Joachim Sauer

List of Publications by Year
in descending order

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351 papers	26,550 citations	3515 90 h-index	8599 146 g-index
389 all docs	389 docs citations	389 times ranked	14809 citing authors

#	Article	IF	Citations
1	Gasâ€Phase Mechanism of O^{.â˙}/Ni²⁺â€Mediated Methane Conversion to Formaldehyde. Angewandte Chemie - International Edition, 2022, 61, .	7.2	6
2	Dimerization of Linear Butenes and Pentenes in an Acidic Zeolite (Hâ€MFI). Angewandte Chemie - International Edition, 2021, 60, 3529-3533.	7.2	11
3	Adsorption and cracking of propane by zeolites of different pore size. Journal of Catalysis, 2021, 395, 117-128.	3.1	29
4	Insights into Reaction Kinetics in Confined Space: Real Time Observation of Water Formation under a Silica Cover. Journal of the American Chemical Society, 2021, 143, 8780-8790.	6.6	22
5	Chemically Accurate Vibrational Free Energies of Adsorption from Density Functional Theory Molecular Dynamics: Alkanes in Zeolites. Journal of Chemical Theory and Computation, 2021, 17, 5849-5862.	2.3	13
6	Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting. Science, 2021, 374, 454-459.	6.0	281
7	The Chemical Nature of Ti4O10â€“: Vibrational Predissociation Spectroscopy Combined with Global Structure Optimization. Journal of Physical Chemistry A, 2021, 125, 9571-9577.	1.1	3
8	Dimerization of Linear Butenes and Pentenes in an Acidic Zeolite (Hâ€MFI). Angewandte Chemie, 2021, 133, 3571-3575.	1.6	1
9	Adsorption of CH4 on the Pt(111) surface: Random phase approximation compared to density functional theory. Journal of Chemical Physics, 2021, 155, 174702.	1.2	10
10	Predicting adsorption selectivities from pure gas isotherms for gas mixtures in metalâ€“organic frameworks. Chemical Science, 2020, 11, 643-655.	3.7	19
11	Valence and Structure Isomerism of Al2FeO4+: Synergy of Spectroscopy and Quantum Chemistry. Journal of the American Chemical Society, 2020, 142, 18050-18059.	6.6	14
12	Isomerization and Selective Hydrogenation of Propyne: Screening of Metalâ€“Organic Frameworks Modified by Atomic Layer Deposition. Journal of the American Chemical Society, 2020, 142, 20380-20389.	6.6	15
13	Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metalâ€“Organic Frameworks. ACS Catalysis, 2020, 10, 10051-10059.	5.5	14
14	Thermochemistry of FeO_mH_n^z Species: Assessment of Some DFT Functionals. Journal of Chemical Theory and Computation, 2020, 16, 2430-2435.	2.3	7
15	Elucidating Surface Structure with Action Spectroscopy. Journal of the American Chemical Society, 2020, 142, 2665-2671.	6.6	16
16	Interaction of C₃â€“C₅Alkenes with Zeolitic BrÃ¸nsted Sites: Ï€-Complexes, Alkoxides, and Carbenium Ions in H-FER. Journal of Physical Chemistry C, 2020, 124, 10067-10078.	1.5	41
17	Reaction dynamics of metal/oxide catalysts: Methanol oxidation at vanadium oxide films on Rh(1Â1Â1) from UHV to 10â˙2 mbar. Journal of Catalysis, 2020, 385, 255-264.	3.1	13
18	Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metalâ€“organic frameworks and in acidic zeolites. Physical Chemistry Chemical Physics, 2020, 22, 7577-7585.	1.3	30

