
497	Trends in electrochemical CO2 reduction activity for open and close-packed metal surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 4720-7	1.1	284

496	Climbing the Activity Volcano: Core□Shell Ru@Pt Electrocatalysts for Oxygen Reduction. *ChemElectroChem*, **2014**, 1, 67-71	1.2	45
495	Lithium and oxygen vacancies and their role in Li2O2 charge transport in Li□O2 batteries. *Energy and Environmental Science*, **2014**, 7, 720-727	10.7	77
494	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. *Science*, **2014**, 345, 197-200	10	244
493	Theoretical Analysis of Transition-Metal Catalysts for Formic Acid Decomposition. *ACS Catalysis*, **2014**, 4, 1226-1233	4.1	169
492	Trends in Hydrodesulfurization Catalysis Based on Realistic Surface Models. *Catalysis Letters*, **2014**, 144, 1425-1432	1	29
491	Active edge sites in MoSe2 and WSe2 catalysts for the hydrogen evolution reaction: a density functional study. *Physical Chemistry Chemical Physics*, **2014**, 16, 13156-64	1.1	364
490	Electronic Structure Effects in Transition Metal Surface Chemistry. *Topics in Catalysis*, **2014**, 57, 25-32	1.1	154
489	Pt Skin Versus Pt Skeleton Structures of Pt3Sc as Electrocatalysts for Oxygen Reduction. *Topics in Catalysis*, **2014**, 57, 245-254	1.1	36
488	Nanoscale limitations in metal oxide electrocatalysts for oxygen evolution. *Nano Letters*, **2014**, 14, 5853-7	3.2	62
487	Reactivity Descriptor in Solid Acid Catalysis: Predicting Turnover Frequencies for Propene Methylation in Zeotypes. *Journal of Physical Chemistry Letters*, **2014**, 5, 1516-21	1.7	85
486	Unifying Kinetic and Thermodynamic Analysis of 2 e□ and 4 e□ Reduction of Oxygen on Metal Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 6706-6718	1.2	227
485	**2014**,		219
484	Catalyst Structure **2014**, 138-149		
483	Poisoning and Promotion of Catalysts **2014**, 150-154		
482	Surface Electrocatalysis **2014**, 155-174		
481	Relation of Activity to Surface Electronic Structure **2014**, 175-194		0
480	Energy Trends in Catalysis **2014**, 85-96		1
479	Kinetics **2014**, 68-84		

478	Rate Constants **2014**, 47-67		
477	The Electronic Factor in Heterogeneous Catalysis **2014**, 114-137		8
476	Activity and Selectivity Maps **2014**, 97-113		0
475	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO2 Reduction. *ChemCatChem*, **2014**, 6, 1899-1905	1.4	194
474	Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2014**, 118, 29252-29259	1.2	66
473	The Potential Energy Diagram **2014**, 6-25		
472	Heterogeneous Catalysis and a Sustainable Future **2014**, 1-5		
471	Exploring the limits: A low-pressure, low-temperature Haber–Bosch process. *Chemical Physics Letters*, **2014**, 598, 108-112	1	275
470	Analysis of sulfur-induced selectivity changes for anhydrous methanol dehydrogenation on Ni(100) surfaces. *Surface Science*, **2013**, 613, 58-62	0.7	4
469	Theoretical investigation of the activity of cobalt oxides for the electrochemical oxidation of water. *Journal of the American Chemical Society*, **2013**, 135, 13521-30	4.3	849
468	On the effect of coverage-dependent adsorbate–adsorbate interactions for CO methanation on transition metal surfaces. *Journal of Catalysis*, **2013**, 307, 275-282	2.3	160
467	Tunneling and Polaron Charge Transport through Li2O2 in Li–O2 Batteries. *Journal of Physical Chemistry Letters*, **2013**, 4, 3494-3499	1.7	141
466	Ni–Fe–S Cubanes in CO2 Reduction Electrocatalysis: A DFT Study. *ACS Catalysis*, **2013**, 3, 2640-2643	4.1	53
465	Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode. *Nature Communications*, **2013**, 4,	5	261
464	Electroreduction of Methanediol on Copper. *Catalysis Letters*, **2013**, 143, 631-635	1	19
463	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO2(110). *Journal of Physical Chemistry C*, **2013**, 117, 460-465	1.2	72
462	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO2 Reduction to CO. *Journal of Physical Chemistry Letters*, **2013**, 4, 388-92	1.7	485
461	CO and CO2 Hydrogenation to Methanol Calculated Using the BEEF-vdW Functional. *Catalysis Letters*, **2013**, 143, 71-73	1	122

460	Insights into C?C Coupling in CO2 Electroreduction on Copper Electrodes. *ChemCatChem*, **2013**, 5, 737-742	4	258
459	First-Principles Calculations of Fischer□Tropsch Processes Catalyzed by Nitrogenase Enzymes. *ChemCatChem*, **2013**, 5, 732-736	1.4	13
458	Comment on □Using Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applications□ *Journal of Physical Chemistry C*, **2013**, 117, 6914-6915	1.2	13
457	Li-O2 Kinetic Overpotentials: Tafel Plots from Experiment and First-Principles Theory. *Journal of Physical Chemistry Letters*, **2013**, 4, 556-60	1.7	134
456	Real-time observation of surface bond breaking with an x-ray laser. *Science*, **2013**, 339, 1302-5	10	162
455	Methanol to Dimethyl Ether over ZSM-22: A Periodic Density Functional Theory Study. *ACS Catalysis* , **2013**, 3, 735-745	4.1	61
454	Modeling CO2 reduction on Pt(111). *Physical Chemistry Chemical Physics*, **2013**, 15, 7114-22	1.1	72
453	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. *Journal of Physical Chemistry Letters*, **2013**, 4, 222-6	1.7	221
452	First principles investigation of zinc-anode dissolution in zinc-air batteries. *Physical Chemistry Chemical Physics*, **2013**, 15, 6416-21	1.1	31
451	Guest□host interactions of arenes in H-ZSM-5 and their impact on methanol-to-hydrocarbons deactivation processes. *Journal of Catalysis*, **2013**, 300, 235-241	2.3	52
450	Theoretical evidence for low kinetic overpotentials in Li-O2 electrochemistry. *Journal of Chemical Physics*, **2013**, 138, 034703	1.3	186
449	In silicosearch for novel methane steam reforming catalysts. *New Journal of Physics*, **2013**, 15, 125021	0.8	55
448	Selective ultrafast probing of transient hot chemisorbed and precursor states of CO on Ru(0001). *Physical Review Letters*, **2013**, 110, 186101	1.9	49
447	Formation energies of group I and II metal oxides using random phase approximation. *Physical Review B*, **2013**, 87,	1	23
446	Calculated formation and reaction energies of 3d transition metal oxides using a hierarchy of exchange-correlation functionals. *Physical Review B*, **2013**, 88,	1	18
445	Effects of a New Electrochemical Cleaning Protocol on Ru@Pt Core-Shell ORR Catalysts. *ECS Transactions*, **2013**, 58, 929-936	0.4	3
444	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. *Journal of Catalysis*, **2012**, 290, 108-117	2.3	84
443	Application of a new informatics tool in heterogeneous catalysis: Analysis of methanol dehydrogenation on transition metal catalysts for the production of anhydrous formaldehyde. *Journal of Catalysis*, **2012**, 291, 133-137	2.3	39

442	CatApp: A Web Application for Surface Chemistry and Heterogeneous Catalysis. *Angewandte Chemie*, **2012**, 124, 278-280	0.7	26
441	CatApp: a web application for surface chemistry and heterogeneous catalysis. *Angewandte Chemie - International Edition*, **2012**, 51, 272-4	4.6	106
440	Energetics of Oxygen Adatoms, Hydroxyl Species and Water Dissociation on Pt(111). *Journal of Physical Chemistry C*, **2012**, 116, 25772-25776	1.2	54
439	The importance of surface morphology in controlling the selectivity of polycrystalline copper for CO2 electroreduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 76-81	1.1	485
438	Modeling van der Waals Interactions in Zeolites with Periodic DFT: Physisorption of n-Alkanes in ZSM-22. *Catalysis Letters*, **2012**, 142, 1057-1060	1	57
437	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. *Journal of Physical Chemistry C*, **2012**, 116, 21077-21082	1.2	236
436	Unifying the 2e(-) and 4e(-) Reduction of Oxygen on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 2948-51	1.7	206
435	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. *Physical Review B*, **2012**, 85,	1	852
434	Identifying active surface phases for metal oxide electrocatalysts: a study of manganese oxide bi-functional catalysts for oxygen reduction and water oxidation catalysis. *Physical Chemistry Chemical Physics*, **2012**, 14, 14010-22	1.1	270
433	Simulating Linear Sweep Voltammetry from First-Principles: Application to Electrochemical Oxidation of Water on Pt(111) and Pt3Ni(111). *Journal of Physical Chemistry C*, **2012**, 116, 4698-4704	1.2	64
432	CO hydrogenation to methanol on CuNi catalysts: Theory and experiment. *Journal of Catalysis*, **2012**, 293, 51-60	2.3	163
431	Twin Problems of Interfacial Carbonate Formation in Nonaqueous Li-O2 Batteries. *Journal of Physical Chemistry Letters*, **2012**, 3, 997-1001	1.7	909
430	Balance of nanostructure and bimetallic interactions in Pt model fuel cell catalysts: in situ XAS and DFT study. *Journal of the American Chemical Society*, **2012**, 134, 9664-71	4.3	95
429	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	1.1	810
428	The active site of methanol synthesis over Cu/ZnO/Al2O3 industrial catalysts. *Science*, **2012**, 336, 893-7	10	1650
427	Finite-Size Effects in O and CO Adsorption for the Late Transition Metals. *Topics in Catalysis*, **2012**, 55, 1276-1282	1.1	54
426	Activity Descriptors for CO2 Electroreduction to Methane on Transition-Metal Catalysts. *Journal of Physical Chemistry Letters*, **2012**, 3, 251-258	1.7	975
425	Photoelectrocatalysis and electrocatalysis on silicon electrodes decorated with cubane-like clusters. *Journal of Photonics for Energy*, **2012**, 2, 026001	0.7	16

