Lars C Grabow

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6112287/publications.pdf

Version: 2024-02-01

86	6,998	87843 38	58549 82
papers	citations	h-index	g-index

96	96	96	9098
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanism of Methanol Synthesis on Cu through CO₂and CO Hydrogenation. ACS Catalysis, 2011, 1, 365-384.	5.5	990
2	The critical role of water at the gold-titania interface in catalytic CO oxidation. Science, 2014, 345, 1599-1602.	6.0	493
3	Mechanism of the Water Gas Shift Reaction on Pt:â€‰ First Principles, Experiments, and Microkinetic Modeling. Journal of Physical Chemistry C, 2008, 112, 4608-4617.	1.5	452
4	Interlayer-Expanded Molybdenum Disulfide Nanocomposites for Electrochemical Magnesium Storage. Nano Letters, 2015, 15, 2194-2202.	4.5	357
5	Universal BrÃ¸nsted-Evans-Polanyi Relations for Câ€“C, Câ€“O, Câ€“N, Nâ€“O, Nâ€“N, and Oâ€“O Dissociation Reactions. Catalysis Letters, 2011, 141, 370-373.	1.4	265
6	Water-Mediated Proton Hopping on an Iron Oxide Surface. Science, 2012, 336, 889-893.	6.0	242
7	Why Au and Cu Are More Selective Than Pt for Preferential Oxidation of CO at Low Temperature. Catalysis Letters, 2004, 93, 93-100.	1.4	238
8	Experimental and Theoretical Insights into the Hydrogen-Efficient Direct Hydrodeoxygenation Mechanism of Phenol over Ru/TiO₂. ACS Catalysis, 2015, 5, 6509-6523.	5.5	219
9	Trends in low-temperature water?gas shift reactivity on transition metals. Journal of Catalysis, 2005, 229, 265-275.	3.1	213
10	Understanding Trends in Catalytic Activity: The Effect of Adsorbateâ€“Adsorbate Interactions for CO Oxidation Over Transition Metals. Topics in Catalysis, 2010, 53, 298-310.	1.3	204
11	Insights into Nitrate Reduction over Indium-Decorated Palladium Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 503-515.	5.5	188
12	Vertically Aligned MoS₂/Mo₂C hybrid Nanosheets Grown on Carbon Paper for Efficient Electrocatalytic Hydrogen Evolution. ACS Catalysis, 2017, 7, 7312-7318.	5.5	181
13	Coverage-Induced Conformational Effects on Activity and Selectivity: Hydrogenation and Decarbonylation of Furfural on Pd(111). ACS Catalysis, 2015, 5, 104-112.	5.5	172
14	Nature of Cu Active Centers in Cu-SSZ-13 and Their Responses to SO₂ Exposure. ACS Catalysis, 2018, 8, 1325-1337.	5.5	172
15	Epitaxial Growth of ZSM-5@Silicalite-1: A Coreâ€“Shell Zeolite Designed with Passivated Surface Acidity. ACS Nano, 2015, 9, 4006-4016.	7.3	134
16	Effects of Catalyst Phase on the Hydrogen Evolution Reaction of Water Splitting: Preparation of Phase-Pure Films of FeP, Fe₂P, and Fe₃P and Their Relative Catalytic Activities. Chemistry of Materials, 2018, 30, 3588-3598.	3.2	123
17	Bifunctional metal phosphide FeMnP films from single source metal organic chemical vapor deposition for efficient overall water splitting. Nano Energy, 2017, 39, 444-453.	8.2	117
18	H₂ Oxidation over Supported Au Nanoparticle Catalysts: Evidence for Heterolytic H₂ Activation at the Metalâ€“Support Interface. Journal of the American Chemical Society, 2018, 140, 16469-16487.	6.6	113

