Andreas Heyden

List of Publications by Year
in descending order

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106 papers	8,667 citations	61984 43 h-index	42399 92 g-index
108 all docs	108 docs citations	108 times ranked	9393 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method. Journal of Chemical Physics, 2005, 123, 224101.	3.0	662
3	A growing string method for determining transition states: Comparison to the nudged elastic band and string methods. Journal of Chemical Physics, 2004, 120, 7877-7886.	3.0	293
4	Upcycling Single-Use Polyethylene into High-Quality Liquid Products. ACS Central Science, 2019, 5, 1795-1803.	11.3	283
5	Analysis of Kinetics and Reaction Pathways in the Aqueous-Phase Hydrogenation of Levulinic Acid To Form Î³-Valerolactone over Ru/C. ACS Catalysis, 2014, 4, 1171-1181.	11.2	265
6	Catalytic upcycling of high-density polyethylene via a processive mechanism. Nature Catalysis, 2020, 3, 893-901.	34.4	262
7	Electronic Properties of Bimetallic Metalâ€“Organic Frameworks (MOFs): Tailoring the Density of Electronic States through MOF Modularity. Journal of the American Chemical Society, 2017, 139, 5201-5209.	13.7	178
8	Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5â€. Journal of Physical Chemistry B, 2005, 109, 1857-1873.	2.6	176
9	Adaptive Partitioning in Combined Quantum Mechanical and Molecular Mechanical Calculations of Potential Energy Functions for Multiscale Simulations. Journal of Physical Chemistry B, 2007, 111, 2231-2241.	2.6	172
10	Synthesis and characterization of Mo-doped SrFeO3â^Î´ as cathode materials for solid oxide fuel cells. Journal of Power Sources, 2012, 202, 63-69.	7.8	147
11	On the importance of metalâ€“oxide interface sites for the waterâ€“gas shift reaction over Pt/CeO2 catalysts. Journal of Catalysis, 2014, 309, 314-324.	6.2	142
12	Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 6624-6647.	11.2	134
13	Î²-O-4 Bond Cleavage Mechanism for Lignin Model Compounds over Pd Catalysts Identified by Combination of First-Principles Calculations and Experiments. ACS Catalysis, 2016, 6, 5589-5598.	11.2	116
14	Theoretical Investigation of the Reaction Mechanism of the Guaiacol Hydrogenation over a Pt(111) Catalyst. ACS Catalysis, 2015, 5, 2423-2435.	11.2	111
15	Liquid-Phase Modeling in Heterogeneous Catalysis. ACS Catalysis, 2018, 8, 2188-2194.	11.2	101
16	Theoretical investigation of the reaction mechanism of the hydrodeoxygenation of guaiacol over a Ru(0 0 0 1) model surface. Journal of Catalysis, 2015, 321, 39-50.	6.2	100
17	Conservative Algorithm for an Adaptive Change of Resolution in Mixed Atomistic/Coarse-Grained Multiscale Simulations. Journal of Chemical Theory and Computation, 2008, 4, 217-221.	5.3	94
18	Active Sites in Copper-Based Metalâ€“Organic Frameworks: Understanding Substrate Dynamics, Redox Processes, and Valence-Band Structure. Journal of Physical Chemistry C, 2015, 119, 27457-27466.	3.1	87

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19	Microkinetic modeling of the decarboxylation and decarbonylation of propanoic acid over Pd(111) model surfaces based on parameters obtained from first principles. Journal of Catalysis, 2013, 305, 56-66.	6.2	81
20	A Reaction Mechanism for the Nitrous Oxide Decomposition on Binuclear Oxygen Bridged Iron Sites in Fe-ZSM-5. Journal of Physical Chemistry C, 2007, 111, 2092-2101.	3.1	80
21	Water-Gas Shift Activity of Atomically Dispersed Cationic Platinum versus Metallic Platinum Clusters on Titania Supports. ACS Catalysis, 2017, 7, 301-309.	11.2	78
22	Nitrous Oxide Decomposition over Fe-ZSM-5 in the Presence of Nitric Oxide: A Comprehensive DFT Study. Journal of Physical Chemistry B, 2006, 110, 17096-17114.	2.6	77
