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	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
2	Decarbonisation of steel mill gases in an energy-neutral chemical looping process. Energy Conversion and Management, 2022, 254, 115248.	9.2	6
3	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
4	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
5	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
6	Reshaping the Role of CO₂ in Propane Dehydrogenation: From Waste Gas to Platform Chemical. ACS Catalysis, 2022, 12, 9339-9358.	11.2	11
7	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
8	Selective silylation boosts propylene epoxidation with H2 and O2 over Au/TS-1. Chem Catalysis, 2021, 1, 761-762.	6.1	5
9	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
10	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
11	Effect of Boron Promotion on Coke Formation during Propane Dehydrogenation over Pt/Î³-Al₂O₃ Catalysts. ACS Catalysis, 2020, 10, 5208-5216.	11.2	39
12	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
13	Autocatalytic Role of Molecular Hydrogen in Copper-Catalyzed Transfer Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 8073-8082.	11.2	16
14	Operando computational catalysis: shape, structure, and coverage under reaction conditions. Current Opinion in Chemical Engineering, 2019, 23, 85-91.	7.8	14
15	Role of Ketoâ€“Enol Tautomerization in the Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 3831-3839.	11.2	17
16	CO Adsorption Site Preference on Platinum: Charge Is the Essence. ACS Catalysis, 2018, 8, 3770-3774.	11.2	51
17	CO Adsorption on Pt(111): From Isolated Molecules to Ordered High-Coverage Structures. ACS Catalysis, 2018, 8, 10225-10233.	11.2	38
18	Role of Surface Hydroxyl Species in Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2018, 8, 7539-7548.	11.2	35

#	Article	IF	Citations
19	Ethylene Hydrogenation over Pt/TiO₂: A Charge-Sensitive Reaction. ACS Catalysis, 2017, 7, 1966-1970.	11.2	40
20	The Chemical Route to a Carbon Dioxide Neutral World. ChemSusChem, 2017, 10, 1039-1055.	6.8	174
21	CO Activation on Realistic Cobalt Surfaces: Kinetic Role of Hydrogen. ACS Catalysis, 2017, 7, 5289-5293.	11.2	26
22	Flexible MgO Barrier Magnetic Tunnel Junctions. Advanced Materials, 2016, 28, 4983-4990.	21.0	59
23	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
24	Energy penalty estimates for CO2 capture: Comparison between fuel types and capture-combustion modes. Energy, 2016, 103, 709-714.	8.8	74
25	Key Role of Surface Hydroxyl Groups in Câ€“O Activation during Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2016, 6, 3660-3664.	11.2	92
26	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. Journal of Physical Chemistry C, 2016, 120, 21685-21690.	3.1	12
27	Single-Molecule Rotational Switch on a Dangling Bond Dimer Bearing. ACS Nano, 2016, 10, 8499-8507.	14.6	33
28	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
29	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
30	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
31	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
32	Origin of the Formation of Nanoislands on Cobalt Catalysts during Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2015, 5, 4756-4760.	11.2	30
33	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
34	CO adsorption on cobalt: Prediction of stable surface phases. Surface Science, 2015, 642, L6-L10.	1.9	44
35	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
36	Highly efficient, NiAu-catalyzed hydrogenolysis of lignin into phenolic chemicals. Green Chemistry, 2014, 16, 2432-2437.	9.0	239

#	Article	IF	Citations
37	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
38	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
39	Strain-enhanced tunneling magnetoresistance in MgO magnetic tunnel junctions. Scientific Reports, 2014, 4, 6505.	3.3	36
40	Effect of the CO coverage on the Fischerâ€“Tropsch synthesis mechanism on cobalt catalysts. Journal of Catalysis, 2013, 297, 217-226.	6.2	97
41	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
42	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
43	Biaxial strain effect of spin dependent tunneling in MgO magnetic tunnel junctions. Applied Physics Letters, 2012, 101, 042407.	3.3	18
44	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
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	Effect of boron promotion on the stability of cobalt Fischerâ€“Tropsch catalysts. Journal of Catalysis, 2011, 280, 50-59.	6.2	65
47	Aryl Fluoride Reductive Elimination from PdII Complexes: a Descriptor to Guide Ligand Selection. ChemCatChem, 2011, 3, 1060-1064.	3.7	11
48	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
49	Construction of an ab initio kinetic model for industrial ethane pyrolysis. AIChE Journal, 2011, 57, 2458-2471.	3.6	19
50	Carbon deposition on Co catalysts during Fischerâ€“Tropsch synthesis: A computational and experimental study. Journal of Catalysis, 2010, 274, 121-129.	6.2	99
51	Improving the Stability of Cobalt Fischerâ^'Tropsch Catalysts by Boron Promotion. Industrial & Engineering Chemistry Research, 2010, 49, 11098-11100.	3.7	36
52	Design of an Oxygen Reduction Catalyst for Direct Methanol Fuel Cells. Industrial & Engineering Chemistry Research, 2010, 49, 10251-10253.	3.7	5
53	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>1</mml:mn></mml:mrow><mml:mo>)</mml:mo></mml:mrow><mml:mo>-</mml:mo><mml:mi>H</mml:mi></mml:mrow></mml:math> atomic wire. Physical Review B, 2010, 81, .	3.2	27
54	Effect of boron on the stability of Ni catalysts during steam methane reforming. Journal of Catalysis, 2009, 261, 158-165.	6.2	143

#	Article	IF	Citations
55	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
56	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
57	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
58	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
59	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
60	Surface reconstruction of MoS2 to Mo2S3. Surface Science, 2008, 602, 2628-2633.	1.9	32
61	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
62	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
63	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
64	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
65	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
66	Adsorption of cyclohexadiene, cyclohexene and cyclohexane on Pt(111). Surface Science, 2006, 600, 3121-3134.	1.9	38
67	Improving the coking resistance of Ni-based catalysts by promotion with subsurface boron. Journal of Catalysis, 2006, 242, 217-226.	6.2	112
68	Ab Initio Group Contribution Method for Activation Energies of Hydrogen Abstraction Reactions. ChemPhysChem, 2006, 7, 188-199.	2.1	66
69	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
70	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
71	Ab initio group contribution method for activation energies for radical additions. AIChE Journal, 2004, 50, 426-444.	3.6	88
72	Kinetic models for catalytic reactions from first principles: benzene hydrogenation. Molecular Physics, 2004, 102, 267-272.	1.7	15

#	Article	IF	Citations
73	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
74	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
75	Density Functional Study of Benzene Adsorption on Pt(111). Journal of Physical Chemistry B, 2002, 106, 7489-7498.	2.6	166
76	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
77	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