

Rutger van Santen

List of Publications by Year in descending order

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83
papers

5,443
citations

81743

39
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82410

72
g-index

123
all docs

123
docs citations

123
times ranked

5497
citing authors

#	ARTICLE	IF	CITATIONS
1	Complementary Structure Sensitive and Insensitive Catalytic Relationships. <i>Accounts of Chemical Research</i> , 2009, 42, 57-66.	7.6	581
2	Reactivity Theory of Zeolitic Brønsted Acidic Sites. <i>Chemical Reviews</i> , 1995, 95, 637-660.	23.0	575
3	Reactivity Theory of Transition-Metal Surfaces: A Brønsted-Evans-Polanyi Linear Activation Energy-Free-Energy Analysis. <i>Chemical Reviews</i> , 2010, 110, 2005-2048.	23.0	492
4	Mechanism and microkinetics of the Fischer-Tropsch reaction. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17038.	1.3	233
5	The Optimally Performing Fischer-Tropsch Catalyst. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12746-12750.	7.2	208
6	Theoretical Study of the Mechanism of Surface Methoxy and Dimethyl Ether Formation from Methanol Catalyzed by Zeolitic Protons. <i>Journal of Physical Chemistry B</i> , 1997, 101, 2292-2305.	1.2	166
7	The Mechanism of Ethylene Epoxidation Catalysis. <i>Catalysis Letters</i> , 2013, 143, 131-141.	1.4	137
8	A Periodic DFT Study of Isobutene Chemisorption in Proton-Exchanged Zeolites: Dependence of Reactivity on the Zeolite Framework Structure. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1309-1315.	1.2	129
9	Structure sensitivity of the Fischer-Tropsch reaction; molecular kinetics simulations. <i>Catalysis Science and Technology</i> , 2011, 1, 891.	2.1	120
10	Structure Sensitivity of the Oxygen Evolution Reaction Catalyzed by Cobalt(II,III) Oxide. <i>Journal of the American Chemical Society</i> , 2015, 137, 14660-14672.	6.6	116
11	Carbonium ion formation in zeolite catalysis. <i>Catalysis Letters</i> , 1994, 27, 91-96.	1.4	106
12	Nature and Location of Cationic Lanthanum Species in High Alumina Containing Faujasite Type Zeolites. <i>Journal of Physical Chemistry C</i> , 2011, 115, 21763-21776.	1.5	105
13	Mesoporous Organic-Inorganic Hybrid Materials Built Using Polyhedral Oligomeric Silsesquioxane Blocks. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5003-5006.	7.2	99
14	Electronic structure calculations and dynamics of methane activation on nickel and cobalt. <i>Journal of Chemical Physics</i> , 1994, 101, 11012-11020.	1.2	85
15	DFT study of oxygen-bridged Zn ²⁺ ion pairs in Zn/ZSM-5 zeolites. <i>Catalysis Letters</i> , 2000, 70, 175-181.	1.4	83
16	Water-Promoted Hydrocarbon Activation Catalyzed by Binuclear Gallium Sites in ZSM-5 Zeolite. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 7273-7276.	7.2	78
17	Enantioselective epoxidation of <i>l</i> -methylstyrene catalyzed by immobilized Mn(salen) catalysts in different mesoporous silica supports. <i>Journal of Catalysis</i> , 2008, 256, 226-236.	3.1	77
18	A Periodic Structure Density Functional Theory Study of Propylene Chemisorption in Acidic Chabazite: Effect of Zeolite Structure Relaxation. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3248-3254.	1.2	76