23	Origin of the unique activity of Pt/TiO2 catalysts for the waterâ€“gas shift reaction. Journal of Catalysis, 2013, 306, 78-90.	6.2	76
24	Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surfaces Using Machine Learning. Journal of Physical Chemistry C, 2018, 122, 28142-28150.	3.1	74
25	Adsorbate-Induced Changes in the Surface Composition of Bimetallic Clusters: Ptâˆ'Au on TiO₂(110). Journal of Physical Chemistry C, 2010, 114, 21652-21663.	3.1	70
26	Theoretical Investigation of the Reaction Mechanism of the Decarboxylation and Decarbonylation of Propanoic Acid on Pd(111) Model Surfaces. Journal of Physical Chemistry C, 2012, 116, 14328-14341.	3.1	70
27	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 based on parameters obtained from first-principles calculations. Journal of Catalysis, 2005, 233, 26-35.	6.2	68
28	Theoretical Investigation of H₂ Oxidation on the Sr₂Fe_{1.5}Mo_{0.5}O₆ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions. Journal of the American Chemical Society, 2014, 136, 8374-8386.	13.7	68
29	Toward rational design of stable, supported metal catalysts for aqueous-phase processing: Insights from the hydrogenation of levulinic acid. Journal of Catalysis, 2015, 329, 10-21.	6.2	65
30	Theoretical Investigation of the Hydrodeoxygenation of Levulinic Acid to Î³-Valerolactone over Ru(0001). ACS Catalysis, 2017, 7, 215-228.	11.2	65
31	Microkinetic modeling of nitrous oxide decomposition on dinuclear oxygen bridged iron sites in Fe-ZSM-5. Journal of Catalysis, 2007, 248, 213-225.	6.2	63
32	Size-Controlled Nanoparticles Embedded in a Mesoporous Architecture Leading to Efficient and Selective Hydrogenolysis of Polyolefins. Journal of the American Chemical Society, 2022, 144, 5323-5334.	13.7	60
33	Modeling the noble metal/TiO2 (110) interface with hybrid DFT functionals: A periodic electrostatic embedded cluster model study. Journal of Chemical Physics, 2010, 133, 164703.	3.0	59
34	Waterâ€“Gas Shift Catalysis at Corner Atoms of Pt Clusters in Contact with a TiO₂ (110) Support Surface. ACS Catalysis, 2014, 4, 3654-3662.	11.2	56
35	Uncertainty Quantification Framework Applied to the Waterâ€“Gas Shift Reaction over Pt-Based Catalysts. Journal of Physical Chemistry C, 2016, 120, 10328-10339.	3.1	56
36	Controlling reaction pathways of selective Câ€“O bond cleavage of glycerol. Nature Communications, 2018, 9, 4612.	12.8	54

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37	Ni modified ceramic anodes for solid oxide fuel cells. Journal of Power Sources, 2012, 201, 43-48.	7.8	52
38	Solvent effects on the hydrodeoxygenation of propanoic acid over Pd(111) model surfaces. Green Chemistry, 2014, 16, 605-616.	9.0	51
39	Identifying Active Sites of the Waterâ€“Gas Shift Reaction over Titania Supported Platinum Catalysts under Uncertainty. ACS Catalysis, 2018, 8, 3990-3998.	11.2	49
40	Understanding the Nature and Activity of Supported Platinum Catalysts for the Waterâ€“Gas Shift Reaction: From Metallic Nanoclusters to Alkali-Stabilized Single-Atom Cations. ACS Catalysis, 2019, 9, 7721-7740.	11.2	48
41	New Implicit Solvation Scheme for Solid Surfaces. Journal of Physical Chemistry C, 2012, 116, 22458-22462.	3.1	47
42	On the Importance of the Associative Carboxyl Mechanism for the Water-Gas Shift Reaction at Pt/CeO₂ Interface Sites. Journal of Physical Chemistry C, 2014, 118, 6314-6323.	3.1	47
43	Combined DFT and Microkinetic Modeling Study of Hydrogen Oxidation at the Ni/YSZ Anode of Solid Oxide Fuel Cells. Journal of Physical Chemistry Letters, 2012, 3, 2767-2772.	4.6	46
