

# 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  
papers

6,998  
citations

87888

38  
h-index

58581

82  
g-index

96  
all docs

96  
docs citations

96  
times ranked

9098  
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of Methanol Synthesis on Cu through CO <sub>2</sub> and CO Hydrogenation. ACS Catalysis, 2011, 1, 365-384.	11.2	990
2	The critical role of water at the gold-titania interface in catalytic CO oxidation. Science, 2014, 345, 1599-1602.	12.6	493
3	Mechanism of the Water Gas Shift Reaction on Pt: First Principles, Experiments, and Microkinetic Modeling. Journal of Physical Chemistry C, 2008, 112, 4608-4617.	3.1	452
4	Interlayer-Expanded Molybdenum Disulfide Nanocomposites for Electrochemical Magnesium Storage. Nano Letters, 2015, 15, 2194-2202.	9.1	357
5	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.	2.6	265
6	Water-Mediated Proton Hopping on an Iron Oxide Surface. Science, 2012, 336, 889-893.	12.6	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.	2.6	238
8	Experimental and Theoretical Insights into the Hydrogen-Efficient Direct Hydrodeoxygenation Mechanism of Phenol over Ru/TiO <sub>2</sub> . ACS Catalysis, 2015, 5, 6509-6523.	11.2	219
9	Trends in low-temperature water-gas shift reactivity on transition metals. Journal of Catalysis, 2005, 229, 265-275.	6.2	213
10	Understanding Trends in Catalytic Activity: The Effect of Adsorbate-Adsorbate Interactions for CO Oxidation Over Transition Metals. Topics in Catalysis, 2010, 53, 298-310.	2.8	204
11	Insights into Nitrate Reduction over Indium-Decorated Palladium Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 503-515.	11.2	188
12	Vertically Aligned MoS <sub>2</sub> /Mo <sub>2</sub> C hybrid Nanosheets Grown on Carbon Paper for Efficient Electrocatalytic Hydrogen Evolution. ACS Catalysis, 2017, 7, 7312-7318.	11.2	181
13	Coverage-Induced Conformational Effects on Activity and Selectivity: Hydrogenation and Decarbonylation of Furfural on Pd(111). ACS Catalysis, 2015, 5, 104-112.	11.2	172
14	Nature of Cu Active Centers in Cu-SSZ-13 and Their Responses to SO <sub>2</sub> Exposure. ACS Catalysis, 2018, 8, 1325-1337.	11.2	172
15	Epitaxial Growth of ZSM-5@Silicalite-1: A Core-Shell Zeolite Designed with Passivated Surface Acidity. ACS Nano, 2015, 9, 4006-4016.	14.6	134
16	Effects of Catalyst Phase on the Hydrogen Evolution Reaction of Water Splitting: Preparation of Phase-Pure Films of FeP, Fe <sub>2</sub> P, and Fe <sub>3</sub> P and Their Relative Catalytic Activities. Chemistry of Materials, 2018, 30, 3588-3598.	6.7	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.	16.0	117
18	H <sub>2</sub> Oxidation over Supported Au Nanoparticle Catalysts: Evidence for Heterolytic H <sub>2</sub> Activation at the Metal-Support Interface. Journal of the American Chemical Society, 2018, 140, 16469-16487.	13.7	113