424	Evidence of Scrambling over Ruthenium-based Catalysts in Supercritical-water Gasification. *ChemCatChem*, **2012**, 4, 1185-1189	1.4	16
423	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	1.1	171
422	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. *ACS Catalysis*, **2012**, 2, 1654-1660	4.1	360
421	Search Directions for Direct H2O2 Synthesis Catalysts Starting from Au12 Nanoclusters. *Topics in Catalysis*, **2012**, 55, 336-344	1.1	35
420	Oral health-related quality of life in patients treated by implant-supported fixed dentures and removable partial dentures. *Clinical Oral Implants Research*, **2012**, 23, 958-62	0.9	33
419	The Computational Materials Repository. *Computing in Science and Engineering*, **2012**, 14, 51-57	0.4	119
418	Electrical conductivity in Li2O2 and its role in determining capacity limitations in non-aqueous Li-O2 batteries. *Journal of Chemical Physics*, **2011**, 135, 214704	1.3	460
417	Ab initio van der waals interactions in simulations of water alter structure from mainly tetrahedral to high-density-like. *Journal of Physical Chemistry B*, **2011**, 115, 14149-60	1	78
416	Hydrogen evolution on Au(111) covered with submonolayers of Pd. *Physical Review B*, **2011**, 84,	1	43
415	Van der Waals effect in weak adsorption affecting trends in adsorption, reactivity, and the view of substrate nobility. *Physical Review B*, **2011**, 83,	1	32
414	Electronic shell structure and chemisorption on gold nanoparticles. *Physical Review B*, **2011**, 84,	1	40
413	Chemistry. Optimizing perovskites for the water-splitting reaction. *Science*, **2011**, 334, 1355-6	10	281
412	Universal transition state scaling relations for (de)hydrogenation over transition metals. *Physical Chemistry Chemical Physics*, **2011**, 13, 20760-5	1.1	295
411	A multifaceted approach to hydrogen storage. *Physical Chemistry Chemical Physics*, **2011**, 13, 16955-72	1.1	58
410	Bioinspired molecular co-catalysts bonded to a silicon photocathode for solar hydrogen evolution. *Nature Materials*, **2011**, 10, 434-8	8.6	556
409	Trends in oxygen reduction and methanol activation on transition metal chalcogenides. *Electrochimica Acta*, **2011**, 56, 9783-9788	2.3	48
408	Scaling relationships for adsorption energies of C2 hydrocarbons on transition metal surfaces. *Chemical Engineering Science*, **2011**, 66, 6318-6323	1.9	93
407	The Pt(111)/electrolyte interface under oxygen reduction reaction conditions: an electrochemical impedance spectroscopy study. *Langmuir*, **2011**, 27, 2058-66	1.3	157

406	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 2244-2252	1.2	46
405	Density functional theory in surface chemistry and catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 937-43	3.3	1141
404	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. *ChemCatChem*, **2011**, 3, 1159-1165	1.4	2321
403	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution. *ChemCatChem*, **2011**, 3, 1607-1611	1.4	146
402	Universal Brønsted-Evans-Polanyi Relations for C–C, C–O, C–N, N–O, N–N, and O–O Dissociation Reactions. *Catalysis Letters*, **2011**, 141, 370-373	1	215
401	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. *Catalysis Letters*, **2011**, 141, 1067-1071		193
400	Atomic-Scale Modeling of Particle Size Effects for the Oxygen Reduction Reaction on Pt. *Catalysis Letters*, **2011**, 141, 909-913	1	193
399	Descriptor-Based Analysis Applied to HCN Synthesis from NH3 and CH4. *Angewandte Chemie*, **2011**, 123, 4697-4701	0.7	11
398	Descriptor-based analysis applied to HCN synthesis from NH3 and CH4. *Angewandte Chemie - International Edition*, **2011**, 50, 4601-5	4.6	68
397	The role of transition metal interfaces on the electronic transport in lithium–air batteries. *Catalysis Today*, **2011**, 165, 2-9	1.8	82
396	On the behavior of Brønsted-Evans-Polanyi relations for transition metal oxides. *Journal of Chemical Physics*, **2011**, 134, 244509	1.3	108
395	First-principles investigations of Ni3Al(111) and NiAl(110) surfaces at metal dusting conditions. *Surface Science*, **2011**, 605, 582-592	0.7	10
394	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. *Surface Science*, **2011**, 605, 1354-1359	0.7	368
393	Bio-inspired co-catalysts bonded to a silicon photocathode for solar hydrogen evolution **2011**,		1
392	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. *Journal of Chemical Physics*, **2010**, 132, 071101	1.3	319
391	CO oxidation on PdO surfaces. *Journal of Chemical Physics*, **2010**, 133, 084704	1.3	62
390	Modeling the Electrochemical Hydrogen Oxidation and Evolution Reactions on the Basis of Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 18182-18197	1.2	743
389	Ammonia dynamics in magnesium ammine from DFT and neutron scattering. *Energy and Environmental Science*, **2010**, 3, 448	10.7	41

388	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	0.7	1092
387	Chemistry. Green gold catalysis. *Science*, **2010**, 327, 278-9	10	82
386	Enzymatic versus inorganic oxygen reduction catalysts: comparison of the energy levels in a free-energy scheme. *Inorganic Chemistry*, **2010**, 49, 3567-72	1.4	53
385	Computational high-throughput screening of electrocatalytic materials for hydrogen evolution **2010**, 280-284		16
384	On the Role of Metal Step-Edges in Graphene Growth. *Journal of Physical Chemistry C*, **2010**, 114, 11221-11227	4.2	102
383	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. *Energy and Environmental Science*, **2010**, 3, 1311	10.7	1861
382	Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. *Topics in Catalysis*, **2010**, 53, 357-364	1.1	42
381	Understanding Trends in Catalytic Activity: The Effect of Adsorbate–Adsorbate Interactions for CO Oxidation Over Transition Metals. *Topics in Catalysis*, **2010**, 53, 298-310	1.1	167
380	Hydrogen Reactions on Nanostructured Surfaces **2010**, 1-70		9
379	Nanoscale Phenomena in Catalyst Layers for PEM Fuel Cells: From Fundamental Physics to Benign Design **2010**, 317-369		
378	Fuel Cells with Neat Proton-Conducting Salt Electrolytes **2010**, 371-393		
377	Vibrational Spectroscopy for the Characterization of PEM Fuel Cell Membrane Materials **2010**, 395-413		4
376	Ab Initio Electrochemical Properties of Electrode Surfaces **2010**, 415-431		14
375	Electronic Structure and Reactivity of Transition Metal Complexes **2010**, 433-455		3
374	Quantitative Description of Electron Transfer Reactions **2010**, 457-487		
373	Understanding Electrocatalysts for Low-Temperature Fuel Cells **2010**, 489-510		2
372	Operando XAS Techniques: Past, Present, and Future **2010**, 511-544		3
371	Operando X-Ray Absorption Spectroscopy of Polymer Electrolyte Fuel Cells **2010**, 545-563		