44	Theoretical investigation of the decarboxylation and decarbonylation mechanism of propanoic acid over a Ru(0 0 0 1) model surface. Journal of Catalysis, 2015, 324, 14-24.	6.2	45
45	Nature of Pt_n/TiO₂(110) Interface under Water-Gas Shift Reaction Conditions: A Constrained ab Initio Thermodynamics Study. Journal of Physical Chemistry C, 2011, 115, 19246-19259.	3.1	44
46	Hybrid Quantum Mechanics/Molecular Mechanics Solvation Scheme for Computing Free Energies of Reactions at Metalâ€“Water Interfaces. Journal of Chemical Theory and Computation, 2014, 10, 3354-3368.	5.3	42
47	Investigation of solvent effects in the hydrodeoxygenation of levulinic acid to Î³-valerolactone over Ru catalysts. Journal of Catalysis, 2019, 379, 164-179.	6.2	42
48	Solvation Effects in the Hydrodeoxygenation of Propanoic Acid over a Model Pd(211) Catalyst. Journal of Physical Chemistry C, 2016, 120, 2724-2736.	3.1	40
49	Solvent effects in the liquid phase hydrodeoxygenation of methyl propionate over a Pd(1 1 1) catalyst model. Journal of Catalysis, 2016, 333, 171-183.	6.2	37
50	Adaptive-Partitioning QM/MM Dynamics Simulations: 3. Solvent Molecules Entering and Leaving Protein Binding Sites. Journal of Chemical Theory and Computation, 2014, 10, 4765-4776.	5.3	36
51	Direct Oxidation of Methane to Methanol Enabled by Electronic Atomic Monolayerâ€“Metal Support Interaction. ACS Catalysis, 2019, 9, 6073-6079.	11.2	36
52	Ethylene glycol reforming on Pt(111): first-principles microkinetic modeling in vapor and aqueous phases. Catalysis Science and Technology, 2016, 6, 8242-8256.	4.1	35
53	Nature of Pt_n/CeO₂ (111) Surface under Waterâ€“Gas Shift Reaction Conditions: A Constrained ab Initio Thermodynamics Study. Journal of Physical Chemistry C, 2012, 116, 9029-9042.	3.1	34
54	Understanding Active Sites in the Waterâ€“Gas Shift Reaction for Ptâ€“Re Catalysts on Titania. ACS Catalysis, 2017, 7, 2597-2606.	11.2	34

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55	Study of molecular shape and non-ideality effects on mixture adsorption isotherms of small molecules in carbon nanotubes: A grand canonical Monte Carlo simulation study. Chemical Engineering Science, 2002, 57, 2439-2448.	3.8	31
56	Nucleation, Growth, and Adsorbate-Induced Changes in Composition for Coâ€“Au Bimetallic Clusters on TiO₂. Journal of Physical Chemistry C, 2012, 116, 24616-24629.	3.1	31
57	Investigation of solvent effects on the hydrodeoxygenation of guaiacol over Ru catalysts. Catalysis Science and Technology, 2019, 9, 6253-6273.	4.1	28
58	Solving the equations of motion for mixed atomistic and coarse-grained systems. Molecular Simulation, 2009, 35, 962-973.	2.0	27
59	Hydrodeoxygenation of propanoic acid over silica-supported palladium: effect of metal particle size. Catalysis Science and Technology, 2014, 4, 3909-3916.	4.1	25
60	Microkinetic analysis of C3â€“C5 ketone hydrogenation over supported Ru catalysts. Journal of Catalysis, 2017, 348, 59-74.	6.2	24
61	Mechanistic study of the ceria supported, re-catalyzed deoxydehydration of vicinal OH groups. Catalysis Science and Technology, 2018, 8, 5750-5762.	4.1	24
62	A Multiple Filter Based Neural Network Approach to the Extrapolation of Adsorption Energies on Metal Surfaces for Catalysis Applications. Journal of Chemical Theory and Computation, 2020, 16, 1105-1114.	5.3	24
63	Mechanism of Sulfur Poisoning of Sr₂Fe_{1.5}Mo_{0.5}O_{6-Î´} Perovskite Anode under Solid Oxide Fuel Cell Conditions. Journal of Physical Chemistry C, 2014, 118, 23545-23552.	3.1	23
64	Titaniaâ€Supported Singleâ€Atom Platinum Catalyst for Waterâ€Gas Shift Reaction. Chemie-Ingenieur-Technik, 2017, 89, 1343-1349.	0.8	22
