Mark Saeys

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4036365/publications.pdf

Version: 2024-02-01

77 papers	3,725 citations	109321 35 h-index	133252 59 g-index
81 all docs	81 docs citations	81 times ranked	4699 citing authors

#	Article	IF	Citations
1	Highly efficient, NiAu-catalyzed hydrogenolysis of lignin into phenolic chemicals. Green Chemistry, 2014, 16, 2432-2437.	9.0	239
2	The Chemical Route to a Carbon Dioxide Neutral World. ChemSusChem, 2017, 10, 1039-1055.	6.8	174
3	Ab Initio Calculations for Hydrocarbons:Â Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. Journal of Physical Chemistry A, 2003, 107, 9147-9159.	2.5	170
4	Density Functional Study of Benzene Adsorption on Pt(111). Journal of Physical Chemistry B, 2002, 106, 7489-7498.	2.6	166
5	Density Functional Theory Study of the CO Insertion Mechanism for Fischerâ˜Tropsch Synthesis over Co Catalysts. Journal of Physical Chemistry C, 2009, 113, 8357-8365.	3.1	153
6	Effect of boron on the stability of Ni catalysts during steam methane reforming. Journal of Catalysis, 2009, 261, 158-165.	6.2	143
7	Group Additive Values for the Gas Phase Standard Enthalpy of Formation of Hydrocarbons and Hydrocarbon Radicals. Journal of Physical Chemistry A, 2005, 109, 7466-7480.	2.5	127
8	Improving the coking resistance of Ni-based catalysts by promotion with subsurface boron. Journal of Catalysis, 2006, 242, 217-226.	6.2	112
9	Carbon deposition on Co catalysts during Fischerâ€“Tropsch synthesis: A computational and experimental study. Journal of Catalysis, 2010, 274, 121-129.	6.2	99
10	Effect of the CO coverage on the Fischerâ€“Tropsch synthesis mechanism on cobalt catalysts. Journal of Catalysis, 2013, 297, 217-226.	6.2	97
11	Computational and experimental study of the Volcano behavior of the oxygen reduction activity of PdM@PdPt/C (M = Pt, Ni, Co, Fe, and Cr) coreâ€“shell electrocatalysts. Journal of Catalysis, 2012, 291, 26-35.	6.2	93
12	Key Role of Surface Hydroxyl Groups in Câ€“O Activation during Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2016, 6, 3660-3664.	11.2	92
13	Ab initio group contribution method for activation energies for radical additions. AICHE Journal, 2004, 50, 426-444.	3.6	88
14	Ab Initio Reaction Path Analysis of Benzene Hydrogenation to Cyclohexane on Pt(111)â€. Journal of Physical Chemistry B, 2005, 109, 2064-2073.	2.6	86
15	Energy penalty estimates for CO2 capture: Comparison between fuel types and capture-combustion modes. Energy, 2016, 103, 709-714.	8.8	74
16	Density Functional Theory Analysis of Benzene (De)hydrogenation on Pt(111):Â Addition and Removal of the First Two H-Atoms. Journal of Physical Chemistry B, 2003, 107, 3844-3855.	2.6	71
17	Controlling the CO oxidation rate over Pt/TiO2 catalysts by defect engineering of the TiO2 support. Journal of Catalysis, 2014, 311, 306-313.	6.2	71
18	Origin of Extraordinary Stability of Squareâ€Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. Angewandte Chemie - International Edition, 2015, 54, 5312-5316.	13.8	67