370	New Concepts in the Chemistry and Engineering of Low-Temperature Fuel Cells **2010**, 565-610		
369	Comparison of Electrocatalysis and Bioelectrocatalysis of Hydrogen and Oxygen Redox Reactions **2010**, 71-110		9
368	Design of Palladium-Based Alloy Electrocatalysts for Hydrogen Oxidation Reaction in Fuel Cells **2010**, 111-146		2
367	Mechanism of an Enhanced Oxygen Reduction Reaction at Platinum-Based Electrocatalysts: Identification and Quantification of Oxygen Species Adsorbed on Electrodes by X-Ray Photoelectron Spectroscopy **2010**, 147-168		4
366	Biocathodes for Dioxygen Reduction in Biofuel Cells **2010**, 169-214		7
365	Platinum Monolayer Electrocatalysts: Improving Structure and Activity **2010**, 215-236		3
364	The Importance of Enzymes: Benchmarks for Electrocatalysts **2010**, 237-255		
363	Approach to Microbial Fuel Cells and Their Applications **2010**, 257-281		1
362	Half-Cell Investigations of Cathode Catalysts for PEM Fuel Cells: From Model Systems to High-Surface-Area Catalysts **2010**, 283-316		1
361	The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations. *Electrochimica Acta*, **2010**, 55, 7975-7981	2.3	387
360	Formation energies of rutile metal dioxides using density functional theory. *Physical Review B*, **2009** , 79,	1	82
359	The effect of Co-promotion on MoS2 catalysts for hydrodesulfurization of thiophene: A density functional study. *Journal of Catalysis*, **2009**, 268, 201-208	2.3	122
358	Towards the computational design of solid catalysts. *Nature Chemistry*, **2009**, 1, 37-46	4.4	2590
357	Alloys of platinum and early transition metals as oxygen reduction electrocatalysts. *Nature Chemistry*, **2009**, 1, 552-6	4.4	2287
356	Ammonia synthesis and decomposition on a Ru-based catalyst modeled by first-principles. *Surface Science*, **2009**, 603, 1731-1739	0.7	68
355	First-principles investigations of the Ni3Sn alloy at steam reforming conditions. *Surface Science*, **2009**, 603, 762-770	0.7	37
354	Trends in CO Oxidation Rates for Metal Nanoparticles and Close-Packed, Stepped, and Kinked Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 10548-10553	1.2	207
353	Chemistry. Rate control and reaction engineering. *Science*, **2009**, 324, 1655-6	10	58

352	Experimental and computational studies on structural transitions in the LiBH4□iI pseudobinary system. *Applied Physics Letters*, **2009**, 94, 141912	1.1	72
351	Modeling ethanol decomposition on transition metals: a combined application of scaling and Br□sted-Evans-Polanyi relations. *Journal of the American Chemical Society*, **2009**, 131, 5809-15	4.3	245
350	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	1.3	74
349	Density functional for van der Waals forces accounts for hydrogen bond in benchmark set of water hexamers. *Journal of Chemical Physics*, **2009**, 131, 046102	1.3	50
348	Magnetic edge states in MoS2 characterized using density-functional theory. *Physical Review B*, **2009**, 80,	1	85
347	Density functional study of the adsorption and van der Waals binding of aromatic and conjugated compounds on the basal plane of MoS(2). *Journal of Chemical Physics*, **2009**, 130, 104709	1.3	93
346	Step Effects on the Dissociation of NO on Close-Packed Rhodium Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 20623-20631	1.2	33
345	Combinatorial Density Functional Theory-Based Screening of Surface Alloys for the Oxygen Reduction Reaction. *Journal of Physical Chemistry C*, **2009**, 113, 4932-4939	1.2	209
344	Hydrogen evolution on nano-particulate transition metal sulfides. *Faraday Discussions*, **2008**, 140, 219-31; discussion 297-317	1.1	672
343	Steady state oxygen reduction and cyclic voltammetry. *Faraday Discussions*, **2008**, 140, 337-46; discussion 417-37	1.1	203
342	Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. *Journal of Catalysis*, **2008**, 255, 6-19	2.3	365
341	First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. *Journal of Catalysis*, **2008**, 259, 147-160	2.3	488
340	Chapter 8 Understanding Heterogeneous Catalysis from the Fundamentals. *Handbook of Surface Science*, **2008**, 3, 269-340		2
339	Oxidation and Photo-Oxidation of Water on TiO2 Surface. *Journal of Physical Chemistry C*, **2008**, 112, 9872-9879	1.2	422
338	The nature of the active site in heterogeneous metal catalysis. *Chemical Society Reviews*, **2008**, 37, 2163-71	14.1	553
337	Surface Pourbaix diagrams and oxygen reduction activity of Pt, Ag and Ni(111) surfaces studied by DFT. *Physical Chemistry Chemical Physics*, **2008**, 10, 3722-30	1.1	351
336	Ammonia for hydrogen storage: challenges and opportunities. *Journal of Materials Chemistry*, **2008**, 18, 2304		687
335	Identification of non-precious metal alloy catalysts for selective hydrogenation of acetylene. *Science*, **2008**, 320, 1320-2	10	795

334	Recent density functional studies of hydrodesulfurization catalysts: insight into structure and mechanism. *Journal of Physics Condensed Matter*, **2008**, 20, 064236	0.7	24
333	BEP relations for N2 dissociation over stepped transition metal and alloy surfaces. *Physical Chemistry Chemical Physics*, **2008**, 10, 5202-6	1.1	63
332	Indirect, reversible high-density hydrogen storage in compact metal ammine salts. *Journal of the American Chemical Society*, **2008**, 130, 8660-8	4.3	143
331	Indirect hydrogen storage in metal ammines **2008**, 533-564		22
330	Heterogeneous Catalysis **2008**, 255-321		48
329	Using scaling relations to understand trends in the catalytic activity of transition metals. *Journal of Physics Condensed Matter*, **2008**, 20, 064239	0.7	80
328	Theoretical Modelling of Catalytic Reactions **2008**, 1479		1
327	Recent STM, DFT and HAADF-STEM studies of sulfide-based hydrotreating catalysts: Insight into mechanistic, structural and particle size effects. *Catalysis Today*, **2008**, 130, 86-96	1.8	228
326	Scaling relationships for adsorption energies on transition metal oxide, sulfide, and nitride surfaces. *Angewandte Chemie - International Edition*, **2008**, 47, 4683-6	4.6	260
325	Trends in the catalytic CO oxidation activity of nanoparticles. *Angewandte Chemie - International Edition*, **2008**, 47, 4835-9	4.6	336
324	On the role of surface modifications of palladium catalysts in the selective hydrogenation of acetylene. *Angewandte Chemie - International Edition*, **2008**, 47, 9299-302	4.6	197
323	Modeling the electrified solid□quid interface. *Chemical Physics Letters*, **2008**, 466, 68-71	1	291
322	Electrochemistry on the computer: Understanding how to tailor the metal overlayers for the oxygen reduction reaction. *Surface Science*, **2008**, 602, 2337-2338	0.7	30
321	A molecular view of heterogeneous catalysis. *Journal of Chemical Physics*, **2008**, 128, 182503	1.3	107
320	Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode. *Physical Chemistry Chemical Physics*, **2007**, 9, 3241-50	1.1	533
319	Comparing Electrochemical and Biological Water Splitting. *Journal of Physical Chemistry C*, **2007**, 111, 18821-18823	1.2	90
318	Estimations of electric field effects on the oxygen reduction reaction based on the density functional theory. *Physical Chemistry Chemical Physics*, **2007**, 9, 5158-61	1.1	215
317	Size-specific chemistry on bimetallic surfaces: a combined experimental and theoretical study. *ChemPhysChem*, **2007**, 8, 2068-71	0.9	57

316	Large-scale, density functional theory-based screening of alloys for hydrogen evolution. *Surface Science*, **2007**, 601, 1590-1598	0.7	135
315	CO methanation over supported bimetallic NiFe catalysts: From computational studies towards catalyst optimization. *Applied Catalysis A: General*, **2007**, 320, 98-104	1.9	207
314	Electrochemical dissolution of surface alloys in acids: Thermodynamic trends from first-principles calculations. *Electrochimica Acta*, **2007**, 52, 5829-5836	2.3	231
313	Electrolysis of water on oxide surfaces. *Journal of Electroanalytical Chemistry*, **2007**, 607, 83-89	1.6	1692
312	Catalytic activity of Au nanoparticles. *Nano Today*, **2007**, 2, 14-18	6.1	927
311	The hydrogenation and direct desulfurization reaction pathway in thiophene hydrodesulfurization over MoS2 catalysts at realistic conditions: A density functional study. *Journal of Catalysis*, **2007**, 248, 188-203	2.3	228
310	Location and coordination of promoter atoms in Co- and Ni-promoted MoS2-based hydrotreating catalysts. *Journal of Catalysis*, **2007**, 249, 220-233	2.3	356
309	Scaling properties of adsorption energies for hydrogen-containing molecules on transition-metal surfaces. *Physical Review Letters*, **2007**, 99, 016105	1.9	1009
308	Discovery of technical methanation catalysts based on computational screening. *Topics in Catalysis*, **2007**, 45, 9-13	1.1	103
307	Trends in catalytic NO decomposition over transition metal surfaces. *Topics in Catalysis*, **2007**, 45, 117-120	1.1	31
306	Insights into the reactivity of supported Au nanoparticles: combining theory and experiments. *Topics in Catalysis*, **2007**, 44, 15-26	1.1	356
305	Ligand effects in heterogeneous catalysis and electrochemistry. *Electrochimica Acta*, **2007**, 52, 5512-5516	2.3	421
304	Theoretical Trends in Particle Size Effects for the Oxygen Reduction Reaction. *Zeitschrift Fur Physikalische Chemie*, **2007**, 221, 1209-1220	0.8	154
303	Cyclic voltammograms for H on Pt(111) and Pt(100) from first principles. *Physical Review Letters*, **2007**, 99, 126101	1.9	159
302	Direct NO decomposition over stepped transition-metal surfaces. *Pure and Applied Chemistry*, **2007**, 79, 1895-1903	0.6	19
301	Ethylene dissociation on flat and stepped Ni(111): A combined STM and DFT study. *Surface Science*, **2006**, 600, 66-77	0.7	89
300	A high-density ammonia storage/delivery system based on Mg(NH3)6Cl2 for SCR DeNOx in vehicles. *Chemical Engineering Science*, **2006**, 61, 2618-2625	1.9	72
299	Toward computational screening in heterogeneous catalysis: Pareto-optimal methanation catalysts. *Journal of Catalysis*, **2006**, 239, 501-506	2.3	284