#	Article	IF	Citations
19	Density functional theory study of Li, Na, and Mg intercalation and diffusion in MoS₂with controlled interlayer spacing. Materials Research Express, 2016, 3, 064001.	0.8	100
20	Lattice strain effects on CO oxidation on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 3369.	1.3	96
21	Synergistic Effects in Bimetallic Palladiumâ€“Copper Catalysts Improve Selectivity in Oxygenate Coupling Reactions. Journal of the American Chemical Society, 2016, 138, 6805-6812.	6.6	94
22	Computational Assessment of the Dominant Factors Governing the Mechanism of Methanol Dehydration over H-ZSM-5 with Heterogeneous Aluminum Distribution. ACS Catalysis, 2016, 6, 2287-2298.	5.5	92
23	Descriptorâ€Based Analysis Applied to HCN Synthesis from NH₃ and CH₄. Angewandte Chemie - International Edition, 2011, 50, 4601-4605.	7.2	80
24	A DFT study of furan hydrogenation and ring opening on Pd(111). Green Chemistry, 2014, 16, 736-747.	4.6	80
25	Periodic, vdW-corrected density functional theory investigation of the effect of Al siting in H-ZSM-5 on chemisorption properties and site-specific acidity. Catalysis Communications, 2014, 52, 98-102.	1.6	77
26	Condition-Dependent Pd Speciation and NO Adsorption in Pd/Zeolites. ACS Catalysis, 2020, 10, 12801-12818.	5.5	74
27	Finite-Size Effects in O and CO Adsorption for the Late Transition Metals. Topics in Catalysis, 2012, 55, 1276-1282.	1.3	68
28	Niâ€“Feâ€“S Cubanes in CO₂ Reduction Electrocatalysis: A DFT Study. ACS Catalysis, 2013, 3, 2640-2643.	5.5	68
29	BrÃ¸nstedâ€“Evansâ€“Polanyi and Transition State Scaling Relations of Furan Derivatives on Pd(111) and Their Relation to Those of Small Molecules. ACS Catalysis, 2014, 4, 604-612.	5.5	68
30	In silicosearch for novel methane steam reforming catalysts. New Journal of Physics, 2013, 15, 125021.	1.2	65
31	Stabilizing the Interface between Sodium Metal Anode and Sulfide-Based Solid-State Electrolyte with an Electron-Blocking Interlayer. ACS Applied Materials & Interfaces, 2019, 11, 9672-9678.	4.0	61
32	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. Surface Science, 2010, 604, 11-20.	0.8	58
33	Tip-Dependent Scanning Tunneling Microscopy Imaging of Ultrathin FeO Films on Pt(111). Journal of Physical Chemistry C, 2011, 115, 2089-2099.	1.5	55
34	Correlating STM contrast and atomic-scale structure by chemical modification: Vacancy dislocation loops on FeO/Pt(111). Surface Science, 2009, 603, L15-L18.	0.8	53
35	Structure of Stoichiometric and Oxygen-Rich Ultrathin FeO(111) Films Grown on Pd(111). Journal of Physical Chemistry C, 2013, 117, 15155-15163.	1.5	52
36	Interaction of carbon dioxide with Cu overlayers on Pt(111). Surface Science, 2008, 602, 702-711.	0.8	44

