Frerich J Keil

List of Publications by Year
in descending order

62	6,631	117453	133063
papers	citations	34 h-index	59 g-index

63	63	63	7225
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method. Journal of Chemical Physics, 2005, 123, 224101.	1.2	662
3	Methanol-to-hydrocarbons: process technology. Microporous and Mesoporous Materials, 1999, 29, 49-66.	2.2	477
4	Modeling of Diffusion in Zeolites. Reviews in Chemical Engineering, 2000, 16, .	2.3	228
5	Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5â€. Journal of Physical Chemistry B, 2005, 109, 1857-1873.	1.2	176
6	Process intensification. Reviews in Chemical Engineering, 2018, 34, 135-200.	2.3	156
7	Quantum Chemical Modeling of Benzene Ethylation over H-ZSM-5 Approaching Chemical Accuracy: A Hybrid MP2:DFT Study. Journal of the American Chemical Society, 2010, 132, 11525-11538.	6.6	144
8	Adsorption of Methane, Ethane, and Their Binary Mixtures on MCM-41:Â Experimental Evaluation of Methods for the Prediction of Adsorption Equilibrium. Langmuir, 2002, 18, 2693-2701.	1.6	141
9	Recent advances in CO2 hydrogenation to value-added products â€" Current challenges and future directions. Progress in Energy and Combustion Science, 2021, 85, 100905.	15.8	134
10	Theoretical study of SN2 reactions. Ab initio computations on HF and CI level. Journal of the American Chemical Society, 1976, 98, 4787-4793.	6.6	111
11	Transport in Nanoporous Materials Including MOFs: The Applicability of Fickâ€™s Laws. Angewandte Chemie - International Edition, 2015, 54, 14580-14583.	7.2	90
12	Catalytic oxidation of 1,2-dichlorobenzene over ABO3-type perovskites. Catalysis Today, 2000, 62, 329-336.	2.2	83
13	A Reaction Mechanism for the Nitrous Oxide Decomposition on Binuclear Oxygen Bridged Iron Sites in Fe-ZSM-5. Journal of Physical Chemistry C, 2007, 111, 2092-2101.	1.5	80
14	Theoretical Investigation of Benzene Alkylation with Ethene over H-ZSM-5. Journal of Physical Chemistry C, 2008, 112, 15402-15411.	1.5	78
15	Nitrous Oxide Decomposition over Fe-ZSM-5 in the Presence of Nitric Oxide: A Comprehensive DFT Study. Journal of Physical Chemistry B, 2006, 110, 17096-17114.	1.2	77
16	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. Adsorption, 2021, 27, 683-760.	1.4	72
17	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 based on parameters obtained from first-principles calculations. Journal of Catalysis, 2005, 233, 26-35.	3.1	68
18	Optimization of three-dimensional catalyst pore structures. Chemical Engineering Science, 1994, 49, 4811-4822.	1.9	67

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19	Modeling of Three-Dimensional Linear Pressure Fields in Sonochemical Reactors with Homogeneous and Inhomogeneous Density Distributions of Cavitation Bubblesâ€. Industrial & Engineering Chemistry Research, 1998, 37, 848-864.	1.8	61
20	Combined Density Functional Theory and Monte Carlo Analysis of Monomolecular Cracking of Light Alkanes Over H-ZSM-5. Journal of Physical Chemistry C, 2012, 116, 23408-23417.	1.5	59
21	A dynamic bifurcation criterion for thermal runaway during the flash sintering of ceramics. Journal of the European Ceramic Society, 2016, 36, 1261-1267.	2.8	57
22	Molecular simulation of alkene adsorption in zeolites. Molecular Physics, 2005, 103, 471-489.	0.8	55
23	Multicomponent Diffusion and Reaction in Three-Dimensional Networks:â€‰ General Kinetics. Industrial & Engineering Chemistry Research, 1997, 36, 3275-3281.	1.8	54
24	Multiplicity of solutions in the optimization of a bifunctional catalyst blend in a tubular reactor. Canadian Journal of Chemical Engineering, 1992, 70, 780-785.	0.9	50
25	Modeling of linear pressure fields in sonochemical reactors considering an inhomogeneous density distribution of cavitation bubbles. Chemical Engineering Science, 1999, 54, 2865-2872.	1.9	50
26	Surface Barriers of Hydrocarbon Transport Triggered by Ideal Zeolite Structures. Journal of Physical Chemistry C, 2012, 116, 3677-3683.	1.5	46
27	Simulation and experiment of multicomponent diffusion and reaction in three-dimensional networks. Chemical Engineering Science, 1999, 54, 3485-3493.	1.9	45
28	Modelling of phenomena within catalyst particles. Chemical Engineering Science, 1996, 51, 1543-1567.	1.9	44
29	Transport into Nanosheets: Diffusion Equations Put to Test. Journal of Physical Chemistry C, 2013, 117, 7384-7390.	1.5	43
30	Process intensification education contributes to sustainable development goals. Part 1. Education for Chemical Engineers, 2020, 32, 1-14.	2.8	42
31	Application of a forced-flow catalytic membrane reactor for the dimerisation of isobutene. Catalysis Today, 2004, 98, 295-308.	2.2	40
32	Complexities in modeling of heterogeneous catalytic reactions. Computers and Mathematics With Applications, 2013, 65, 1674-1697.	1.4	39
33	Molecular simulation of adsorption and transport diffusion of model fluids in carbon nanotubes. Molecular Physics, 2002, 100, 3741-3751.	0.8	38
34	Predicting Local Transport Coefficients at Solidâ€“Gas Interfaces. Journal of Physical Chemistry C, 2012, 116, 18878-18883.	1.5	37
35	Theoretical Investigation of the Mechanism of the Selective Catalytic Reduction of Nitric Oxide with Ammonia on H-Form Zeolites. Journal of Physical Chemistry C, 2008, 112, 17378-17387.	1.5	36
36	Olefin/Paraffin Separation Potential of ZIFâ€9 and ZIFâ€71: A Combined Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2016, 2016, 4440-4449.	1.0	33

