Lars C Grabow

List of Publications by Year
in descending order

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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	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
2	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
3	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
4	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
5	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
6	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
7	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	18
8	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
9	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
10	NOx adsorption with CO and C2H4 on Pd/SSZ-13: Experiments and modeling. Applied Catalysis B: Environmental, 2021, 286, 119871.	10.8	26
11	The Synergy of Dilute Pd and Surface Oxygen Species for Methane Upgrading on Au₃Pd(111). Energy Technology, 2020, 8, 1900732.	1.8	3
12	Condition-Dependent Pd Speciation and NO Adsorption in Pd/Zeolites. ACS Catalysis, 2020, 10, 12801-12818.	5.5	74
13	Accelerated Modeling of Lithium Diffusion in Solid State Electrolytes using Artificial Neural Networks. Advanced Theory and Simulations, 2020, 3, 2000097.	1.3	11
14	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
15	Ethylene Dehydroaromatization over Gaâ€ZSMâ€5 Catalysts: Nature and Role of Gallium Speciation. Angewandte Chemie - International Edition, 2020, 59, 19592-19601.	7.2	38
16	Ethylene Dehydroaromatization over Gaâ€ZSMâ€5 Catalysts: Nature and Role of Gallium Speciation. Angewandte Chemie, 2020, 132, 19760-19769.	1.6	0
17	Extendable Machine Learning Model for the Stability of Single Atom Alloys. Topics in Catalysis, 2020, 63, 728-741.	1.3	25
18	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

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19	Enhancing Technological Applications through Density Functional Theory Modeling of Nanomaterials. ACS Applied Nano Materials, 2020, 3, 6127-6130.	2.4	3
20	Passive NOx adsorption on Pd/H-ZSM-5: Experiments and modeling. Applied Catalysis B: Environmental, 2020, 269, 118802.	10.8	43
21	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
22	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
23	Frequencies and Thermal Stability of Isolated Surface Hydroxyls on Pyrogenic TiO₂ Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 24533-24548.	1.5	30
24	Titania surface chemistry and its influence on supported metal catalysts. Polyhedron, 2019, 170, 41-50.	1.0	11
25	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
26	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
27	Learning from the past: Are catalyst design principles transferrable between hydrodesulfurization and deoxygenation?. AIChE Journal, 2018, 64, 3121-3133.	1.8	9
28	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
29	Nature of Cu Active Centers in Cu-SSZ-13 and Their Responses to SO₂ Exposure. ACS Catalysis, 2018, 8, 1325-1337.	5.5	172
30	Insights into Nitrate Reduction over Indium-Decorated Palladium Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 503-515.	5.5	188
31	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
32	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
33	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
34	Silverâ€Promoted Dehydroaromatization of Ethylene over ZSMâ€5 Catalysts. ChemCatChem, 2017, 9, 1675-1682.	1.8	31
35	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
36	Mechanistic Insights into Ethylene Transformations on Ir(111) by Density Functional Calculations and Microkinetic Modeling. ChemPhysChem, 2017, 18, 906-916.	1.0	10

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37	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
38	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
39	Vertically Aligned MoS₂/Mo₂C hybrid Nanosheets Grown on Carbon Paper for Efficient Electrocatalytic Hydrogen Evolution. ACS Catalysis, 2017, 7, 7312-7318.	5.5	181
40	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
41	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
42	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
43	Strategy to improve catalytic trend predictions for methane oxidation and reforming. AICHE Journal, 2017, 63, 66-77.	1.8	15
44	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
45	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. Chemistry - A European Journal, 2016, 22, 16078-16088.	1.7	31
46	Water-assisted oxygen activation during selective oxidation reactions. Current Opinion in Chemical Engineering, 2016, 13, 100-108.	3.8	19
47	Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations. Chemistry - A European Journal, 2016, 22, 15961-15961.	1.7	2
48	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
49	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
50	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
51	Novel 2D RuPt core-edge nanocluster catalyst for CO electro-oxidation. Surface Science, 2015, 640, 50-58.	0.8	15
52	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
53	Interlayer-Expanded Molybdenum Disulfide Nanocomposites for Electrochemical Magnesium Storage. Nano Letters, 2015, 15, 2194-2202.	4.5	357
54	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

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55	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
56	Advanced solution methods for microkinetic models of catalytic reactions: A methanol synthesis case study. AICHE Journal, 2014, 60, 1336-1346.	1.8	19
57	A DFT study of furan hydrogenation and ring opening on Pd(111). Green Chemistry, 2014, 16, 736-747.	4.6	80
58	The critical role of water at the gold-titania interface in catalytic CO oxidation. Science, 2014, 345, 1599-1602.	6.0	493
59	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
60	Trends in Hydrodesulfurization Catalysis Based on Realistic Surface Models. Catalysis Letters, 2014, 144, 1425-1432.	1.4	32
61	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
62	Niâ€“Feâ€“S Cubanes in CO₂ Reduction Electrocatalysis: A DFT Study. ACS Catalysis, 2013, 3, 2640-2643.	5.5	68
63	Computational Catalyst Screening. RSC Catalysis Series, 2013, , 1-58.	0.1	11
64	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
65	In silicosearch for novel methane steam reforming catalysts. New Journal of Physics, 2013, 15, 125021.	1.2	65
66	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
67	When Outliers Make All The Difference. ChemCatChem, 2012, 4, 1887-1888.	1.8	6
68	Finite-Size Effects in O and CO Adsorption for the Late Transition Metals. Topics in Catalysis, 2012, 55, 1276-1282.	1.3	68
69	Water-Mediated Proton Hopping on an Iron Oxide Surface. Science, 2012, 336, 889-893.	6.0	242
70	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
71	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
72	Mechanism of Methanol Synthesis on Cu through CO₂and CO Hydrogenation. ACS Catalysis, 2011, 1, 365-384.	5.5	990

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73	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
74	Descriptorâ€Based Analysis Applied to HCN Synthesis from NH₃ and CH₄. Angewandte Chemie - International Edition, 2011, 50, 4601-4605.	7.2	80
75	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
76	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. Surface Science, 2010, 604, 11-20.	0.8	58
77	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
78	Effectiveness of in situ NH3 annealing treatments for the removal of oxygen from GaN surfaces. Surface Science, 2009, 603, 387-399.	0.8	29
79	Practical Surface Treatments and Surface Chemistry of n-Type and p-Type GaN. Journal of Electronic Materials, 2008, 37, 439-447.	1.0	25
80	Nanocatalysis Beyond the Goldâ€Rush Era. Angewandte Chemie - International Edition, 2008, 47, 7390-7392.	7.2	34
81	Interaction of carbon dioxide with Cu overlayers on Pt(111). Surface Science, 2008, 602, 702-711.	0.8	44
82	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
83	Molecular-scale structural distortion near vacancies in pentacene. Applied Physics Letters, 2008, 92, 153313.	1.5	7
84	Lattice strain effects on CO oxidation on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 3369.	1.3	96
85	Trends in low-temperature water?gas shift reactivity on transition metals. Journal of Catalysis, 2005, 229, 265-275.	3.1	213
86	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