#	Article	IF	Citations
19	Ab Initio Group Contribution Method for Activation Energies of Hydrogen Abstraction Reactions. ChemPhysChem, 2006, 7, 188-199.	2.1	66
20	Minimizing CO₂ emissions with renewable energy: a comparative study of emerging technologies in the steel industry. Energy and Environmental Science, 2020, 13, 1923-1932.	30.8	66
21	Effect of boron promotion on the stability of cobalt Fischerâ€“Tropsch catalysts. Journal of Catalysis, 2011, 280, 50-59.	6.2	65
22	A Triphenylamineâ€Based Conjugated Polymer with Donorâ€Ïâ€Acceptor Architecture as Organic Sensitizer for Dyeâ€Sensitized Solar Cells. Macromolecular Rapid Communications, 2009, 30, 1533-1537.	3.9	60
23	Flexible MgO Barrier Magnetic Tunnel Junctions. Advanced Materials, 2016, 28, 4983-4990.	21.0	59
24	Etherification of Functionalized Phenols with Chloroheteroarenes at Low Palladium Loading: Theoretical Assessment of the Role of Triphosphane Ligands in Cï£¿O Reductive Elimination. Advanced Synthesis and Catalysis, 2011, 353, 3403-3414.	4.3	51
25	CO Adsorption Site Preference on Platinum: Charge Is the Essence. ACS Catalysis, 2018, 8, 3770-3774.	11.2	51
26	Evaluating the Structure of Catalysts Using Core-Level Binding Energies Calculated from First Principles. Journal of Physical Chemistry C, 2013, 117, 1684-1691.	3.1	45
27	CO adsorption on cobalt: Prediction of stable surface phases. Surface Science, 2015, 642, L6-L10.	1.9	44
28	Solid micellar Ru single-atom catalysts for the water-free hydrogenation of CO2 to formic acid. Applied Catalysis B: Environmental, 2021, 290, 120036.	20.2	43
29	Calculation of the conductance of a finite atomic line of sulfur vacancies created on a molybdenum disulfide surface. Physical Review B, 2008, 77, .	3.2	42
30	Ethylene Hydrogenation over Pt/TiO₂: A Charge-Sensitive Reaction. ACS Catalysis, 2017, 7, 1966-1970.	11.2	40
31	First Principles Study of the Effect of Carbon and Boron on the Activity of a Ni Catalyst. Journal of Physical Chemistry C, 2009, 113, 4099-4106.	3.1	39
32	Effect of Boron Promotion on Coke Formation during Propane Dehydrogenation over Pt/Î³-Al₂O₃ Catalysts. ACS Catalysis, 2020, 10, 5208-5216.	11.2	39
33	Adsorption of cyclohexadiene, cyclohexene and cyclohexane on Pt(111). Surface Science, 2006, 600, 3121-3134.	1.9	38
34	Thioetherification of Chloroheteroarenes: A Binuclear Catalyst Promotes Wide Scope and High Functionalâ€Group Tolerance. Chemistry - A European Journal, 2014, 20, 12584-12594.	3.3	38
35	CO Adsorption on Pt(111): From Isolated Molecules to Ordered High-Coverage Structures. ACS Catalysis, 2018, 8, 10225-10233.	11.2	38
36	First Principles Study of the Stability and the Formation Kinetics of Subsurface and Bulk Carbon on a Ni Catalyst. Journal of Physical Chemistry C, 2008, 112, 9679-9685.	3.1	37

#	Article	IF	Citations
37	Improving the Stability of Cobalt Fischerâ˜Tropsch Catalysts by Boron Promotion. Industrial & Engineering Chemistry Research, 2010, 49, 11098-11100.	3.7	36
38	Strain-enhanced tunneling magnetoresistance in MgO magnetic tunnel junctions. Scientific Reports, 2014, 4, 6505.	3.3	36
39	Role of Surface Hydroxyl Species in Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2018, 8, 7539-7548.	11.2	35
40	Single-Molecule Rotational Switch on a Dangling Bond Dimer Bearing. ACS Nano, 2016, 10, 8499-8507.	14.6	33
41	Surface reconstruction of MoS2 to Mo2S3. Surface Science, 2008, 602, 2628-2633.	1.9	32
42	Shape and Size of Cobalt Nanoislands Formed Spontaneously on Cobalt Terraces during Fischerâ€“Tropsch Synthesis. Journal of Physical Chemistry Letters, 2016, 7, 1996-2001.	4.6	32
43	Origin of the Formation of Nanoislands on Cobalt Catalysts during Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2015, 5, 4756-4760.	11.2	30
44	The combination of deconvolution and density functional theory for the mid-infrared vibrational spectra of stable and unstable rhodium carbonyl clusters. Vibrational Spectroscopy, 2006, 41, 101-111.	2.2	28
45	Negative Tunneling Magnetoresistance by Canted Magnetization in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>MgO</mml:mi><mml:mo>/</mml:mo><mml:mi>NiO</mml:mi></mml:math>Tunnel Barriers. Physical Review Letters, 2011, 106, 167201.	7.8	28
46	Contacting a Conjugated Molecule with a Surface Dangling Bond Dimer on a Hydrogenated Ge(001) Surface Allows Imaging of the Hidden Ground Electronic State. ACS Nano, 2013, 7, 10105-10111.	14.6	28
47	Density functional study of the adsorption of 1,4-cyclohexadiene on Pt(111): origin of the Câ€“H stretch red shift. Surface Science, 2002, 513, 315-327.	1.9	27
48	First principles study of the coking resistance and the activity of a boron promoted Ni catalyst. Chemical Engineering Science, 2007, 62, 5039-5041.	3.8	27
49	Conductance decay of a surface hydrogen tunneling junction fabricated along a Si(001)-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mo>Â—</mml:mo><mml:mn atomic wire. Physical Review B, 2010, 81, .	3.2	27
50	CO Activation on Realistic Cobalt Surfaces: Kinetic Role of Hydrogen. ACS Catalysis, 2017, 7, 5289-5293.	11.2	26
51	Shape of Cobalt and Platinum Nanoparticles Under a CO Atmosphere: A Combined In Situ TEM and Computational Catalysis Study. ACS Catalysis, 2019, 9, 7449-7456.	11.2	21
52	first principles Study of the Reaction of Formic and Acetic Acids with Hydroxyl Radicals. Journal of Physical Chemistry A, 2008, 112, 6918-6928.	2.5	20
53	Construction of an ab initio kinetic model for industrial ethane pyrolysis. AICHE Journal, 2011, 57, 2458-2471.	3.6	19
54	Biaxial strain effect of spin dependent tunneling in MgO magnetic tunnel junctions. Applied Physics Letters, 2012, 101, 042407.	3.3	18