298	Changing the activity of electrocatalysts for oxygen reduction by tuning the surface electronic structure. *Angewandte Chemie - International Edition*, **2006**, 45, 2897-901	4.6	1451
297	Hydrogen evolution over bimetallic systems: understanding the trends. *ChemPhysChem*, **2006**, 7, 1032-5	0.9	310
296	Changing the Activity of Electrocatalysts for Oxygen Reduction by Tuning the Surface Electronic Structure. *Angewandte Chemie*, **2006**, 118, 2963-2967	0.7	458
295	Electronic-Structure-Based Design of Ordered Alloys. *MRS Bulletin*, **2006**, 31, 986-990	1.1	11
294	Response to [Comment on "Trends in the Exchange Current for Hydrogen Evolution" [J. Electrochem. Soc., 152, J23 (2005)]] *Journal of the Electrochemical Society*, **2006**, 153, L33	1.3	26
293	Multidimensional effects on dissociation of N2 on Ru(0001). *Physical Review Letters*, **2006**, 96, 096102	1.9	85
292	The effect of surface relaxation on the N2 dissociation rate on stepped Ru: a transition state theory study. *Journal of Chemical Physics*, **2006**, 124, 026102	1.3	5
291	Generation of nanopores during desorption of NH3 from Mg(NH3)6Cl2. *Journal of the American Chemical Society*, **2006**, 128, 16-7	4.3	80
290	Mechanisms for catalytic carbon nanofiber growth studied by ab initio density functional theory calculations. *Physical Review B*, **2006**, 73,	1	229
289	Chemistry. Toward efficient hydrogen production at surfaces. *Science*, **2006**, 312, 1322-3	10	343
288	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	1	168
287	Calculated phase diagrams for the electrochemical oxidation and reduction of water over Pt(111). *Journal of Physical Chemistry B*, **2006**, 110, 21833-9	1	341
286	Reactive and nonreactive scattering of N2 from Ru(0001): a six-dimensional adiabatic study. *Journal of Chemical Physics*, **2006**, 125, 114706	1.3	40
285	Density Functional Theory in Surface Science and Heterogeneous Catalysis. *MRS Bulletin*, **2006**, 31, 669-674	1.1	95
284	Computational high-throughput screening of electrocatalytic materials for hydrogen evolution. *Nature Materials*, **2006**, 5, 909-13	8.6	2624
283	Towards an ammonia-mediated hydrogen economy?. *Catalysis Today*, **2006**, 111, 140-144	1.8	262
282	A density functional study of inhibition of the HDS hydrogenation pathway by pyridine, benzene, and H2S on MoS2-based catalysts. *Catalysis Today*, **2006**, 111, 44-51	1.8	83
281	Insights into ammonia synthesis from first-principles. *Surface Science*, **2006**, 600, 4264-4268	0.7	34

280	Catalysis by Enzymes: The Biological Ammonia Synthesis. *Topics in Catalysis*, **2006**, 37, 55-70	1.1	78
279	Step sites in syngas catalysis. *Topics in Catalysis*, **2006**, 40, 45-48	1.1	69
278	Molecular Modeling and High-Throughput Experimentation (HTE): Meeting the Challenges of Catalysts, Chemicals and Materials Design. *Oil and Gas Science and Technology*, **2006**, 61, 579-592	0.6	2
277	Bayesian error estimation in density-functional theory. *Physical Review Letters*, **2005**, 95, 216401	1.9	145
276	Ammonia synthesis from first-principles calculations. *Science*, **2005**, 307, 555-8	10	916
275	Trends in hydride formation energies for magnesium-3d transition metal alloys. *Journal of Alloys and Compounds*, **2005**, 386, 1-7	2.4	80
274	Biomimetic hydrogen evolution: MoS2 nanoparticles as catalyst for hydrogen evolution. *Journal of the American Chemical Society*, **2005**, 127, 5308-9	4.3	2895
273	A density functional study of the chemical differences between Type I and Type II MoS2-based structures in hydrotreating catalysts. *Journal of Physical Chemistry B*, **2005**, 109, 2245-53	1	153
272	A general scheme for the estimation of oxygen binding energies on binary transition metal surface alloys. *Surface Science*, **2005**, 592, 104-111	0.7	152
271	Trends in the chemical properties of early transition metal carbide surfaces: A density functional study. *Catalysis Today*, **2005**, 105, 66-73	1.8	247
270	Electrolysis of water on (oxidized) metal surfaces. *Chemical Physics*, **2005**, 319, 178-184	0.8	997
269	CO oxidation on gold nanoparticles: Theoretical studies. *Applied Catalysis A: General*, **2005**, 291, 13-20	1.9	161
268	Trends in the Exchange Current for Hydrogen Evolution. *Journal of the Electrochemical Society*, **2005**, 152, J23	1.3	2860
267	Metal ammine complexes for hydrogen storage. *Journal of Materials Chemistry*, **2005**, 15, 4106		148
266	Controlling the catalytic bond-breaking selectivity of Ni surfaces by step blocking. *Nature Materials*, **2005**, 4, 160-2	8.6	248
265	Negative surface energy clearing up confusion. *Nature Materials*, **2005**, 4, 186-186	8.6	13
264	Why the optimal ammonia synthesis catalyst is not the optimal ammonia decomposition catalyst. *Journal of Catalysis*, **2005**, 230, 309-312	2.3	171
263	The Ligand Effect: CO Desorption from Pt/Ru Catalysts. *Fuel Cells*, **2005**, 5, 429-435	0.9	58

262	CO oxidation on rutile-supported au nanoparticles. *Angewandte Chemie - International Edition*, **2005**, 44, 1824-6	4.6	349
261	CO Oxidation on Rutile-Supported Au Nanoparticles. *Angewandte Chemie*, **2005**, 117, 1858-1860	0.7	78
260	In vivo diffusion weighted 19F MRI using SF6. *Magnetic Resonance in Medicine*, **2005**, 54, 460-3	1.1	33
259	The role of reaction pathways and support interactions in the development of high activity hydrotreating catalysts. *Catalysis Today*, **2005**, 107-108, 12-22	1.8	130
258	Methane activation on Ni(1 1 1): Effects of poisons and step defects. *Surface Science*, **2005**, 590, 127-137	0.7	211
257	The electronic structure effect in heterogeneous catalysis. *Catalysis Letters*, **2005**, 100, 111-114	1	253
256	Understanding the Effect of Steps, Strain, Poisons, and Alloying: Methane Activation on Ni Surfaces. *Catalysis Letters*, **2005**, 105, 9-13	1	67
255	The reaction rate for dissociative adsorption of N2 on stepped Ru(0001): six-dimensional quantum calculations. *Journal of Chemical Physics*, **2005**, 122, 234702	1.3	43
254	Spectroscopic link between adsorption site occupation and local surface chemical reactivity. *Physical Review Letters*, **2004**, 93, 046101	1.9	36
253	A negative surface energy for alumina. *Nature Materials*, **2004**, 3, 289-93	8.6	162
252	Atomic-scale imaging of carbon nanofibre growth. *Nature*, **2004**, 427, 426-9	16.4	1195
251	Atomic-scale insight into structure and morphology changes of MoS2 nanoclusters in hydrotreating catalysts. *Journal of Catalysis*, **2004**, 221, 510-522	2.3	324
250	Modification of the surface electronic and chemical properties of Pt(111) by subsurface 3d transition metals. *Journal of Chemical Physics*, **2004**, 120, 10240-6	1.3	1003
249	Role of strain and ligand effects in the modification of the electronic and chemical properties of bimetallic surfaces. *Physical Review Letters*, **2004**, 93, 156801	1.9	1048
248	CO Desorption Rate Dependence on CO Partial Pressure over Platinum Fuel Cell Catalysts. *Fuel Cells*, **2004**, 4, 309-319	0.9	42
247	On the origin of the catalytic activity of gold nanoparticles for low-temperature CO oxidation. *Journal of Catalysis*, **2004**, 223, 232-235	2.3	1017
246	Sintering of nickel steam-reforming catalysts: effects of temperature and steam and hydrogen pressures. *Journal of Catalysis*, **2004**, 223, 432-443	2.3	235
245	Hydrodesulfurization reaction pathways on MoS2 nanoclusters revealed by scanning tunneling microscopy. *Journal of Catalysis*, **2004**, 224, 94-106	2.3	260

