Rutger van Santen

List of Publications by Year
in descending order

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83 papers	5,443 citations	81743 39 h-index	82410 72 g-index
123 all docs	123 docs citations	123 times ranked	5497 citing authors

#	Article	IF	Citations
1	Solid acid catalysis. Part II, Catalytic chemistry of proton activation. , 2021, , .		0
2	Dynamic restructuring of supported metal nanoparticles and its implications for structure insensitive catalysis. Nature Communications, 2021, 12, 7096.	5.8	33
3	Deactivation Kinetics of the Catalytic Alkylation Reaction. ACS Catalysis, 2020, 10, 6988-7006.	5.5	9
4	Theory of Zeolite Catalysis. , 2018, , 151-188.		1
5	The challenge of catalyst prediction. Faraday Discussions, 2018, 208, 35-52.	1.6	8
6	A density functional theory study of propylene epoxidation mechanism on Ag₂O(001) surface. Physical Chemistry Chemical Physics, 2018, 20, 26681-26687.	1.3	13
7	Deactivation Kinetics of Solid Acid Catalyst with Laterally Interacting Protons. ACS Catalysis, 2018, 8, 9016-9033.	5.5	13
8	Scaling Relations for Acidity and Reactivity of Zeolites. Journal of Physical Chemistry C, 2017, 121, 23520-23530.	1.5	74
9	Hydride Transfer versus Deprotonation Kinetics in the Isobutaneâ€“Propene Alkylation Reaction: A Computational Study. ACS Catalysis, 2017, 7, 8613-8627.	5.5	49
10	Lattice model of reduced jamming by a barrier. Physical Review E, 2016, 94, 042115.	0.8	18
11	How molecular is the chemisorptive bond?. Physical Chemistry Chemical Physics, 2016, 18, 20868-20894.	1.3	41
12	Quantum chemistry of the oxygen evolution reaction on cobalt(<scp>ii</scp>,<scp>iii</scp>) oxide â€“ implications for designing the optimal catalyst. Faraday Discussions, 2016, 188, 199-226.	1.6	18
13	Water Splitting on TiO₂-Based Electrochemical Cells: A Small Cluster Study. Journal of Physical Chemistry C, 2016, 120, 437-449.	1.5	21
14	Structure Sensitivity of the Oxygen Evolution Reaction Catalyzed by Cobalt(II,III) Oxide. Journal of the American Chemical Society, 2015, 137, 14660-14672.	6.6	116
15	Carbon-Induced Surface Transformations of Cobalt. ACS Catalysis, 2015, 5, 596-601.	5.5	44
16	DFT Simulations of Water Adsorption and Activation on Lowâ€Index Î±â€Ga₂O₃ Surfaces. Chemistry - A European Journal, 2014, 20, 6915-6926.	1.7	32
17	Structure sensitivity in the ruthenium nanoparticle catalyzed aqueous-phase Fischerâ€“Tropsch reaction. Catalysis Science and Technology, 2014, 4, 3510-3523.	2.1	26
18	The Optimally Performing Fischerâ€“Tropsch Catalyst. Angewandte Chemie - International Edition, 2014, 53, 12746-12750.	7.2	208

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19	Mechanistic studies in catalysis. Catalysis Science and Technology, 2014, 4, 3408-3408.	2.1	1
20	Site Stability on Cobalt Nanoparticles: A Molecular Dynamics ReaxFF Reactive Force Field Study. Journal of Physical Chemistry C, 2014, 118, 6882-6886.	1.5	36
21	Quantum chemistry of the Fischerâ€“Tropsch reaction catalysed by a stepped ruthenium surface. Catalysis Science and Technology, 2014, 4, 3129-3140.	2.1	51
22	Microkinetics of oxygenate formation in the Fischerâ€“Tropsch reaction. Physical Chemistry Chemical Physics, 2014, 16, 10041-10058.	1.3	21
23	Mechanism and microkinetics of the Fischerâ€“Tropsch reaction. Physical Chemistry Chemical Physics, 2013, 15, 17038.	1.3	233
24	The Mechanism of Ethylene Epoxidation Catalysis. Catalysis Letters, 2013, 143, 131-141.	1.4	137
25	Reconstruction of Clean and Oxygen-Covered Pt(110) Surfaces. Journal of Physical Chemistry C, 2013, 117, 11251-11257.	1.5	24
26	Monomer Formation Model versus Chain Growth Model of the Fischerâ€“Tropsch Reaction. Journal of Physical Chemistry C, 2013, 117, 4488-4504.	1.5	55
27	Catalyst nano-particle size dependence of the Fischerâ€“Tropsch reaction. Faraday Discussions, 2013, 162, 267.	1.6	16
28	Effect of Surface and Oxygen Coverage on Ethylene Epoxidation. Topics in Catalysis, 2012, 55, 710-717.	1.3	45
29	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
30	Methane Dissociation on High and Low Indices Rh Surfaces. Journal of Physical Chemistry C, 2011, 115, 13027-13034.	1.5	35
31	Nature and Location of Cationic Lanthanum Species in High Alumina Containing Faujasite Type Zeolites. Journal of Physical Chemistry C, 2011, 115, 21763-21776.	1.5	105
32	Structure sensitivity of the Fischerâ€“Tropsch reaction; molecular kinetics simulations. Catalysis Science and Technology, 2011, 1, 891.	2.1	120
33	Stability and reactivity of active sites for direct benzene oxidation to phenol in Fe/ZSM-5: A comprehensive periodic DFT study. Journal of Catalysis, 2011, 284, 194-206.	3.1	69
34	Epoxidation of Ethylene by Silver Oxide (Ag2O) Cluster: A Density Functional Theory Study. Catalysis Letters, 2011, 141, 762-771.	1.4	20
35	Editorial: Problem Solvers and Thinkers. Angewandte Chemie - International Edition, 2011, 50, 11808-11809.	7.2	1
36	Symmetric Transition State Analysis: An Analysis of Dissociative Methane Adsorption on Rh{111} Using Quantum Chemical Calculations. Topics in Catalysis, 2010, 53, 403-416.	1.3	4

