Ivo A W Filot

List of Publications by Year
in descending order

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66 papers	3,887 citations	109137 35 h-index	123241 61 g-index
70 all docs	70 docs citations	70 times ranked	4917 citing authors

#	Article	IF	Citations
1	On the Potential of Gallium- and Indium-Based Liquid Metal Membranes for Hydrogen Separation. Membranes, 2022, 12, 75.	1.4	3
2	Lateral Interactions of Dynamic Adlayer Structures from Artificial Neural Networks. Journal of Physical Chemistry C, 2022, 126, 5529-5540.	1.5	5
3	Promoted Fischer-Tropsch catalysts. , 2021, , .		0
4	Improved Pd/CeO₂ Catalysts for Low-Temperature NO Reduction: Activation of CeO₂ Lattice Oxygen by Fe Doping. ACS Catalysis, 2021, 11, 5614-5627.	5.5	44
5	Consequences of Amide Connectivity in the Supramolecular Polymerization of Porphyrins: Spectroscopic Observations Rationalized by Theoretical Modelling. Chemistry - A European Journal, 2021, 27, 9700-9707.	1.7	16
6	Atomistic Insights Into the Degradation of Inorganic Halide Perovskite CsPbI₃: A Reactive Force Field Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2021, 12, 5519-5525.	2.1	31
7	Enumerating Active Sites on Metal Nanoparticles: Understanding the Size Dependence of Cobalt Particles for CO Dissociation. ACS Catalysis, 2021, 11, 8484-8492.	5.5	26
8	Niâ€"In Synergy in CO₂ Hydrogenation to Methanol. ACS Catalysis, 2021, 11, 11371-11384.	5.5	79
9	A quantum-chemical study of the CO dissociation mechanism on low-index Miller planes of Ï´-Fe3C. Catalysis Today, 2020, 342, 152-160.	2.2	15
10	First-principles based microkinetic modeling of transient kinetics of CO hydrogenation on cobalt catalysts. Catalysis Today, 2020, 342, 131-141.	2.2	29
11	A theoretical study of the reverse waterâ€gas shift reaction on Ni(111) and Ni(311) surfaces. Canadian Journal of Chemical Engineering, 2020, 98, 740-748.	0.9	25
12	First-principles microkinetics simulations of electrochemical reduction of CO2 over Cu catalysts. Electrochimica Acta, 2020, 335, 135665.	2.6	32
13	Stability of heterogeneous single-atom catalysts: a scaling law mapping thermodynamics to kinetics. Npj Computational Materials, 2020, 6, .	3.5	44
14	The Vital Role of Step-Edge Sites for Both CO Activation and Chain Growth on Cobalt Fischerâ€"Tropsch Catalysts Revealed through First-Principles-Based Microkinetic Modeling Including Lateral Interactions. ACS Catalysis, 2020, 10, 9376-9400.	5.5	37
15	Detailed chemomechanistic sensitivity study on the alkoxylation of fatty amines. International Journal of Chemical Kinetics, 2020, 52, 861-871.	1.0	1
16	Dynamics of gold clusters on ceria during CO oxidation. Journal of Catalysis, 2020, 392, 39-47.	3.1	20
17	Bioorthogonal Tetrazine Carbamate Cleavage by Highly Reactive trans-Cyclooctene. Journal of the American Chemical Society, 2020, 142, 10955-10963.	6.6	58
18	Design of Nonideal Eutectic Mixtures Based on Correlations with Molecular Properties. Journal of Physical Chemistry B, 2020, 124, 5209-5219.	1.2	16