#	ARTICLE	IF	CITATIONS
19	Density functional theory study of Li, Na, and Mg intercalation and diffusion in MoS <sub>2</sub> with controlled interlayer spacing. <i>Materials Research Express</i> , 2016, 3, 064001.	1.6	100
20	Lattice strain effects on CO oxidation on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3369.	2.8	96
21	Synergistic Effects in Bimetallic Palladium-Copper Catalysts Improve Selectivity in Oxygenate Coupling Reactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 6805-6812.	13.7	94
22	Computational Assessment of the Dominant Factors Governing the Mechanism of Methanol Dehydration over H-ZSM-5 with Heterogeneous Aluminum Distribution. <i>ACS Catalysis</i> , 2016, 6, 2287-2298.	11.2	92
23	Descriptor-Based Analysis Applied to HCN Synthesis from NH <sub>3</sub> and CH <sub>4</sub> . <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4601-4605.	13.8	80
24	A DFT study of furan hydrogenation and ring opening on Pd(111). <i>Green Chemistry</i> , 2014, 16, 736-747.	9.0	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. <i>Catalysis Communications</i> , 2014, 52, 98-102.	3.3	77
26	Condition-Dependent Pd Speciation and NO Adsorption in Pd/Zeolites. <i>ACS Catalysis</i> , 2020, 10, 12801-12818.	11.2	74
27	Finite-Size Effects in O and CO Adsorption for the Late Transition Metals. <i>Topics in Catalysis</i> , 2012, 55, 1276-1282.	2.8	68
28	Ni-Fe-S Cubanes in CO <sub>2</sub> Reduction Electrocatalysis: A DFT Study. <i>ACS Catalysis</i> , 2013, 3, 2640-2643.	11.2	68
29	Brønsted-Evans-Polanyi and Transition State Scaling Relations of Furan Derivatives on Pd(111) and Their Relation to Those of Small Molecules. <i>ACS Catalysis</i> , 2014, 4, 604-612.	11.2	68
30	<i>In silico</i> search for novel methane steam reforming catalysts. <i>New Journal of Physics</i> , 2013, 15, 125021.	2.9	65
31	Stabilizing the Interface between Sodium Metal Anode and Sulfide-Based Solid-State Electrolyte with an Electron-Blocking Interlayer. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 9672-9678.	8.0	61
32	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. <i>Surface Science</i> , 2010, 604, 11-20.	1.9	58
33	Tip-Dependent Scanning Tunneling Microscopy Imaging of Ultrathin FeO Films on Pt(111). <i>Journal of Physical Chemistry C</i> , 2011, 115, 2089-2099.	3.1	55
34	Correlating STM contrast and atomic-scale structure by chemical modification: Vacancy dislocation loops on FeO/Pt(111). <i>Surface Science</i> , 2009, 603, L15-L18.	1.9	53
35	Structure of Stoichiometric and Oxygen-Rich Ultrathin FeO(111) Films Grown on Pd(111). <i>Journal of Physical Chemistry C</i> , 2013, 117, 15155-15163.	3.1	52
36	Interaction of carbon dioxide with Cu overlayers on Pt(111). <i>Surface Science</i> , 2008, 602, 702-711.	1.9	44

#	ARTICLE	IF	CITATIONS
37	Passive NO <sub>x</sub> adsorption on Pd/H-ZSM-5: Experiments and modeling. Applied Catalysis B: Environmental, 2020, 269, 118802.	20.2	43
38	Experimental and First-Principles Evidence for Interfacial Activity of Ru/TiO <sub>2</sub> for the Direct Conversion of m-Cresol to Toluene. ChemCatChem, 2017, 9, 2642-2651.	3.7	42
39	Ethylene Dehydroaromatization over Ga-ZSM-5 Catalysts: Nature and Role of Gallium Speciation. Angewandte Chemie - International Edition, 2020, 59, 19592-19601.	13.8	38
40	Water Poisons H <sub>2</sub> Activation at the Au-TiO <sub>2</sub> Interface by Slowing Proton and Electron Transfer between Au and Titania. Journal of the American Chemical Society, 2020, 142, 5760-5772.	13.7	36
41	Nanocatalysis Beyond the Gold-Rush Era. Angewandte Chemie - International Edition, 2008, 47, 7390-7392.	13.8	34
42	Trends in Hydrodesulfurization Catalysis Based on Realistic Surface Models. Catalysis Letters, 2014, 144, 1425-1432.	2.6	32
43	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. Chemistry - A European Journal, 2016, 22, 16078-16088.	3.3	31
44	Silver-Promoted Dehydroaromatization of Ethylene over ZSM-5 Catalysts. ChemCatChem, 2017, 9, 1675-1682.	3.7	31
45	Frequencies and Thermal Stability of Isolated Surface Hydroxyls on Pyrogenic TiO <sub>2</sub> Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 24533-24548.	3.1	30
46	Effectiveness of in situ NH <sub>3</sub> annealing treatments for the removal of oxygen from GaN surfaces. Surface Science, 2009, 603, 387-399.	1.9	29
47	NaBr Poisoning of Au/TiO <sub>2</sub> Catalysts: Effects on Kinetics, Poisoning Mechanism, and Estimation of the Number of Catalytic Active Sites. ACS Catalysis, 2012, 2, 684-694.	11.2	29
48	CO-Induced Embedding of Pt Adatoms in a Partially Reduced FeO <sub>x</sub> Film on Pt(111). Journal of the American Chemical Society, 2011, 133, 10692-10695.	13.7	27
49	NO <sub>x</sub> adsorption with CO and C <sub>2</sub> H <sub>4</sub> on Pd/SSZ-13: Experiments and modeling. Applied Catalysis B: Environmental, 2021, 286, 119871.	20.2	26
50	Practical Surface Treatments and Surface Chemistry of n-Type and p-Type GaN. Journal of Electronic Materials, 2008, 37, 439-447.	2.2	25
51	Extendable Machine Learning Model for the Stability of Single Atom Alloys. Topics in Catalysis, 2020, 63, 728-741.	2.8	25
52	Finite Size Effects in Submonolayer Catalysts Investigated by CO Electrosorption on Pt <sub>sML</sub> /Pd(100). Journal of the American Chemical Society, 2017, 139, 13676-13679.	13.7	23
53	Selectivity tuning over monometallic and bimetallic dehydrogenation catalysts: effects of support and particle size. Catalysis Science and Technology, 2018, 8, 314-327.	4.1	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.	3.1	22