#	Article	IF	Citations
37	Passive NOx adsorption on Pd/H-ZSM-5: Experiments and modeling. Applied Catalysis B: Environmental, 2020, 269, 118802.	10.8	43
38	Experimental and Firstâ€Principles Evidence for Interfacial Activity of Ru/TiO₂ for the Direct Conversion of mâ€Cresol to Toluene. ChemCatChem, 2017, 9, 2642-2651.	1.8	42
39	Ethylene Dehydroaromatization over Gaâ€ZSMâ€5 Catalysts: Nature and Role of Gallium Speciation. Angewandte Chemie - International Edition, 2020, 59, 19592-19601.	7.2	38
40	Water Poisons H₂ Activation at the Auâ€“TiO₂ Interface by Slowing Proton and Electron Transfer between Au and Titania. Journal of the American Chemical Society, 2020, 142, 5760-5772.	6.6	36
41	Nanocatalysis Beyond the Goldâ€Rush Era. Angewandte Chemie - International Edition, 2008, 47, 7390-7392.	7.2	34
42	Trends in Hydrodesulfurization Catalysis Based on Realistic Surface Models. Catalysis Letters, 2014, 144, 1425-1432.	1.4	32
43	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. Chemistry - A European Journal, 2016, 22, 16078-16088.	1.7	31
44	Silverâ€Promoted Dehydroaromatization of Ethylene over ZSMâ€5 Catalysts. ChemCatChem, 2017, 9, 1675-1682.	1.8	31
45	Frequencies and Thermal Stability of Isolated Surface Hydroxyls on Pyrogenic TiO₂ Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 24533-24548.	1.5	30
46	Effectiveness of in situ NH3 annealing treatments for the removal of oxygen from GaN surfaces. Surface Science, 2009, 603, 387-399.	0.8	29
47	NaBr Poisoning of Au/TiO₂ Catalysts: Effects on Kinetics, Poisoning Mechanism, and Estimation of the Number of Catalytic Active Sites. ACS Catalysis, 2012, 2, 684-694.	5.5	29
48	CO-Induced Embedding of Pt Adatoms in a Partially Reduced FeOxFilm on Pt(111). Journal of the American Chemical Society, 2011, 133, 10692-10695.	6.6	27
49	NOx adsorption with CO and C2H4 on Pd/SSZ-13: Experiments and modeling. Applied Catalysis B: Environmental, 2021, 286, 119871.	10.8	26
50	Practical Surface Treatments and Surface Chemistry of n-Type and p-Type GaN. Journal of Electronic Materials, 2008, 37, 439-447.	1.0	25
51	Extendable Machine Learning Model for the Stability of Single Atom Alloys. Topics in Catalysis, 2020, 63, 728-741.	1.3	25
52	Finite Size Effects in Submonolayer Catalysts Investigated by CO Electrosorption on Pt_{sML}/Pd(100). Journal of the American Chemical Society, 2017, 139, 13676-13679.	6.6	23
53	Selectivity tuning over monometallic and bimetallic dehydrogenation catalysts: effects of support and particle size. Catalysis Science and Technology, 2018, 8, 314-327.	2.1	23
54	Nature of Acid Sites in Silica-Supported Zirconium Oxide: A Combined Experimental and Periodic DFT Study. Journal of Physical Chemistry C, 2015, 119, 15150-15159.	1.5	22

#	Article	IF	Citations
55	Advanced solution methods for microkinetic models of catalytic reactions: A methanol synthesis case study. AICHE Journal, 2014, 60, 1336-1346.	1.8	19
56	Water-assisted oxygen activation during selective oxidation reactions. Current Opinion in Chemical Engineering, 2016, 13, 100-108.	3.8	19
57	Spatiotemporal Coke Coupling Enhances para-Xylene Selectivity in Highly Stable MCM-22 Catalysts. Journal of the American Chemical Society, 2022, 144, 7861-7870.	6.6	19
58	Kinetics of H₂ Adsorption at the Metalâ€“Support Interface of Au/TiO₂ Catalysts Probed by Broad Background IR Absorbance. Angewandte Chemie - International Edition, 2021, 60, 7735-7743.	7.2	16
59	Novel 2D RuPt core-edge nanocluster catalyst for CO electro-oxidation. Surface Science, 2015, 640, 50-58.	0.8	15
60	From Activeâ€Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation. ChemCatChem, 2017, 9, 1594-1600.	1.8	15
61	Strategy to improve catalytic trend predictions for methane oxidation and reforming. AICHE Journal, 2017, 63, 66-77.	1.8	15
62	Evaluating the benefits of kinetic Monte Carlo and microkinetic modeling for catalyst design studies in the presence of lateral interactions. Catalysis Today, 2022, 387, 150-158.	2.2	15
63	Activity Trends for Catalytic CO and NO Co-Oxidation at Low Temperature Diesel Emission Conditions. Industrial & Engineering Chemistry Research, 2018, 57, 12715-12725.	1.8	13
64	Magnetocapacitance effect and magnetoelectric coupling in type-II multiferroic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>HoFeWO</mml:mi><mml:mn>6</mml:mn></mml:msub> Physical Review B, 2021, 103, .	1.1	13
65	Computational Catalyst Screening. RSC Catalysis Series, 2013, , 1-58.	0.1	11
66	Titania surface chemistry and its influence on supported metal catalysts. Polyhedron, 2019, 170, 41-50.	1.0	11
67	Accelerated Modeling of Lithium Diffusion in Solid State Electrolytes using Artificial Neural Networks. Advanced Theory and Simulations, 2020, 3, 2000097.	1.3	11
68	Mechanistic Insights into Ethylene Transformations on Ir(111) by Density Functional Calculations and Microkinetic Modeling. ChemPhysChem, 2017, 18, 906-916.	1.0	10
69	Learning from the past: Are catalyst design principles transferrable between hydrodesulfurization and deoxygenation?. AICHE Journal, 2018, 64, 3121-3133.	1.8	9
70	Linking low and high temperature NO oxidation mechanisms over BrÃ¸nsted acidic chabazite to dynamic changes of the active site. Journal of Catalysis, 2020, 389, 195-206.	3.1	9
71	On the Limited Role of Electronic Support Effects in Selective Alkyne Hydrogenation: A Kinetic Study of Au/MO_x Catalysts Prepared from Oleylamineâ€Capped Colloidal Nanoparticles. ChemCatChem, 2019, 11, 1650-1664.	1.8	9
72	Molecular-scale structural distortion near vacancies in pentacene. Applied Physics Letters, 2008, 92, 153313.	1.5	7