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37	Effect of the catalyst pore structure on fixed-bed reactor performance of partial oxidation of n-butane: A simulation study. Chemical Engineering Science, 2016, 142, 299-309.	1.9	32
38	Molecular Modelling for Reactor Design. Annual Review of Chemical and Biomolecular Engineering, 2018, 9, 201-227.	3.3	31
39	Theoretical Investigation of the Mechanism of the Selective Catalytic Reduction of Nitrogen Dioxide with Ammonia on H-Form Zeolites and the Role of Nitric and Nitrous Acids as Intermediates. Journal of Physical Chemistry C, 2010, 114, 6567-6587.	1.5	26
40	Multiscale Modeling of Reaction and Diffusion in Zeolites: From the Molecular Level to the Reactor. Soft Materials, 2012, 10, 179-201.	0.8	25
41	Optimizing catalyst pore network structure in the presence of deactivation by coking. AICHE Journal, 2019, 65, e16687.	1.8	25
42	Modeling of Sound Fields in Liquids with a Nonhomogeneous Distribution of Cavitation Bubbles as a Basis for the Design of Sonochemical Reactors. Chemical Engineering and Technology, 1998, 21, 873-877.	0.9	23
43	Grand canonical molecular dynamics simulations of transport diffusion in geometrically heterogeneous pores. Physical Chemistry Chemical Physics, 2003, 5, 369-375.	1.3	23
44	Unveiling the role of 2D monolayer Mn-doped MoS₂material: toward an efficient electrocatalyst for H₂evolution reaction. Physical Chemistry Chemical Physics, 2021, 24, 265-280.	1.3	21
45	Theoretical Investigation of the Mechanism of the Selective Catalytic Oxidation of Ammonia on H-Form Zeolites. Journal of Physical Chemistry C, 2009, 113, 13860-13876.	1.5	20
46	Increasing yield and operating time of SLP-catalyst processes by flow reversal and instationary operation. Chemical Engineering Science, 2003, 58, 841-847.	1.9	16
47	Kinetic parameters estimation via dragonfly algorithm (DA) and comparison of cylindrical and spherical reactors performance for CO2 hydrogenation to hydrocarbons. Energy Conversion and Management, 2020, 226, 113550.	4.4	16
48	Adsorption and diffusion in zeolites: the pitfall of isotypic crystal structures. Molecular Simulation, 2011, 37, 986-989.	0.9	13
49	A high-speed method for obtaining kinetic data for exothermic or endothermic catalytic reactions under non-isothermal conditions illustrated for the ammonia synthesis. Applied Catalysis A: General, 2003, 240, 95-110.	2.2	12
50	Theoretical Investigation of the Mechanism of the Oxidation of Nitrogen Oxide on Iron-Form Zeolites in the Presence of Water. Journal of Physical Chemistry C, 2011, 115, 2114-2133.	1.5	12
51	Deactivation and regeneration of Claus catalyst particles unraveled by pore network model. Chemical Engineering Science, 2020, 211, 115305.	1.9	12
52	Catalytic reactions and reactors. Chemical Engineering Science, 2004, 59, 5473-5478.	1.9	9
53	The temperature-scanning plug flow reactor (TSPFR) applied to complex reactionsâ€"Oxidative dehydrogenation of propane as an example. Chemical Engineering Journal, 2005, 108, 219-226.	6.6	9
54	An alternative procedure for modeling of Knudsen flow and surface diffusion. Periodica Polytechnica: Chemical Engineering, 2008, 52, 37.	0.5	8

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55	Kinetics of N2O catalytic decomposition over three-dimensional fractals. Chemical Physics Letters, 2000, 330, 410-416.	1.2	7
56	Experimental and Theoretical Analysis of the Influence of Different Linker Molecules in Imidazolate Frameworks Potsdam (IFP-n) on the Separation of Olefinâ€“Paraffin Mixtures. Langmuir, 2017, 33, 11170-11179.	1.6	5
57	Development of microkinetic expressions by instationary methods. Studies in Surface Science and Catalysis, 2001, , 41-55.	1.5	4
58	Modeling of Process Intensificationâ€“ An Introduction and Overview. , 0, , 1-7.		3
59	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations. Catalysis Science and Technology, 2021, 11, 3539-3555.	2.1	3
60	Ethylene Hydrogenation in Pellets with Different Pore Structures, Measured in a One-Sided Single-Pellet Reactor. International Journal of Chemical Reactor Engineering, 2019, 17, .	0.6	1
61	A mathematical model of dehydroisomerization of methylcyclopentane using a bifunctional catalyst blend. Chemical Engineering and Technology, 1993, 16, 191-199.	0.9	0
62	Rigorous Lower Bounds for the Ground State Energy of Molecules by Employing Necessary N-Representability Conditions. Journal of Chemical Theory and Computation, 2020, 16, 7342-7356.	2.3	0