#	ARTICLE	IF	CITATIONS
55	Advanced solution methods for microkinetic models of catalytic reactions: A methanol synthesis case study. <i>AIChE Journal</i> , 2014, 60, 1336-1346.	3.6	19
56	Water-assisted oxygen activation during selective oxidation reactions. <i>Current Opinion in Chemical Engineering</i> , 2016, 13, 100-108.	7.8	19
57	Spatiotemporal Coke Coupling Enhances <i>p</i> -Xylene Selectivity in Highly Stable MCM-22 Catalysts. <i>Journal of the American Chemical Society</i> , 2022, 144, 7861-7870.	13.7	19
58	Kinetics of H <sub>2</sub> Adsorption at the Metal-Support Interface of Au/TiO <sub>2</sub> Catalysts Probed by Broad Background IR Absorbance. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7735-7743.	13.8	16
59	Novel 2D RuPt core-edge nanocluster catalyst for CO electro-oxidation. <i>Surface Science</i> , 2015, 640, 50-58.	1.9	15
60	From Active-Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation. <i>ChemCatChem</i> , 2017, 9, 1594-1600.	3.7	15
61	Strategy to improve catalytic trend predictions for methane oxidation and reforming. <i>AIChE Journal</i> , 2017, 63, 66-77.	3.6	15
62	Evaluating the benefits of kinetic Monte Carlo and microkinetic modeling for catalyst design studies in the presence of lateral interactions. <i>Catalysis Today</i> , 2022, 387, 150-158.	4.4	15
63	Activity Trends for Catalytic CO and NO Co-Oxidation at Low Temperature Diesel Emission Conditions. <i>Industrial &amp; Engineering Chemistry Research</i> , 2018, 57, 12715-12725.	3.7	13
64	Magnetocapacitance effect and magnetoelectric coupling in type-II multiferroic $\text{HoFeWO}_6$ . <i>Physical Review B</i> , 2021, 103, .	3.2	13
65	Computational Catalyst Screening. <i>RSC Catalysis Series</i> , 2013, , 1-58.	0.1	11
66	Titania surface chemistry and its influence on supported metal catalysts. <i>Polyhedron</i> , 2019, 170, 41-50.	2.2	11
67	Accelerated Modeling of Lithium Diffusion in Solid State Electrolytes using Artificial Neural Networks. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000097.	2.8	11
68	Mechanistic Insights into Ethylene Transformations on Ir(111) by Density Functional Calculations and Microkinetic Modeling. <i>ChemPhysChem</i> , 2017, 18, 906-916.	2.1	10
69	Learning from the past: Are catalyst design principles transferrable between hydrodesulfurization and deoxygenation?. <i>AIChE Journal</i> , 2018, 64, 3121-3133.	3.6	9
70	Linking low and high temperature NO oxidation mechanisms over Brønsted acidic chabazite to dynamic changes of the active site. <i>Journal of Catalysis</i> , 2020, 389, 195-206.	6.2	9
71	On the Limited Role of Electronic Support Effects in Selective Alkyne Hydrogenation: A Kinetic Study of Au/MO <sub>x</sub> Catalysts Prepared from Oleylamine-Capped Colloidal Nanoparticles. <i>ChemCatChem</i> , 2019, 11, 1650-1664.	3.7	9
72	Molecular-scale structural distortion near vacancies in pentacene. <i>Applied Physics Letters</i> , 2008, 92, 153313.	3.3	7