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37	Site Structure Sensitivity Differences for Dissociation of Diatomic Molecules. Topics in Catalysis, 2010, 53, 969-975.	1.3	10
38	Molecular recognition in cationâ€exchanged zeolites. International Journal of Quantum Chemistry, 2010, 110, 210-220.	1.0	10
39	On Shustorovich's Bond-Order conservation method as applied to chemisorption. Recueil Des Travaux Chimiques Des Pays-Bas, 2010, 109, 59-63.	0.0	19
40	Reactivity Theory of Transition-Metal Surfaces: A BrÃ¸nstedâˆ'Evansâˆ'Polanyi Linear Activation Energyâˆ'Free-Energy Analysis. Chemical Reviews, 2010, 110, 2005-2048.	23.0	492
41	Density functional theory studies of the hydrogenation properties of Mg and Ti. Physical Review B, 2009, 79, .	1.1	35
42	Multi-level Modeling of Silicaâ€“Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
43	Complementary Structure Sensitive and Insensitive Catalytic Relationships. Accounts of Chemical Research, 2009, 42, 57-66.	7.6	581
44	Enantioselective epoxidation of Î²-methylstyrene catalyzed by immobilized Mn(salen) catalysts in different mesoporous silica supports. Journal of Catalysis, 2008, 256, 226-236.	3.1	77
45	Computational modeling of catalytic reactivity. Molecular Simulation, 2007, 33, 327-336.	0.9	10
46	An Efficient Hybrid, Nanostructured, Epoxidation Catalyst: Titanium Silsesquioxaneâ€“Polystyrene Copolymer Supported on SBA-15. Chemistry - A European Journal, 2007, 13, 1210-1221.	1.7	56
47	Mesoporous Organicâ€“Inorganic Hybrid Materials Built Using Polyhedral Oligomeric Silsesquioxane Blocks. Angewandte Chemie - International Edition, 2007, 46, 5003-5006.	7.2	99
48	Waterâ€Promoted Hydrocarbon Activation Catalyzed by Binuclear Gallium Sites in ZSMâ€5 Zeolite. Angewandte Chemie - International Edition, 2007, 46, 7273-7276.	7.2	78
49	Organo-bridged silsesquioxane titanates for heterogeneous catalytic epoxidation with aqueous hydrogen peroxide. Journal of Catalysis, 2007, 251, 453-458.	3.1	10
50	Theory of surface chemical reactivity. Russian Journal of Physical Chemistry B, 2007, 1, 261-291.	0.2	22
51	Controlling Reaction Pathways for Alcohol Dehydration and Dehydrogenation over FeSBA-15 Catalysts. Catalysis Letters, 2007, 117, 18-24.	1.4	28
52	Positron Emission Profiling â€" The Ammonia Oxidation Reaction as a Case Study. Catalytic Science Series, 2006, , 213-260.	0.6	0
53	Positron Emission Profiling Study of the Diffusion of 3-Methylpentane in Silicalite-1. Topics in Catalysis, 2003, 24, 103-113.	1.3	6
54	Title is missing!. Catalysis Letters, 2003, 86, 25-31.	1.4	68