#	Article	IF	Citations
55	Electronic characterization of a single dangling bond on n- and p-type Si(001)-(2 Ã— 1):H. Surface Science, 2016, 645, 88-92.	1.9	17
56	Role of Ketoâ€“Enol Tautomerization in the Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 3831-3839.	11.2	17
57	Autocatalytic Role of Molecular Hydrogen in Copper-Catalyzed Transfer Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 8073-8082.	11.2	16
58	Kinetic models for catalytic reactions from first principles: benzene hydrogenation. Molecular Physics, 2004, 102, 267-272.	1.7	15
59	Ab Initio Reaction Path Analysis for the Initial Hydrogen Abstraction from Organic Acids by Hydroxyl Radicals. Journal of Physical Chemistry A, 2009, 113, 7852-7860.	2.5	15
60	Interaction of a conjugated polyaromatic molecule with a single dangling bond quantum dot on a hydrogenated semiconductor. Physical Chemistry Chemical Physics, 2016, 18, 3854-3861.	2.8	14
61	Operando computational catalysis: shape, structure, and coverage under reaction conditions. Current Opinion in Chemical Engineering, 2019, 23, 85-91.	7.8	14
62	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. Journal of Physical Chemistry C, 2016, 120, 21685-21690.	3.1	12
63	Ru(III) single site solid micellar catalyst for selective aqueous phase hydrogenation of carbonyl groups in biomass-derived compounds. Applied Catalysis B: Environmental, 2022, 300, 120730.	20.2	12
64	Aryl Fluoride Reductive Elimination from PdII Complexes: a Descriptor to Guide Ligand Selection. ChemCatChem, 2011, 3, 1060-1064.	3.7	11
65	Carbon monoxide production using a steel mill gas in a combined chemical looping process. Journal of Energy Chemistry, 2022, 68, 811-825.	12.9	11
66	Reshaping the Role of CO₂ in Propane Dehydrogenation: From Waste Gas to Platform Chemical. ACS Catalysis, 2022, 12, 9339-9358.	11.2	11
67	Carbon nanotube formation during propane decomposition on boron-modified Co/Al 2 O 3 catalysts: A kinetic study. International Journal of Hydrogen Energy, 2014, 39, 18016-18026.	7.1	10
68	Origin of the contrast inversion in the STM image of CO on Cu(1 1 1). Surface Science, 2009, 603, 3286-3291.	1.9	9
69	Bismuth mobile promoter and cobalt-bismuth nanoparticles in carbon nanotube supported Fischer-Tropsch catalysts with enhanced stability. Journal of Catalysis, 2021, 401, 102-114.	6.2	9
70	Dielsâ€“Alder attachment of a planar organic molecule to a dangling bond dimer on a hydrogenated semiconductor surface. Physical Chemistry Chemical Physics, 2016, 18, 16757-16765.	2.8	7
71	Decarbonisation of steel mill gases in an energy-neutral chemical looping process. Energy Conversion and Management, 2022, 254, 115248.	9.2	6
72	Dynamic pressure-swing chemical looping process for the recovery of CO from blast furnace gas. Energy Conversion and Management, 2022, 258, 115515.	9.2	6

#	Article	IF	Citations
73	Design of an Oxygen Reduction Catalyst for Direct Methanol Fuel Cells. Industrial & Engineering Chemistry Research, 2010, 49, 10251-10253.	3.7	5
74	Selective silylation boosts propylene epoxidation with H2 and O2 over Au/TS-1. Chem Catalysis, 2021, 1, 761-762.	6.1	5
75	Development of an Active and Mechanically Stable Catalyst for the Oxidative Coupling of Methane in a Gasâ€“Solid Vortex Reactor. Industrial & Engineering Chemistry Research, 2022, 61, 7748-7759.	3.7	5
76	Preferential Oxidation of H₂ in CO-Rich Streams over a Ni/Î³-Al₂O₃ Catalyst: An Experimental and First-Principles Microkinetic Study. ACS Catalysis, 0, , 9011-9022.	11.2	3
77	Frontispiece: Origin of Extraordinary Stability of Squareâ€Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. Angewandte Chemie - International Edition, 2015, 54, .	13.8	1