#	Article	IF	Citations
73	Atomic Properties of Monoclinic Ag₂Se Thin Film Grown on SrTiO₃Substrate by Molecular Beam Epitaxy. Journal of Physical Chemistry Letters, 2021, 12, 4140-4147.	2.1	7
74	When Outliers Make All The Difference. ChemCatChem, 2012, 4, 1887-1888.	1.8	6
75	Kinetics of H₂ Adsorption at the Metalâ€“Support Interface of Au/TiO₂ Catalysts Probed by Broad Background IR Absorbance. Angewandte Chemie, 2021, 133, 7814-7822.	1.6	5
76	CH₄ steam reforming on Pt + Pd/Al₂O₃ monolith: impact of Mn_{0.5}Fe_{2.5}O₄ spinel addition. Catalysis Science and Technology, 2022, 12, 2618-2633.	2.1	4
77	Oxygenate Reactions over PdCu and PdAg Catalysts: Distinguishing Electronic and Geometric Effects on Reactivity and Selectivity. ACS Catalysis, 2022, 12, 5766-5775.	5.5	4
78	Experimental and First-Principles Evidence for Interfacial Activity of Ru/TiO2 for the Direct Conversion of m -Cresol to Toluene. ChemCatChem, 2017, 9, 2612-2612.	1.8	3
79	Quantification and Statistical Analysis of Errors Related to the Approximate Description of Active Site Models in Metalâ€Exchanged Zeolites. ChemCatChem, 2019, 11, 5055-5067.	1.8	3
80	The Synergy of Dilute Pd and Surface Oxygen Species for Methane Upgrading on Au₃Pd(111). Energy Technology, 2020, 8, 1900732.	1.8	3
81	Enhancing Technological Applications through Density Functional Theory Modeling of Nanomaterials. ACS Applied Nano Materials, 2020, 3, 6127-6130.	2.4	3
82	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. Chemistry - A European Journal, 2016, 22, 15961-15961.	1.7	2
83	Electroless Pb Monolayer Depositionâ€”Prelude for Further Advances in Catalyst Monolayer Synthesis via Surface Limited Redox Replacement Reaction. ACS Catalysis, 2021, 11, 4650-4659.	5.5	2
84	From Activeâ€Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation. ChemCatChem, 2017, 9, 1520-1520.	1.8	1
85	Catalytic Encounters at the Molecular Level: Gabor A. Somorjai Award Symposium for Creative Research in Catalysis in Honor of Professor Manos Mavrikakis. Topics in Catalysis, 2020, 63, 617-617.	1.3	0
86	Ethylene Dehydroaromatization over Gaâ€ZSMâ€5 Catalysts: Nature and Role of Gallium Speciation. Angewandte Chemie, 2020, 132, 19760-19769.	1.6	0