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19	N2O Decomposition Catalysed by Transition Metal Ions. <i>Catalysis Letters</i> , 2001, 75, 45-48.	1.4	75
20	Scaling Relations for Acidity and Reactivity of Zeolites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23520-23530.	1.5	74
21	Ab initio molecular dynamics simulation of liquid water and water-vapor interface. <i>Journal of Chemical Physics</i> , 2001, 115, 9815-9820.	1.2	71
22	Stability and reactivity of active sites for direct benzene oxidation to phenol in Fe/ZSM-5: A comprehensive periodic DFT study. <i>Journal of Catalysis</i> , 2011, 284, 194-206.	3.1	69
23	Adsorption and Diffusion of n-Hexane/2-Methylpentane Mixtures in Zeolite Silicalite: Experiments and Modeling. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7690-7698.	1.2	68
24	Title is missing!. <i>Catalysis Letters</i> , 2003, 86, 25-31.	1.4	68
25	Commensurate Freezing of n-Alkanes in Silicalite. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2543-2544.	4.4	58
26	An Efficient Hybrid, Nanostructured, Epoxidation Catalyst: Titanium Silsesquioxane-Polystyrene Copolymer Supported on SBA-15. <i>Chemistry - A European Journal</i> , 2007, 13, 1210-1221.	1.7	56
27	The quantum chemical basis of the Fischer-Tropsch reaction. <i>Catalysis Letters</i> , 1990, 7, 1-14.	1.4	55
28	Monomer Formation Model versus Chain Growth Model of the Fischer-Tropsch Reaction. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4488-4504.	1.5	55
29	Quantum chemistry of the Fischer-Tropsch reaction catalysed by a stepped ruthenium surface. <i>Catalysis Science and Technology</i> , 2014, 4, 3129-3140.	2.1	51
30	Chain Length Effects of Linear Alkanes in Zeolite Ferrierite. 1. Sorption and ¹³ C NMR Experiments. <i>Journal of Physical Chemistry B</i> , 1998, 102, 3945-3951.	1.2	49
31	Hydride Transfer versus Deprotonation Kinetics in the Isobutane-Propene Alkylation Reaction: A Computational Study. <i>ACS Catalysis</i> , 2017, 7, 8613-8627.	5.5	49
32	The Molecular Basis of Zeolite Catalysis: A Review of Theoretical Simulations. <i>Advances in Catalysis</i> , 1998, 42, 1-114.	0.1	48
33	Size and Topological Effects of Rhodium Surfaces, Clusters and Nanoparticles on the Dissociation of CO. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14204-14212.	1.5	48
34	Effect of Surface and Oxygen Coverage on Ethylene Epoxidation. <i>Topics in Catalysis</i> , 2012, 55, 710-717.	1.3	45
35	Theoretical investigation of the insertion of nickel in the CH bond of CH ₄ . Electronic structure calculations and dynamics. <i>Journal of Chemical Physics</i> , 1993, 98, 8810-8818.	1.2	44
36	Chain Length Effects of Linear Alkanes in Zeolite Ferrierite. 2. Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 1998, 102, 3952-3958.	1.2	44

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37	Carbon-Induced Surface Transformations of Cobalt. ACS Catalysis, 2015, 5, 596-601.	5.5	44
38	How molecular is the chemisorptive bond?. Physical Chemistry Chemical Physics, 2016, 18, 20868-20894.	1.3	41
39	Microkinetics Modeling of the Hydroisomerization of n-Hexane. Industrial & Engineering Chemistry Research, 1997, 36, 3116-3125.	1.8	40
40	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
41	Density functional theory studies of the hydrogenation properties of Mg and Ti. Physical Review B, 2009, 79, .	1.1	35
42	Methane Dissociation on High and Low Indices Rh Surfaces. Journal of Physical Chemistry C, 2011, 115, 13027-13034.	1.5	35
43	Dynamic restructuring of supported metal nanoparticles and its implications for structure insensitive catalysis. Nature Communications, 2021, 12, 7096.	5.8	33
44	Theoretical study of the enhanced Brønsted acidity of Zn ²⁺ -exchanged zeolites. Catalysis Letters, 1999, 63, 97-106.	1.4	32
45	DFT Simulations of Water Adsorption and Activation on Low-Index Ga ₂ O ₃ Surfaces. Chemistry - A European Journal, 2014, 20, 6915-6926.	1.7	32
46	Multi-level Modeling of Silica-Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
47	Controlling Reaction Pathways for Alcohol Dehydration and Dehydrogenation over FeSBA-15 Catalysts. Catalysis Letters, 2007, 117, 18-24.	1.4	28
48	Structure sensitivity in the ruthenium nanoparticle catalyzed aqueous-phase Fischer-Tropsch reaction. Catalysis Science and Technology, 2014, 4, 3510-3523.	2.1	26
49	Reconstruction of Clean and Oxygen-Covered Pt(110) Surfaces. Journal of Physical Chemistry C, 2013, 117, 11251-11257.	1.5	24
50	Theory of surface chemical reactivity. Russian Journal of Physical Chemistry B, 2007, 1, 261-291.	0.2	22
51	Microkinetics of oxygenate formation in the Fischer-Tropsch reaction. Physical Chemistry Chemical Physics, 2014, 16, 10041-10058.	1.3	21
52	Water Splitting on TiO ₂ -Based Electrochemical Cells: A Small Cluster Study. Journal of Physical Chemistry C, 2016, 120, 437-449.	1.5	21
53	Epoxidation of Ethylene by Silver Oxide (Ag ₂ O) Cluster: A Density Functional Theory Study. Catalysis Letters, 2011, 141, 762-771.	1.4	20
54	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