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19	A theoretical study of CO oxidation and O2 activation for transition metal overlayers on SrTiO3 perovskite. Journal of Catalysis, 2020, 391, 229-240.	3.1	5
20	Supramolecular interactions between catalytic species allow rational control over reaction kinetics. Chemical Science, 2019, 10, 9115-9124.	3.7	6
21	Efficient Base-Metal NiMn/TiO₂ Catalyst for CO₂ Methanation. ACS Catalysis, 2019, 9, 7823-7839.	5.5	124
22	Coverage Effects in CO Dissociation on Metallic Cobalt Nanoparticles. ACS Catalysis, 2019, 9, 7365-7372.	5.5	37
23	Understanding the Impact of Defects on Catalytic CO Oxidation of LaFeO₃-Supported Rh, Pd, and Pt Single-Atom Catalysts. Journal of Physical Chemistry C, 2019, 123, 7290-7298.	1.5	36
24	Theoretical Approach To Predict the Stability of Supported Single-Atom Catalysts. ACS Catalysis, 2019, 9, 3289-3297.	5.5	101
25	Understanding carbon dioxide activation and carbonâ€“carbon coupling over nickel. Nature Communications, 2019, 10, 5330.	5.8	124
26	Linear Activation Energy-Reaction Energy Relations for LaBO3 (B = Mn, Fe, Co, Ni) Supported Single-Atom Platinum Group Metal Catalysts for CO Oxidation. Journal of Physical Chemistry C, 2019, 123, 31130-31141.	1.5	12
27	A Linear Scaling Relation for CO Oxidation on CeO₂-Supported Pd. Journal of the American Chemical Society, 2018, 140, 4580-4587.	6.6	126
28	Mechanism of Carbon Monoxide Dissociation on a Cobalt Fischer-Tropsch Catalyst. ChemCatChem, 2018, 10, 5-5.	1.8	1
29	Optimum Particle Size for Gold-Catalyzed CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 8327-8340.	1.5	45
30	Quantum-Chemical DFT Study of Direct and H- and C-Assisted CO Dissociation on the Ï‡-Fe₅C₂ HÃgg Carbide. Journal of Physical Chemistry C, 2018, 122, 9929-9938.	1.5	34
31	An Active Alkali-Exchanged Faujasite Catalyst for p-Xylene Production via the One-Pot Dielsâ€“Alder Cycloaddition/Dehydration Reaction of 2,5-Dimethylfuran with Ethylene. ACS Catalysis, 2018, 8, 760-769.	5.5	54
32	Optimum Cu nanoparticle catalysts for CO2 hydrogenation towards methanol. Nano Energy, 2018, 43, 200-209.	8.2	133
33	Stable Pd-Doped Ceria Structures for CH₄ Activation and CO Oxidation. ACS Catalysis, 2018, 8, 75-80.	5.5	111
34	Mechanism of Carbon Monoxide Dissociation on a Cobalt Fischerâ€“Tropsch Catalyst. ChemCatChem, 2018, 10, 136-140.	1.8	39
35	Reversible Restructuring of Silver Particles during Ethylene Epoxidation. ACS Catalysis, 2018, 8, 11794-11800.	5.5	42
36	Potential enthalpic energy of water in oils exploited to control supramolecular structure. Nature, 2018, 558, 100-103.	13.7	123