244	The Brønsted–Evans–Polanyi relation and the volcano curve in heterogeneous catalysis. *Journal of Catalysis*, **2004**, 224, 206-217	2.3	1054
243	The adhesion and shape of nanosized Au particles in a Au/TiO2 catalyst. *Journal of Catalysis*, **2004**, 225, 86-94	2.3	208
242	Nano-scale effects in electrochemistry. *Chemical Physics Letters*, **2004**, 390, 440-444	1	120
241	Structure of the FeFe-cofactor of the iron-only nitrogenase and possible mechanism for dinitrogen reduction. *Physical Chemistry Chemical Physics*, **2004**, 6, 843-853	1.1	22
240	Elastic effects behind cooperative bonding in beta-sheets. *Journal of the American Chemical Society*, **2004**, 126, 13140-3	4.3	22
239	Chemical activity of the nitrogenase FeMo cofactor with a central nitrogen ligand: density functional study. *Journal of the American Chemical Society*, **2004**, 126, 3920-7	4.3	109
238	DFT Study of Formaldehyde and Methanol Synthesis from CO and H2 on Ni(111)□ *Journal of Physical Chemistry B*, **2004**, 108, 14535-14540	1	98
237	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *Journal of Physical Chemistry B*, **2004**, 108, 17886-17892	1	5882
236	On the Compensation Effect in Heterogeneous Catalysis. *Journal of Physical Chemistry B*, **2003**, 107, 9325-9331	1	127
235	Ammonia synthesis over a Ru(0001) surface studied by density functional calculations. *Journal of Catalysis*, **2003**, 220, 273-279	2.3	208
234	Modeling the electro-oxidation of CO and H2/CO on Pt, Ru, PtRu and Pt3Sn. *Electrochimica Acta*, **2003**, 48, 3731-3742	2.3	243
233	High Throughput Experimental and Theoretical Predictive Screening of Materials □A Comparative Study of Search Strategies for New Fuel Cell Anode Catalysts. *Journal of Physical Chemistry B*, **2003**, 107, 11013-11021	1	206
232	Chemistry of one-dimensional metallic edge states in MoS2nanoclusters. *Nanotechnology*, **2003**, 14, 385-389	1.2	163
231	Atomic and electronic structure of MoS2 nanoparticles. *Physical Review B*, **2003**, 67,	1	312
230	Beta-sheet preferences from first principles. *Journal of the American Chemical Society*, **2003**, 125, 16383-6	4.3	21
229	The stability of the hydroxylated (0001) surface of □Al2O3. *Journal of Chemical Physics*, **2003**, 118, 11179-11188	1.3	132
228	Modeling a central ligand in the nitrogenase FeMo cofactor. *Journal of the American Chemical Society*, **2003**, 125, 1466-7	4.3	123
227	A simple and realistic model system for studying hydrogen bonds in □sheets. *Journal of Chemical Physics*, **2003**, 118, 9783-9794	1.3	18

226	Pareto-optimal alloys. *Applied Physics Letters*, **2003**, 83, 4527-4529	1.1	39
225	Bonding of gold nanoclusters to oxygen vacancies on rutile TiO2(110). *Physical Review Letters*, **2003**, 90, 026101	1.9	340
224	Publisher Note: Atomic and electronic structure of MoS2 nanoparticles [Phys. Rev. B 67, 085410 (2003)]. *Physical Review B*, **2003**, 67,	1	4
223	Theoretical study of the Au/TiO2(110) interface. *Surface Science*, **2002**, 515, 175-186	0.7	117
222	Interaction of Pd with steps on Al2O3(). *Surface Science*, **2002**, 518, L577-L582	0.7	18
221	Optimal Catalyst Curves: Connecting Density Functional Theory Calculations with Industrial Reactor Design and Catalyst Selection. *Journal of Catalysis*, **2002**, 205, 382-387	2.3	62
220	Steam Reforming and Graphite Formation on Ni Catalysts. *Journal of Catalysis*, **2002**, 209, 365-384	2.3	867
219	Universality in Heterogeneous Catalysis. *Journal of Catalysis*, **2002**, 209, 275-278	2.3	1007
218	Catalytic CO oxidation by a gold nanoparticle: a density functional study. *Journal of the American Chemical Society*, **2002**, 124, 11262-3	4.3	643
217	Structure Sensitivity of CO Dissociation on Rh Surfaces. *Catalysis Letters*, **2002**, 81, 153-156	1	135
216	Electronic structure and catalysis on metal surfaces. *Annual Review of Physical Chemistry*, **2002**, 53, 319-48	12	801
215	Atomic and molecular adsorption on Rh(111). *Journal of Chemical Physics*, **2002**, 117, 6737-6744	1.3	187
214	Combined electronic structure and evolutionary search approach to materials design. *Physical Review Letters*, **2002**, 88, 255506	1.9	225
213	The surface science of enzymes. *Surface Science*, **2002**, 500, 678-698	0.7	18
212	Monte Carlo simulations of adsorption-induced segregation. *Surface Science*, **2002**, 505, 200-214	0.7	62
211	Hydrogen and synthesis gas by steam- and C02 reforming. *Advances in Catalysis*, **2002**, 47, 65-139	0.2	476
210	Adsorption-induced restructuring of gold nanochains. *Physical Review B*, **2002**, 66,	1	93
209	Electronic factors in catalysis: the volcano curve and the effect of promotion in catalytic ammonia synthesis. *Applied Catalysis A: General*, **2001**, 222, 19-29	1.9	174

208	Kinetics of the Anode Processes in PEM Fuel Cells The Promoting Effect of Ru in PtRu Anodes. *Fuel Cells*, **2001**, 1, 192-201	0.9	70
207	The BrEstedEvansPolanyi Relation and the Volcano Plot for Ammonia Synthesis over Transition Metal Catalysts. *Journal of Catalysis*, **2001**, 197, 229-231	2.3	471
206	Anode Materials for Low-Temperature Fuel Cells: A Density Functional Theory Study. *Journal of Catalysis*, **2001**, 199, 123-131	2.3	286
205	Ligand and ensemble effects in adsorption on alloy surfaces. *Physical Chemistry Chemical Physics*, **2001**, 3, 3814-3818	1.1	386
204	Adsorption-induced step formation. *Physical Review Letters*, **2001**, 87, 126102	1.9	58
203	One-dimensional metallic edge states in MoS2. *Physical Review Letters*, **2001**, 87, 196803	1.9	506
202	Density functional theory studies of the adsorption of ethylene and oxygen on Pt(111) and Pt[sub 3]Sn(111). *Journal of Chemical Physics*, **2001**, 114, 4663	1.3	69
201	Oxygen vacancies as active sites for water dissociation on rutile TiO(2)(110). *Physical Review Letters* , **2001**, 87, 266104	1.9	786
200	Adsorption of Cu and Pd on Al2O3(0001) surfaces with different stoichiometries. *Journal of Chemical Physics*, **2001**, 115, 11261-11267	1.3	83
199	Catalyst design by interpolation in the periodic table: bimetallic ammonia synthesis catalysts. *Journal of the American Chemical Society*, **2001**, 123, 8404-5	4.3	488
198	Structure and Reactivity of NiAu Nanoparticle Catalysts. *Journal of Physical Chemistry B*, **2001**, 105, 5450-5458		164
197	Synergetic effects in CO adsorption on CuPd(111) alloys. *Surface Science*, **2001**, 477, 59-75	0.7	105
196	The effect of strain for N2 dissociation on Fe surfaces. *Surface Science*, **2001**, 489, 135-143	0.7	41
195	N2 dissociation on Fe(110) and Fe/Ru(0001): what is the role of steps?. *Surface Science*, **2001**, 491, 183-194	0.7	55
194	The CO/Pt(111) Puzzle. *Journal of Physical Chemistry B*, **2001**, 105, 4018-4025	1	579
193	Surface chemistry in three dimensions: CO dissociation between two surfaces. *Chemical Physics Letters*, **2000**, 322, 307-311	1	2
192	Steps, kinks, and segregation at metallic surfaces. *Progress in Surface Science*, **2000**, 64, 193-198	1.6	12
191	Molecular aspects of the H2 activation on MoS2 based catalysts the role of dynamic surface arrangements. *Journal of Molecular Catalysis A*, **2000**, 163, 117-122		50