#	ARTICLE	IF	CITATIONS
73	Atomic Properties of Monoclinic Ag <sub>2</sub> Se Thin Film Grown on SrTiO <sub>3</sub> Substrate by Molecular Beam Epitaxy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4140-4147.	4.6	7
74	When Outliers Make All The Difference. <i>ChemCatChem</i> , 2012, 4, 1887-1888.	3.7	6
75	Kinetics of H <sub>2</sub> Adsorption at the Metal-Support Interface of Au/TiO <sub>2</sub> Catalysts Probed by Broad Background IR Absorbance. <i>Angewandte Chemie</i> , 2021, 133, 7814-7822.	2.0	5
76	CH <sub>4</sub> steam reforming on Pt + Pd/Al <sub>2</sub> O <sub>3</sub> monolith: impact of Mn <sub>0.5</sub> Fe <sub>2.5</sub> O <sub>4</sub> spinel addition. <i>Catalysis Science and Technology</i> , 2022, 12, 2618-2633.	4.1	4
77	Oxygenate Reactions over PdCu and PdAg Catalysts: Distinguishing Electronic and Geometric Effects on Reactivity and Selectivity. <i>ACS Catalysis</i> , 2022, 12, 5766-5775.	11.2	4
78	Experimental and First-Principles Evidence for Interfacial Activity of Ru/TiO <sub>2</sub> for the Direct Conversion of m-Cresol to Toluene. <i>ChemCatChem</i> , 2017, 9, 2612-2612.	3.7	3
79	Quantification and Statistical Analysis of Errors Related to the Approximate Description of Active Site Models in Metal-Exchanged Zeolites. <i>ChemCatChem</i> , 2019, 11, 5055-5067.	3.7	3
80	The Synergy of Dilute Pd and Surface Oxygen Species for Methane Upgrading on Au <sub>3</sub> Pd(111). <i>Energy Technology</i> , 2020, 8, 1900732.	3.8	3
81	Enhancing Technological Applications through Density Functional Theory Modeling of Nanomaterials. <i>ACS Applied Nano Materials</i> , 2020, 3, 6127-6130.	5.0	3
82	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. <i>Chemistry - A European Journal</i> , 2016, 22, 15961-15961.	3.3	2
83	Electroless Pb Monolayer Deposition—Prelude for Further Advances in Catalyst Monolayer Synthesis via Surface Limited Redox Replacement Reaction. <i>ACS Catalysis</i> , 2021, 11, 4650-4659.	11.2	2
84	From Active Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation. <i>ChemCatChem</i> , 2017, 9, 1520-1520.	3.7	1
85	Catalytic Encounters at the Molecular Level: Gabor A. Somorjai Award Symposium for Creative Research in Catalysis in Honor of Professor Manos Mavrikakis. <i>Topics in Catalysis</i> , 2020, 63, 617-617.	2.8	0
86	Ethylene Dehydroaromatization over Ga-ZSM-5 Catalysts: Nature and Role of Gallium Speciation. <i>Angewandte Chemie</i> , 2020, 132, 19760-19769.	2.0	0