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37	Transition metal doping of Pd(1 1 1) for the NOâ€¯+â€¯CO reaction. Journal of Catalysis, 2018, 363, 154-163.	3.1	34
38	Highly Active and Stable CH₄ Oxidation by Substitution of Ce⁴⁺ by Two Pd²⁺ Ions in CeO₂(111). ACS Catalysis, 2018, 8, 6552-6559.	5.5	90
39	CO oxidation on Rh-doped hexadecagold clusters. Catalysis Science and Technology, 2017, 7, 75-83.	2.1	15
40	Unravelling the Pathway Complexity in Conformationally Flexible Nâ€Centered Triarylamine Trisamides. Chemistry - A European Journal, 2017, 23, 6103-6110.	1.7	64
41	Theoretical Study of Ripening Mechanisms of Pd Clusters on Ceria. Chemistry of Materials, 2017, 29, 9456-9462.	3.2	67
42	Mechanism of Cobalt-Catalyzed CO Hydrogenation: 1. Methanation. ACS Catalysis, 2017, 7, 8050-8060.	5.5	53
43	Mechanism of Cobalt-Catalyzed CO Hydrogenation: 2. Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2017, 7, 8061-8071.	5.5	94
44	Kinetic aspects of chain growth in Fischerâ€“Tropsch synthesis. Faraday Discussions, 2017, 197, 153-164.	1.6	18
45	A quantum-chemical DFT study of CO dissociation on Fe-promoted stepped Rh surfaces. Catalysis Today, 2016, 275, 111-118.	2.2	12
46	Charge Transport over the Defective CeO₂(111) Surface. Chemistry of Materials, 2016, 28, 5652-5658.	3.2	52
47	Identification of step-edge sites on Rh nanoparticles for facile CO dissociation. Catalysis Communications, 2016, 77, 5-8.	1.6	18
48	Microkinetic Modeling of the Oxygen Reduction Reaction at the Pt(111)/Gas Interface. Catalysis Letters, 2015, 145, 451-457.	1.4	12
49	First-Principles-Based Microkinetics Simulations of Synthesis Gas Conversion on a Stepped Rhodium Surface. ACS Catalysis, 2015, 5, 5453-5467.	5.5	124
50	Development of a Benzimidazoleâ€Derived Bidentate P,Nâ€Ligand for Enantioselective Iridiumâ€Catalyzed Hydrogenations. European Journal of Organic Chemistry, 2014, 2014, 350-362.	1.2	11
51	Correlating Fischerâ€“Tropsch activity to Ru nanoparticle surface structure as probed by high-energy X-ray diffraction. Chemical Communications, 2014, 50, 6005-6008.	2.2	40
52	The Optimally Performing Fischerâ€“Tropsch Catalyst. Angewandte Chemie - International Edition, 2014, 53, 12746-12750.	7.2	208
53	The Optimally Performing Fischerâ€“Tropsch Catalyst. Angewandte Chemie, 2014, 126, 12960-12964.	1.6	35
54	Reactivity of CO on Carbon-Covered Cobalt Surfaces in Fischerâ€“Tropsch Synthesis. Journal of Physical Chemistry C, 2014, 118, 5317-5327.	1.5	42

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55	Innentitelbild: The Optimally Performing Fischerâ€“Tropsch Catalyst (Angew. Chem. 47/2014). Angewandte Chemie, 2014, 126, 12856-12856.	1.6	3
56	Conformational Analysis of Chiral Supramolecular Aggregates: Modeling the Subtle Difference between Hydrogen and Deuterium. Journal of the American Chemical Society, 2013, 135, 16497-16506.	6.6	31
57	Catalytic properties of extraframework iron-containing species in ZSM-5 for N2O decomposition. Journal of Catalysis, 2013, 308, 386-397.	3.1	43
58	Mechanism and microkinetics of the Fischerâ€“Tropsch reaction. Physical Chemistry Chemical Physics, 2013, 15, 17038.	1.3	233
59	Microkinetics of steam methane reforming on platinum and rhodium metal surfaces. Journal of Catalysis, 2013, 297, 227-235.	3.1	43
60	Self-healing systems based on disulfideâ€“thiol exchange reactions. Polymer Chemistry, 2013, 4, 4955.	1.9	383
61	The origin of isotope-induced helical-sense bias in supramolecular polymers of benzene-1,3,5-tricarboxamides. Physical Chemistry Chemical Physics, 2012, 14, 13997.	1.3	3
62	Cooperative Two-Component Self-Assembly of Mono- and Ditopic Monomers. Macromolecules, 2011, 44, 6581-6587.	2.2	35
63	Size and Topological Effects of Rhodium Surfaces, Clusters and Nanoparticles on the Dissociation of CO. Journal of Physical Chemistry C, 2011, 115, 14204-14212.	1.5	48
64	Dynamic Supramolecular Polymers Based on Benzeneâ€1,3,5â€tricarboxamides: The Influence of Amide Connectivity on Aggregate Stability and Amplification of Chirality. Chemistry - A European Journal, 2010, 16, 810-821.	1.7	93
65	Understanding Cooperativity in Hydrogen-Bond-Induced Supramolecular Polymerization: A Density Functional Theory Study. Journal of Physical Chemistry B, 2010, 114, 13667-13674.	1.2	119
66	Tuning the Extent of Chiral Amplification by Temperature in a Dynamic Supramolecular Polymer. Journal of the American Chemical Society, 2010, 132, 611-619.	6.6	165