190	Making gold less noble. *Catalysis Letters*, **2000**, 64, 101-106	1	569
189	Edge termination of MoS2 and CoMoS catalyst particles. *Catalysis Letters*, **2000**, 64, 95-99	1	106
188	Asymmetric pair distribution functions in catalysts. *Topics in Catalysis*, **2000**, 10, 221-230	1.1	52
187	Theoretical Studies of Stability and Reactivity of CHx Species on Ni(111). *Journal of Catalysis*, **2000**, 189, 16-30	2.3	169
186	First principles analysis of hydrogen chemisorption on PdRe alloyed overlayers and alloyed surfaces. *Journal of Chemical Physics*, **2000**, 112, 5435-5439	1.3	67
185	Atomic-scale structure of single-layer MoS2 nanoclusters. *Physical Review Letters*, **2000**, 84, 951-4	1.9	704
184	Diffusion of N adatoms on the Fe(100) surface. *Physical Review Letters*, **2000**, 84, 4898-901	1.9	60
183	SURFACE SCIENCE: How to Power a Nanomotor. *Science*, **2000**, 290, 1520	10	11
182	Ammonia synthesis at low temperatures. *Journal of Chemical Physics*, **2000**, 112, 5343-5347	1.3	170
181	A Comparative Theoretical Study of the Hydrogen, Methyl, and Ethyl Chemisorption on the Pt(111) Surface. *Journal of the American Chemical Society*, **2000**, 122, 4129-4144	4.3	175
180	Theoretical Studies of Stability and Reactivity of C2Hydrocarbon Species on Pt Clusters, Pt(111), and Pt(211). *Journal of Physical Chemistry B*, **2000**, 104, 2299-2310	1	107
179	Modeling the Nitrogenase FeMo Cofactor. *Journal of the American Chemical Society*, **2000**, 122, 12751-12763	4.3	88
178	Mechanisms of self-diffusion on Pt(110). *Physical Review B*, **1999**, 60, R5149-R5152	1	44
177	Theoretical analysis of hydrogen chemisorption on Pd(111), Re(0001) and PdML/Re(0001), ReML/Pd(111) pseudomorphic overlayers. *Physical Review B*, **1999**, 60, 6146-6154	1	183
176	Molecular N2 chemisorptionSpecific adsorption on step defect sites on Pt surfaces. *Journal of Chemical Physics*, **1999**, 111, 8651-8658	1.3	49
175	Nitrogen Adsorption and Hydrogenation on a MoFe6S9 Complex. *Physical Review Letters*, **1999**, 82, 4054-4057	1.9	68
174	Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen. *Nature*, **1999**, 398, 134-136	10	194
173	Nitrogen Adsorption and Dissociation on Fe(111). *Journal of Catalysis*, **1999**, 182, 479-488	2.3	133

172	DFT Calculations of Unpromoted and Promoted MoS2-Based Hydrodesulfurization Catalysts. *Journal of Catalysis*, **1999**, 187, 109-122	2.3	330
171	Chemisorption of Methane on Ni(100) and Ni(111) Surfaces with Preadsorbed Potassium. *Journal of Catalysis*, **1999**, 187, 238-244	2.3	86
170	Advances in deep desulfurization. *Studies in Surface Science and Catalysis*, **1999**, 121, 13-22	0.4	24
169	Surface segregation energies in transition-metal alloys. *Physical Review B*, **1999**, 59, 15990-16000	1	794
168	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. *Physical Review B*, **1999**, 59, 7413-7421	1	5077
167	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. *Surface Science*, **1999**, 422, 8-16	0.7	88
166	How a gold substrate can increase the reactivity of a Pt overlayer. *Surface Science*, **1999**, 426, 395-409	0.7	245
165	Oxygen adsorption on Pt(110)-(1□2): new high-coverage structures. *Surface Science*, **1999**, 430, L533-L539	0.7	37
164	Catalysis from first principles. *Studies in Surface Science and Catalysis*, **1999**, 3-10	0.4	11
163	Role of Steps in N2 Activation on Ru(0001). *Physical Review Letters*, **1999**, 83, 1814-1817	1.9	597
162	Effect of Strain on the Reactivity of Metal Surfaces. *Physical Review Letters*, **1998**, 81, 2819-2822	1.9	1680
161	Design of a surface alloy catalyst for steam reforming. *Science*, **1998**, 279, 1913-5	10	852
160	A theoretical study of adsorbate□adsorbate interactions on Ru(0001). *Surface Science*, **1998**, 414, 315-329	0.7	109
159	Alkali Promotion of N2 Dissociation over Ru(0001). *Physical Review Letters*, **1998**, 80, 4333-4336	1.9	158
158	Crystal-Structure Contribution to the Solid Solubility in Transition Metal Alloys. *Physical Review Letters*, **1998**, 80, 1240-1243	1.9	27
157	N2 Interaction with Fe Surfaces. *Israel Journal of Chemistry*, **1998**, 38, 279-284	1	8
156	Sulphur Bonding in Transition Metal Sulphides and MoS2 Based Structures **1998**, 155-168		3
155	Scattering and conductance quantization in three-dimensional metal nanocontacts. *Physical Review B*, **1997**, 55, 2637-2650	1	87

154	Comment on "Cs-Induced Relaxation of the Cu(110) Surface". *Physical Review Letters*, **1997**, 78, 158-158	1.9	3
153	Adsorbate Reorganization at Steps: NO on Pd(211). *Physical Review Letters*, **1997**, 79, 4441-4444	1.9	60
152	Phase diagrams for surface alloys. *Physical Review B*, **1997**, 56, 5822-5834	1	362
151	Importance of Dynamics in real catalyst systems. *Studies in Surface Science and Catalysis*, **1997**, 121-139	0.4	22
150	A Comparison of N2 and CO Adsorption on Ru(001). *Zeitschrift Fur Physikalische Chemie*, **1997**, 198, 113-128	0.2	27
149	Growth of Co on Cu(111): subsurface growth of trilayer Co islands. *Surface Science*, **1997**, 387, 86-101	0.7	99
148	CO adsorption and dissociation on Pt(111) and Ni(111) surfaces. *Surface Science*, **1997**, 386, 67-72	0.7	85
147	Kinetic Implications of Dynamical Changes in Catalyst Morphology during Methanol Synthesis over Cu/ZnO Catalysts. *Journal of Catalysis*, **1997**, 168, 133-142	2.3	208
146	Density Functional Calculations of N2Adsorption and Dissociation on a Ru(0001) Surface. *Journal of Catalysis*, **1997**, 169, 85-92	2.3	97
145	Sulfur bonding in MoS2 and Co-Mo-S structures. *Catalysis Letters*, **1997**, 47, 177-182	1	120
144	Structure sensitivity in adsorption: CO interaction with stepped and reconstructed Pt surfaces. *Catalysis Letters*, **1997**, 46, 31-35	1	382
143	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19–20 February 1996.1. *Journal of Molecular Catalysis A*, **1997**, 115, 421-429		1000
142	Theory of Adsorption and Surface Reactions **1997**, 285-351		60
141	STABILITY OF ADSORBED HYDROGEN ON Si(100) UNDER CHANGES OF THE SURFACE POTENTIAL. *Surface Review and Letters*, **1996**, 03, 1227-1233	0.3	3
140	Anisotropic corner diffusion as origin for dendritic growth on hexagonal substrates. *Surface Science* , **1996**, 349, L115-L122	0.7	106
139	Geometric and electronic factors determining the differences in reactivity of H2 on Cu(100) and Cu(111). *Surface Science*, **1996**, 359, 45-53	0.7	88
138	Island shapes in homoepitaxial growth of Pt(111). *Surface Science*, **1996**, 359, 37-44	0.7	53
137	Erratum to Electronic factors determining the reactivity of metal surfaces[Surface Science 343 (1995) 211]. *Surface Science*, **1996**, 359, 306	0.7	43

136	Incomplete melting of the Si(100) surface from molecular-dynamics simulations using the effective-medium tight-binding model. *Surface Science*, **1996**, 360, 221-228	0.7	9
135	A semi-empirical effective medium theory for metals and alloys. *Surface Science*, **1996**, 366, 394-402	0.7	185
134	CO chemisorption at metal surfaces and overlayers. *Physical Review Letters*, **1996**, 76, 2141-2144	1.9	1135
133	A Microkinetic Analysis of the Water Gas Shift Reaction under Industrial Conditions. *Journal of Catalysis*, **1996**, 158, 170-180	2.3	194
132	Designing surface alloys with specific active sites. *Catalysis Letters*, **1996**, 40, 131-135	1	65
131	A theoretical study of CH4 dissociation on pure and gold-alloyed Ni(111) surfaces. *Journal of Chemical Physics*, **1996**, 105, 5595-5604	1.3	234
130	Why gold is the noblest of all the metals. *Nature*, **1995**, 376, 238-240	16.4	2251
129	A Kinetic Model of Methanol Synthesis. *Journal of Catalysis*, **1995**, 156, 229-242	2.3	209
128	Surface stress, surface elasticity, and the size effect in surface segregation. *Physical Review B*, **1995**, 51, 10937-10946	1	66
127	Quantized conductance in atom-sized wires between two metals. *Physical Review B*, **1995**, 52, 8499-8514	1	260
126	Atomic-scale determination of misfit dislocation loops at metal-metal interfaces. *Physical Review Letters*, **1995**, 75, 489-492	1.9	149
125	Olesen et al. reply. *Physical Review Letters*, **1995**, 74, 2147	1.9	71
124	"Dealloying" phase separation during growth of Au on Ni(110). *Physical Review Letters*, **1995**, 74, 1159-1162	1.9	77
123	Direct pathway for sticking/desorption of H2 on Si(100). *Physical Review B*, **1995**, 51, 13432-13440	1	82
122	Island shape-induced transition from 2D to 3D growth for Pt/Pt(111). *Physical Review Letters*, **1995**, 74, 2295-2298	1.9	164
121	Electronic factors determining the reactivity of metal surfaces. *Surface Science*, **1995**, 343, 211-220	0.7	1679
120	Effect of strain on surface diffusion and nucleation. *Physical Review B*, **1995**, 52, 14380-14383	1	257
119	Size dependence of phase separation in small bimetallic clusters. *Journal of Physics Condensed Matter*, **1995**, 7, 1047-1057	0.7	68