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55	A Periodic DFT Study of Isobutene Chemisorption in Proton-Exchanged Zeolites:Â Dependence of Reactivity on the Zeolite Framework Structure. Journal of Physical Chemistry B, 2003, 107, 1309-1315.	1.2	129
56	A Periodic Structure Density Functional Theory Study of Propylene Chemisorption in Acidic Chabazite:Â Effect of Zeolite Structure Relaxation. Journal of Physical Chemistry B, 2002, 106, 3248-3254.	1.2	76
57	Ab initio molecular dynamics simulation of liquid water and waterâ€“vapor interface. Journal of Chemical Physics, 2001, 115, 9815-9820.	1.2	71
58	Adsorption and Diffusion ofn-Hexane/2-Methylpentane Mixtures in Zeolite Silicalite:Â Experiments and Modeling. Journal of Physical Chemistry B, 2001, 105, 7690-7698.	1.2	68
59	N2O Decomposition Catalysed by Transition Metal Ions. Catalysis Letters, 2001, 75, 45-48.	1.4	75
60	Development of a New Combinatorial Approach to Multifunctional Catalysts: Metal Silsesquioxanes as Precursors to Microporous Metallosilicates. Chinese Journal of Chemistry, 2001, 19, 30-39.	2.6	11
61	DFT study of oxygen-bridged Zn2+ ion pairs in Zn/ZSM-5 zeolites. Catalysis Letters, 2000, 70, 175-181.	1.4	83
62	Theoretical study of the enhanced BrÃ¸nsted acidity of Zn2+â€exchanged zeolites. Catalysis Letters, 1999, 63, 97-106.	1.4	32
63	Alkylation and Transalkylation Reactions of Aromatics. ACS Symposium Series, 1999, , 307-320.	0.5	6
64	n-Pentane hopping in zeolite ZK-5 studied with13C NMR. Magnetic Resonance in Chemistry, 1999, 37, S108-S117.	1.1	14
65	Chain Length Effects of Linear Alkanes in Zeolite Ferrierite. 1. Sorption and13C NMR Experiments1. Journal of Physical Chemistry B, 1998, 102, 3945-3951.	1.2	49
66	Chain Length Effects of Linear Alkanes in Zeolite Ferrierite. 2. Molecular Simulations1. Journal of Physical Chemistry B, 1998, 102, 3952-3958.	1.2	44
67	The Molecular Basis of Zeolite Catalysis:A Review of Theoretical Simulations. Advances in Catalysis, 1998, 42, 1-114.	0.1	48
68	Configurational-Bias Monte Carlo (CB-MC) Calculations ofn-Alkane Sorption in Zeolites Rho and Fer. Molecular Simulation, 1997, 19, 301-318.	0.9	8
69	Microkinetics Modeling of the Hydroisomerization of n-Hexane. Industrial & Engineering Chemistry Research, 1997, 36, 3116-3125.	1.8	40
70	Theoretical Study of the Mechanism of Surface Methoxy and Dimethyl Ether Formation from Methanol Catalyzed by Zeolitic Protons. Journal of Physical Chemistry B, 1997, 101, 2292-2305.	1.2	166
71	The cluster approach to molecular heterogeneous catalysis. Journal of Computer-Aided Materials Design, 1996, 3, 265-266.	0.7	0
72	SELECTIVE CATALYTIC OXIDATION BY HETEROGENEOUS TRANSITION METAL CATALYSTS. , 1995, , .		2

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73	Kommensurables Einfrieren von nâ€Alkanen im Silicalit. Angewandte Chemie, 1995, 107, 2765-2767.	1.6	8
74	Commensurate Freezing ofn-Alkanes in Silicalite. Angewandte Chemie International Edition in English, 1995, 34, 2543-2544.	4.4	58
75	Reactivity Theory of Zeolitic Broensted Acidic Sites. Chemical Reviews, 1995, 95, 637-660.	23.0	575
76	Electronic structure calculations and dynamics of CC coupling on nickel and cobalt. Journal of Chemical Physics, 1995, 103, 6562-6570.	1.2	14
77	Carbonium ion formation in zeolite catalysis. Catalysis Letters, 1994, 27, 91-96.	1.4	106
78	Electronic structure calculations and dynamics of methane activation on nickel and cobalt. Journal of Chemical Physics, 1994, 101, 11012-11020.	1.2	85
79	Theoretical investigation of the insertion of nickel in the CH bond of CH4. Electronic structure calculations and dynamics. Journal of Chemical Physics, 1993, 98, 8810-8818.	1.2	44
80	Relation between crystal symmetry and ionicity in silica polymorphs. Nature, 1991, 351, 636-638.	13.7	13
81	The Influence of Cations on Growth Kinetics of Silica Aggregates. Materials Research Society Symposia Proceedings, 1990, 180, 273.	0.1	2
82	The quantum chemical basis of the Fischer-Tropsch reaction. Catalysis Letters, 1990, 7, 1-14.	1.4	55
83	CO adsorption and dissociation on Rh(111). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1988, 6, 1128-1133.	0.9	13