65	Microkinetic analysis of acetone hydrogenation over Pt/SiO2. Journal of Catalysis, 2019, 374, 183-198.	6.2	22
66	Importance of Angelica Lactone Formation in the Hydrodeoxygenation of Levulinic Acid to Î³-Valerolactone over a Ru(0001) Model Surface. Journal of Physical Chemistry C, 2017, 121, 18746-18761.	3.1	21
67	Computational Investigation of Aqueous Phase Effects on the Dehydrogenation and Dehydroxylation of Polyols over Pt(111). Journal of Physical Chemistry C, 2019, 123, 19052-19065.	3.1	21
68	Prediction of Transition-State Energies of Hydrodeoxygenation Reactions on Transition-Metal Surfaces Based on Machine Learning. Journal of Physical Chemistry C, 2019, 123, 29804-29810.	3.1	21
69	Enhanced reducibility and conductivity of Na/K-doped SrTi0.8Nb0.2O3. Journal of Materials Chemistry A, 2013, 1, 10546.	10.3	20
70	Effect of Palladium Surface Structure on the Hydrodeoxygenation of Propanoic Acid: Identification of Active Sites. Journal of Physical Chemistry C, 2015, 119, 1928-1942.	3.1	20
71	In Situ Ambient Pressure X-ray Photoelectron Spectroscopy Studies of Methanol Oxidation on Pt(111) and Ptâ€“Re Alloys. Journal of Physical Chemistry C, 2015, 119, 23082-23093.	3.1	20
72	Obtaining mixed ionic/electronic conductivity in perovskite oxides in a reducing environment: A computational prediction for doped SrTiO3. Solid State Ionics, 2012, 228, 37-45.	2.7	19

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73	Rational design of mixed ionic and electronic conducting perovskite oxides for solid oxide fuel cell anode materials: A case study for doped SrTiO3. Journal of Power Sources, 2014, 245, 875-885.	7.8	19
74	Investigation of the high-temperature redox chemistry of Sr₂Fe_{1.5}Mo_{0.5}O_{6â^'Î´}via in situ neutron diffraction. Journal of Materials Chemistry A, 2014, 2, 4045-4054.	10.3	19
75	Theoretical investigation of the hydrodeoxygenation of methyl propionate over Pd (111) model surfaces. Catalysis Science and Technology, 2014, 4, 3981-3992.	4.1	18
76	Density functional theory study on the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type doped SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>at anodic solid oxide fuel cell conditions. Physical	3.2	16
77	Optimum Reaction Conditions for 1,4-Anhydroerythritol and Xylitol Hydrodeoxygenation over a ReO_xâ€“Pd/CeO₂ Catalyst via Design of Experiments. Industrial & Engineering Chemistry Research, 2019, 58, 8681-8689.	3.7	16
78	Dependency of solvation effects on metal identity in surface reactions. Communications Chemistry, 2020, 3, .	4.5	15
79	Propane Dehydrogenation on Platinum Catalysts: Identifying the Active Sites through Bayesian Analysis. ACS Catalysis, 2022, 12, 2487-2498.	11.2	15
80	Unraveling the mechanism of the hydrodeoxygenation of propionic acid over a Pt (1ÂĪÂĪ1) surface in vapor and liquid phases. Journal of Catalysis, 2020, 381, 547-560.	6.2	14
81	Reaction kinetics of the electrochemical oxidation of CO and syngas fuels on a Sr₂Fe_{1.5}Mo_{0.5}O_{6â^'Î´} perovskite anode. Journal of Materials Chemistry A, 2015, 3, 21618-21629.	10.3	13
82	Deoxydehydration of 1,4-anhydroerythritol over anatase TiO₂(101)-supported ReO_x and MoO_x. Catalysis Science and Technology, 2020, 10, 3731-3738.	4.1	13
83	Unraveling the mechanism of propanoic acid hydrodeoxygenation on palladium using deuterium kinetic isotope effects. Journal of Molecular Catalysis A, 2015, 406, 85-93.	4.8	12
84	Understanding the effect of Mo2C support on the activity of Cu for the hydrodeoxygenation of glycerol. Journal of Catalysis, 2020, 388, 141-153.	6.2	12