118	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). *Physical Review B*, **1995**, 52, 14954-14962	1	110
117	Fractal and Dendritic Growth of Surface Aggregates. *Materials Research Society Symposia Proceedings*, **1995**, 407, 379		4
116	Construction of transferable spherically averaged electron potentials. *Journal of Physics Condensed Matter*, **1994**, 6, 5415-5421	0.7	5
115	Quantized conductance in an atom-sized point contact. *Physical Review Letters*, **1994**, 72, 2251-2254	1.9	402
114	Surface alloying in metal-on-metal epitaxial growth. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1994**, 12, 1787-1789	0.9	10
113	Effective-medium tight-binding model for silicon. *Physical Review B*, **1994**, 50, 10727-10741	1	24
112	The coupling between adsorption dynamics and the surface structure: H2 on Si(100). *Chemical Physics Letters*, **1994**, 229, 645-649	1	63
111	Determination of metal particle sizes from EXAFS. *Catalysis Today*, **1994**, 21, 49-55	1.8	29
110	Methanol synthesis on Cu(100) from a binary gas mixture of CO2 and H2. *Catalysis Letters*, **1994**, 26, 373-381	1	203
109	The surface science based ammonia kinetics revisited. *Topics in Catalysis*, **1994**, 1, 253-263	1.1	32
108	Wetting/ non-wetting phenomena during catalysis: Evidence from in situ on-line EXAFS studies of Cu-based catalysts. *Topics in Catalysis*, **1994**, 1, 367-376	1.1	137
107	From quantum physics to heterogeneous catalysis. *Topics in Catalysis*, **1994**, 1, 385-403	1.1	5
106	Melting a Copper Cluster: Critical-Droplet Theory. *Europhysics Letters*, **1994**, 26, 51-56	0.5	42
105	The mobility of Pt atoms and small Pt clusters on Pt(111) and its implications for the early stages of epitaxial growth. *Surface Science*, **1994**, 321, 161-171	0.7	49
104	Theory of adsorption and adsorbate-induced reconstruction. *Surface Science*, **1994**, 299-300, 690-705	0.7	34
103	The energetics and dynamics of H2 dissociation on Al(110). *Surface Science*, **1994**, 304, 131-144	0.7	43
102	Multidimensional potential energy surface for H2 dissociation over Cu(111). *Physical Review Letters*, **1994**, 73, 1400-1403	1.9	313
101	Melting a Copper Cluster: Critical-Droplet Theory. *Europhysics Letters*, **1994**, 26, 557-557	0.5	2

100	Polarization and charge transfer during the dissociation of H2 on Al(110). *Surface Science*, **1993**, 297, L68-L72	0.7	17
99	Activation free energy and entropy for the normal and exchange selfdiffusion processes on Cu(100). *Surface Science*, **1993**, 289, 68-74	0.7	32
98	Chemisorption and vibration of hydrogen on Cu(111). *Surface Science*, **1993**, 285, 27-30	0.7	39
97	Many-atom interactions in metals. *Surface Science*, **1993**, 283, 277-282	0.7	46
96	Initial growth of Au on Ni(110): Surface alloying of immiscible metals. *Physical Review Letters*, **1993**, 71, 754-757	1.9	308
95	The Effect of Anharmonicity on the EXAFS Coordination Number in Small Metallic Particles. *Japanese Journal of Applied Physics*, **1993**, 32, 95	0.5	23
94	Accommodation and diffusion of Cu deposited on flat and stepped Cu(111) surfaces. *Physical Review B*, **1993**, 48, 5607-5611	1	58
93	Role of nonlocal exchange correlation in activated adsorption. *Physical Review Letters*, **1993**, 70, 3971-3974	1.9	155
92	A New Procedure for Particle Size Determination by EXAFS Based on Molecular Dynamics Simulations. *Journal of Catalysis*, **1993**, 141, 368-379	2.3	101
91	Modeling the potassium promotion of CO bonding to Ni (100). *Chemical Physics Letters*, **1993**, 214, 443-446	1.4	15
90	Oxygen chemisorption on metal surfaces: General trends for Cu, Ni and Ag. *Progress in Surface Science*, **1993**, 44, 5-66	1.6	432
89	An effective-medium theory approach to ordering in Cu-Au alloys. *Journal of Physics Condensed Matter*, **1992**, 4, 7191-7202	0.7	17
88	Multidimensional effects in dissociative chemisorption: H2 on Cu and Ni surfaces. *Physical Review B*, **1992**, 45, 11362-11365	1	55
87	Ab initio potential for solids. *Physical Review B*, **1992**, 46, 3798-3809	1	40
86	Chemisorption of H, O, and S on Ni(110): general trends. *Surface Science*, **1992**, 272, 334-341	0.7	65
85	Dissociation path for H2 on Al(110). *Physical Review Letters*, **1992**, 69, 1971-1974	1.9	76
84	Understanding the trends in the hydrodesulfurization activity of the transition metal sulfides. *Catalysis Letters*, **1992**, 13, 1-8	1	130
83	A kinetic model of the water gas shift reaction. *Journal of Catalysis*, **1992**, 134, 445-468	2.3	209

82	The reactivity of metal surfaces. *Catalysis Letters*, **1991**, 9, 173-182	1	9
81	Electronic factors in catalysis. *Progress in Surface Science*, **1991**, 38, 103-144	1.6	90
80	Self-diffusion on copper surfaces. *Physical Review B*, **1991**, 44, 6523-6526	1	150
79	Anharmonicity and disorder on the Cu(110) surface. *Physical Review B*, **1991**, 44, 13002-13009	1	65
78	Optimized and transferable densities from first-principles local density calculations. *Journal of Physics Condensed Matter*, **1991**, 3, 5437-5443	0.7	20
77	Vibrational properties of aluminum, nickel and copper surfaces. *Surface Science*, **1991**, 254, 261-274	0.7	31
76	Cu cluster shell structure at elevated temperatures. *Physical Review Letters*, **1991**, 66, 2219-2222	1.9	90
75	Chemisorption on metal surfaces. *Reports on Progress in Physics*, **1990**, 53, 1253-1295	4.3	244
74	Interaction of hydrogen isotopes with metals: Deuterium trapped at lattice defects in palladium. *Journal of Fusion Energy*, **1990**, 9, 257-261	0.3	15
73	The surface phonons of Cu(111). *Journal of Electron Spectroscopy and Related Phenomena*, **1990**, 54-55, 237-244	0.7	15
72	Oxygen chemisorption on Cu(110): A model for the c(6 x 2) structure. *Physical Review Letters*, **1990**, 65, 2027-2030	1.9	119
71	The dissociative adsorption of hydrogen: Two-, three-, and four-dimensional quantum simulations. *Journal of Chemical Physics*, **1990**, 93, 2879-2884	1.3	90
70	Energies controlling nucleation and growth processes: The case of Ag/W(110). *Physical Review Letters*, **1990**, 65, 3317-3320	1.9	75
69	Theory of the oxygen-induced restructuring of Cu(110) and Cu(100) surfaces. *Physical Review Letters*, **1990**, 65, 1788-1791	1.9	139
68	Effective-medium calculations for hydrogen in Ni, Pd, and Pt. *Physical Review B*, **1990**, 41, 12413-12423	1	23
67	Is there a contraction of the interatomic distance in small metal particles?. *Physical Review Letters*, **1990**, 64, 3155-3158	1.9	80
66	Electrostatic interactions between coadsorbed Xe and CO. *Surface Science*, **1990**, 226, L48-L50	0.7	22
65	H-H interactions in Pd. *Physical Review B*, **1989**, 40, 1993-1996	1	41