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55	Lattice model of reduced jamming by a barrier. <i>Physical Review E</i> , 2016, 94, 042115.	0.8	18
56	Quantum chemistry of the oxygen evolution reaction on cobalt(<i>ii</i>),(<i>iii</i>) oxide – implications for designing the optimal catalyst. <i>Faraday Discussions</i> , 2016, 188, 199-226.	1.6	18
57	Catalyst nano-particle size dependence of the Fischer–Tropsch reaction. <i>Faraday Discussions</i> , 2013, 162, 267.	1.6	16
58	Electronic structure calculations and dynamics of CC coupling on nickel and cobalt. <i>Journal of Chemical Physics</i> , 1995, 103, 6562-6570.	1.2	14
59	n-Pentane hopping in zeolite ZK-5 studied with ¹³ C NMR. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, S108-S117.	1.1	14
60	CO adsorption and dissociation on Rh(111). <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1988, 6, 1128-1133.	0.9	13
61	Relation between crystal symmetry and ionicity in silica polymorphs. <i>Nature</i> , 1991, 351, 636-638.	13.7	13
62	A density functional theory study of propylene epoxidation mechanism on Ag ₂ O(001) surface. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26681-26687.	1.3	13
63	Deactivation Kinetics of Solid Acid Catalyst with Laterally Interacting Protons. <i>ACS Catalysis</i> , 2018, 8, 9016-9033.	5.5	13
64	Development of a New Combinatorial Approach to Multifunctional Catalysts: Metal Silsesquioxanes as Precursors to Microporous Metallosilicates. <i>Chinese Journal of Chemistry</i> , 2001, 19, 30-39.	2.6	11
65	Computational modeling of catalytic reactivity. <i>Molecular Simulation</i> , 2007, 33, 327-336.	0.9	10
66	Organo-bridged silsesquioxane titanates for heterogeneous catalytic epoxidation with aqueous hydrogen peroxide. <i>Journal of Catalysis</i> , 2007, 251, 453-458.	3.1	10
67	Site Structure Sensitivity Differences for Dissociation of Diatomic Molecules. <i>Topics in Catalysis</i> , 2010, 53, 969-975.	1.3	10
68	Molecular recognition in cation-exchanged zeolites. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 210-220.	1.0	10
69	Deactivation Kinetics of the Catalytic Alkylation Reaction. <i>ACS Catalysis</i> , 2020, 10, 6988-7006.	5.5	9
70	Kommensurables Einfrieren von <i>n</i> -Alkanen im Silicalit. <i>Angewandte Chemie</i> , 1995, 107, 2765-2767.	1.6	8
71	Configurational-Bias Monte Carlo (CB-MC) Calculations of <i>n</i> -Alkane Sorption in Zeolites Rho and Fer. <i>Molecular Simulation</i> , 1997, 19, 301-318.	0.9	8
72	The challenge of catalyst prediction. <i>Faraday Discussions</i> , 2018, 208, 35-52.	1.6	8

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73	Alkylation and Transalkylation Reactions of Aromatics. ACS Symposium Series, 1999, , 307-320.	0.5	6
74	Positron Emission Profiling Study of the Diffusion of 3-Methylpentane in Silicalite-1. Topics in Catalysis, 2003, 24, 103-113.	1.3	6
75	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
76	The Influence of Cations on Growth Kinetics of Silica Aggregates. Materials Research Society Symposia Proceedings, 1990, 180, 273.	0.1	2
77	SELECTIVE CATALYTIC OXIDATION BY HETEROGENEOUS TRANSITION METAL CATALYSTS. , 1995, , .		2
78	Editorial: Problem Solvers and Thinkers. Angewandte Chemie - International Edition, 2011, 50, 11808-11809.	7.2	1
79	Mechanistic studies in catalysis. Catalysis Science and Technology, 2014, 4, 3408-3408.	2.1	1
80	Theory of Zeolite Catalysis. , 2018, , 151-188.		1
81	The cluster approach to molecular heterogeneous catalysis. Journal of Computer-Aided Materials Design, 1996, 3, 265-266.	0.7	0
82	Solid acid catalysis. Part II, Catalytic chemistry of proton activation. , 2021, , .		0
83	Positron Emission Profiling â€” The Ammonia Oxidation Reaction as a Case Study. Catalytic Science Series, 2006, , 213-260.	0.6	0