85	Supported Bifunctional Molybdenum Oxide-Palladium Catalysts for Selective Hydrodeoxygenation of Biomass-Derived Polyols and 1,4-Anhydroerythritol. ACS Sustainable Chemistry and Engineering, 2022, 10, 5719-5727.	6.7	12
86	In-Situ Oxygen Isotopic Exchange Vibrational Spectroscopy of Rhenium Oxide Surface Structures on Cerium Oxide. Journal of Physical Chemistry C, 2020, 124, 7174-7181.	3.1	11
87	Kinetics Study of the Hydrodeoxygenation of Xylitol over a ReOx-Pd/CeO2 Catalyst. Catalysts, 2021, 11, 108.	3.5	11
88	Highly Efficient Deoxydehydration and Hydrodeoxygenation on MoS₂-Supported Transition-Metal Atoms through a Câ€“H Activation Mechanism. ACS Catalysis, 2020, 10, 11346-11355.	11.2	10
89	Theoretical Investigation of Solvent Effects on the Hydrodeoxygenation of Propionic Acid over a Ni(111) Catalyst Model. Journal of Physical Chemistry C, 2020, 124, 16488-16500.	3.1	10
90	Oxidative dehydrogenation of propane on the oxygen adsorbed edges of boron nitride nanoribbons. Catalysis Science and Technology, 2020, 10, 5181-5195.	4.1	10

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91	Comparative Study on the Machine Learning-Based Prediction of Adsorption Energies for Ring and Chain Species on Metal Catalyst Surfaces. Journal of Physical Chemistry C, 2021, 125, 17742-17748.	3.1	10
92	Unraveling Unique Surface Chemistry of Transition Metal Nitrides in Controlling Selective Câ€“O Bond Scission Pathways of Glycerol. Jacs Au, 2022, 2, 367-379.	7.9	10
93	Tight-Binding Configuration Interaction (TBCI): A Noniterative Approach to Incorporating Electrostatics into Tight Binding. Journal of Chemical Theory and Computation, 2008, 4, 804-818.	5.3	9
94	Investigation of the reaction mechanism of the hydrodeoxygenation of propionic acid over a Rh(1 1 1) surface: A first principles study. Journal of Catalysis, 2020, 391, 98-110.	6.2	8
95	Preferential Oxidation of CO in Hydrogen at Nonmetal Active Sites with High Activity and Selectivity. ACS Catalysis, 2020, 10, 5362-5370.	11.2	8
96	Probing surface-adsorbate interactions through active particle dynamics. Journal of Colloid and Interface Science, 2022, 614, 425-435.	9.4	7
97	Selective activation of methane C H bond in the presence of methanol. Journal of Catalysis, 2020, 386, 12-18.	6.2	6
98	An ab initio study of the oxygen defect formation and oxide ion migration in (Sr1-xPrx)2FeO4Â±Î´. Journal of Power Sources, 2021, 515, 230602.	7.8	5
99	Surface structure sensitivity of hydrodeoxygenation of biomass-derived organic acids over palladium catalysts: a microkinetic modeling approach. Catalysis Science and Technology, 2021, 11, 6163-6181.	4.1	4
100	Dilute Limit Alloy Pdâ€“Cu Bimetallic Catalysts Prepared by Simultaneous Strong Electrostatic Adsorption: A Combined Infrared Spectroscopic and Density Functional Theory Investigation. Journal of Physical Chemistry C, 2022, 126, 11111-11128.	3.1	4
101	Computational Investigation of the Catalytic Hydrodeoxygenation of Propanoic Acid over a Cu(111) Surface. Journal of Physical Chemistry C, 2021, 125, 19276-19293.	3.1	3
102	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations. Catalysis Science and Technology, 2021, 11, 3539-3555.	4.1	3
103	Aqueous-phase effects on ethanol decomposition over Ru-based catalysts. Catalysis Science and Technology, 2021, 11, 6695-6707.	4.1	2
104	Kinetic and Mechanistic Analysis of the Hydrodeoxygenation of Propanoic Acid on Pt/SiO₂. Industrial & Engineering Chemistry Research, 2021, 60, 16171-16187.	3.7	2
105	Understanding Selective Hydrodeoxygenation of 1,2- and 1,3-Propanediols on Cu/Mo₂C via Multiscale Modeling. ACS Catalysis, 2022, 12, 4581-4596.	11.2	2
106	Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5.. ChemInform, 2005, 36, no.	0.0	0