64	The onset of disorder in Al(110) surfaces below the melting point. *Surface Science*, **1989**, 220, L693-L700	0.7	63
63	Multiple deuterium occupancy of vacancies in Pd and related metals. *Physical Review B*, **1989**, 40, 1990-1992	3	89
62	Effective medium potentials for molecule-surface interactions: H2 on Cu and Ni surfaces. *Journal of Chemical Physics*, **1989**, 90, 7461-7471	1.3	95
61	An interpretation of the high-pressure kinetics of ammonia synthesis based on a microscopic model. *Journal of Catalysis*, **1988**, 110, 1-10	2.3	116
60	Comment on the application of surface kinetic data to the industrial synthesis of ammonia by M. Bowker, I. Parker and K.C. Waugh. *Surface Science*, **1988**, 197, L230-L232	0.7	33
59	Disordering and melting of aluminum surfaces. *Physical Review Letters*, **1988**, 61, 440-443	1.9	199
58	Theory of alkali-metal-induced reconstruction of fcc (110) surfaces. *Physical Review Letters*, **1988**, 60, 2496-2498	1.9	114
57	Monte Carlo calculation of the thermal expansion coefficient of Al. *Physical Review B*, **1987**, 36, 5035-5036	3	31
56	Theoretical aspects of surface reactions. *Surface Science*, **1987**, 189-190, 91-105	0.7	59
55	Interatomic interactions in the effective-medium theory. *Physical Review B*, **1987**, 35, 7423-7442	1	768
54	Theory of adsorbate-induced surface relaxations: Hydrogen on Cu(110). *Physical Review Letters*, **1987**, 59, 2764-2767	1.9	66
53	Theory of hydrogen interaction with metals. *Journal of the Less Common Metals*, **1987**, 130, 475-490		135
52	Dynamics of molecule-surface interactions. *Surface Science*, **1987**, 179, L41-L48	0.7	83
51	A description of the high-pressure ammonia synthesis reaction based on surface science. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1987**, 5, 581-585	0.9	26
50	Multiple hydrogen occupancy of vacancies in Fe. *Journal of Applied Physics*, **1987**, 61, 1788-1794	1	91
49	Electrostatic interactions and their role in coadsorption phenomena. *Journal of the Chemical Society Faraday Transactions I*, **1987**, 83, 1935		43
48	Quantum motion of chemisorbed hydrogen. *Journal of Electron Spectroscopy and Related Phenomena*, **1986**, 38, 313-315	0.7	5
47	Calculated Diabatic Atom-Surface Potential-Energy Curves. *Physica Scripta*, **1986**, 34, 77-83	0.9	17

46	Trends in hydrogen heats of solution and vacancy trapping energies in transition metals. *Journal of Physics F: Metal Physics*, **1986**, 16, 1161-1171		93
45	Theoretical examination of the trapping of ion-implanted hydrogen in metals. *Physical Review B*, **1986**, 33, 854-863	1	99
44	A theoretical study of carbon chemisorption on nickel surfaces. *Surface Science*, **1986**, 166, 539-553	0.7	21
43	Interaction of hydrogen with defects in metals. *Nuclear Instruments & Methods in Physics Research B*, **1985**, 7-8, 55-66	0.5	74
42	Adsorbate–surface and adsorbate–adsorbate interactions and their role in surface reactions. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1985**, 3, 1668-1672	0.9	26
41	Excitation of hydrogen motion inside a nickel vacancy. *Physical Review Letters*, **1985**, 55, 852-855	1.9	26
40	Bridging the "pressure gap" between ultrahigh-vacuum surface physics and high-pressure catalysis. *Physical Review Letters*, **1985**, 55, 2502-2505	1.9	242
39	Electrostatic adsorbate-adsorbate interactions: The poisoning and promotion of the molecular adsorption reaction. *Surface Science*, **1985**, 150, 24-38	0.7	327
38	Oxygen chemisorption and incorporation on transition metal surfaces. *Surface Science*, **1985**, 152-153, 660-683	0.7	70
37	Immobilization mechanisms for ion-implanted deuterium in aluminum. *Journal of Applied Physics*, **1985**, 58, 1841-1850	1	50
36	Vibrational excitation, harpooning, and sticking in molecule–surface collisions. *Journal of Chemical Physics*, **1984**, 81, 2828-2838	1.3	98
35	Repulsive interaction of the helium atom with a metal surface. *Physical Review B*, **1984**, 29, 2314-2316	1	113
34	Interaction of deuterium with lattice defects in nickel. *Nuclear Instruments & Methods in Physics Research B*, **1984**, 4, 374-387	0.5	29
33	Changes in the vibrational frequencies of adsorbed molecules due to an applied electric field. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1984**, 161, 193-198		93
32	Theory nof chemisorption and heterogeneous catalysis. *Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics*, **1984**, 127, 193-202		6
31	Hydrogen adsorption on metal surfaces. *Surface Science*, **1984**, 136, 59-81	0.7	373
30	Microscopic model for the poisoning and promotion of adsorption rates by electronegative and electropositive atoms. *Surface Science*, **1984**, 137, 65-78	0.7	296
29	Theoretical studies of molecular adsorption on metal surfaces. *International Journal of Quantum Chemistry*, **1983**, 23, 1083-1090	0.6	2

28	Interaction of helium with a metal surface. *Physical Review B*, **1983**, 27, 4612-4616	1	127
27	Quantum Motion of Chemisorbed Hydrogen on Ni Surfaces. *Physical Review Letters*, **1983**, 51, 1081-1084	1.9	145
26	The Theory of Ionization Probability in Sputtering. *Physica Scripta*, **1983**, T6, 15-18	0.9	69
25	Rare-gas-metal pair potential: He-vacancy interaction. *Journal of Physics F: Metal Physics*, **1982**, 12, L7-L11		48
24	Calculated Binding Properties of Hydrogen on Nickel Surfaces. *Physical Review Letters*, **1982**, 48, 1620-1624	1.9	103
23	Interaction of Hydrogen with Defects in Metals: Interplay between Theory and Experiment. *Physical Review Letters*, **1982**, 49, 1420-1423	1.9	102
22	Calculation of the helium diffraction from the reconstructed Au(110) surface. *Surface Science*, **1982**, 119, L393-L400	0.7	50
21	Covalent effects in the effective-medium theory of chemical binding: Hydrogen heats of solution in the 3d metals. *Physical Review B*, **1982**, 26, 2875-2885	1	390
20	Adsorption and Dissociation of H2 on Mg Surfaces. *Physical Review Letters*, **1981**, 46, 257-260	1.9	201
19	Dynamical aspects of electronic structure during adsorption. *Journal of Vacuum Science and Technology*, **1981**, 18, 420-426		79
18	Variation of Adatom Valence-Level Positions With the Distance to a Metal Surface. *Physica Scripta*, **1980**, 22, 165-170	0.9	39
17	Dependence of the He-Scattering Potential at Surfaces on the Surface-Electron-Density Profile. *Physical Review Letters*, **1980**, 45, 807-810	1.9	381
16	Effective-medium theory of chemical binding: Application to chemisorption. *Physical Review B*, **1980**, 21, 2131-2136	1	414
15	Calculated energies and geometries for hydrogen impurities in Al and Mg. *Journal of Physics F: Metal Physics*, **1979**, 9, 1975-1982		63
14	Theoretical description of molecule-metal interaction and surface reactions. *Surface Science*, **1979**, 89, 196-225	0.7	146
13	Correlation between sticking probability and adsorbate-induced electron structure. *Surface Science*, **1979**, 89, 251-261	0.7	120
12	Photon and electron emission as indicators of intermediate states in surface reactions. *Surface Science*, **1979**, 89, 554-565	0.7	147
11	Molecular orbital description of surface chemiluminescence. *Surface Science*, **1979**, 80, 179-188	0.7	143

10	Picture of adsorption and desorption of hydrogen emerging from self-consistent model calculations. *Surface Science*, **1979**, 80, 441-449	0.7	40
9	Self-Consistent Calculation of Molecular Chemisorption on Metals. *Physica Scripta*, **1979**, 20, 192-201	0.9	61
8	Secondary-ion emission probability in sputtering. *Physical Review B*, **1979**, 19, 5661-5665	1	339
7	Electron structure of single and interacting hydrogen impurities in free-electron-like metals. *Physical Review B*, **1979**, 20, 446-454	1	118
6	Contraction of diatomic molecules upon chemisorption. *Solid State Communications*, **1978**, 28, 899-902	0.6	12
5	Impurity interactions and pseudo-molecule formation in metals. *Solid State Communications*, **1978**, 25, 995-998	0.6	19
4	Electronic structure of H and He in metal vacancies. *Solid State Communications*, **1977**, 24, 691-693	0.6	54
3	The Electronic Factor in Heterogeneous Catalysis. *Advances in Catalysis*, **1955**, 7, 1-45	0.2	21
2	Increasing Current Density of Li-Mediated Ammonia Synthesis with High Surface Area Copper Electrodes. *ACS Energy Letters*,36-41	6.8	10
1	Sustainable Ammonia Synthesis Exploring the scientific challenges associated with discovering alternative, sustainable processes for ammonia production		32