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19	Acid strength of zeolitic BrÃ¸nsted sitesâ€"Dependence on dielectric properties. Catalysis Today, 2019, 323, 86-93.	2.2	18
20	Hydrogen Atom or Proton Coupled Electron Transfer? Câ€"H Bond Activation by Transition-Metal Oxides. Journal of the American Chemical Society, 2019, 141, 14603-14611.	6.6	25
21	Characterization of Phonon Vibrations of Silica Bilayer Films. Journal of Physical Chemistry C, 2019, 123, 7110-7117.	1.5	8
22	Students, Postdoctoral Associates, and Collaborators of Joachim Sauer. Journal of Physical Chemistry C, 2019, 123, 7527-7528.	1.5	0
23	Curriculum Vitae of Joachim Sauer. Journal of Physical Chemistry C, 2019, 123, 7529-7530.	1.5	0
24	Autobiography of Joachim Sauer. Journal of Physical Chemistry C, 2019, 123, 7521-7526.	1.5	0
25	Publications of Joachim Sauer. Journal of Physical Chemistry C, 2019, 123, 7531-7539.	1.5	1
26	Ab Initio Calculations for Moleculeâ€"Surface Interactions with Chemical Accuracy. Accounts of Chemical Research, 2019, 52, 3502-3510.	7.6	70
27	Chemically Accurate Adsorption Energies: CO and H2O on the MgO(001) Surface. Journal of Chemical Theory and Computation, 2019, 15, 1329-1344.	2.3	23
28	Interaction of Water Molecules with the Î±-Fe₂O₃(0001) Surface: A Combined Experimental and Computational Study. Journal of Physical Chemistry C, 2019, 123, 8324-8335.	1.5	26
29	Structure and Reactivity of Alâ€'O(H)â€'Al Moieties in Siloxide Frameworks: Solution and Gasâ€Phase Model Studies. Angewandte Chemie - International Edition, 2019, 58, 902-906.	7.2	16
30	Struktur und ReaktivitÃ¤t der Alâ€O(H)â€Alâ€Einheiten in SiloxidgerÃ¼stverbindungen â€" Modellstudien in LÃ¶sung und in Isolation. Angewandte Chemie, 2019, 131, 912-917.	1.6	6
31	A Two-Dimensional â€˜Zigzagâ€™ Silica Polymorph on a Metal Support. Journal of the American Chemical Society, 2018, 140, 6164-6168.	6.6	14
32	Vanadium Oxide Oligomers and Ordered Monolayers Supported on CeO₂(111): Structure and Stability Studied by Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 9101-9110.	1.5	19
33	Kooperative Bildung einer langreichweitig geordneten Wasserschicht auf der Fe₃O₄(111)â€OberflÃche. Angewandte Chemie, 2018, 130, 1423-1428.	1.6	7
34	Chemically accurate adsorption energies for methane and ethane monolayers on the MgO(001) surface. Physical Chemistry Chemical Physics, 2018, 20, 9760-9769.	1.3	26
35	Surface Termination of Fe₃O₄(111) Films Studied by CO Adsorption Revisited. Journal of Physical Chemistry B, 2018, 122, 527-533.	1.2	46
36	Cooperative Formation of Longâ€Range Ordering in Water Adâ€layers on Fe₃O₄(111) Surfaces. Angewandte Chemie - International Edition, 2018, 57, 1409-1413.	7.2	59

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37	Ab Initio Prediction of Proton Exchange Barriers for Alkanes at BrÃ¸nsted Sites of Zeolite H-MFI. Journal of the American Chemical Society, 2018, 140, 18151-18161.	6.6	50
38	Hydrogen Spillover to Copper Clusters on Hydroxylated Î³-Al₂O₃. Journal of Physical Chemistry C, 2018, 122, 18445-18455.	1.5	44
39	Ab initio study of methanol and ethanol adsorption on BrÃ¸nsted sites in zeolite H-MFI. Physical Chemistry Chemical Physics, 2018, 20, 19964-19970.	1.3	29
40	Water adsorption on the Fe₃O₄(111) surface: dissociation and network formation. Physical Chemistry Chemical Physics, 2018, 20, 15764-15774.	1.3	26
41	Initial stages of CO₂ adsorption on CaO: a combined experimental and computational study. Physical Chemistry Chemical Physics, 2017, 19, 4231-4242.	1.3	47
42	Gasâ€Phase Vibrational Spectroscopy of the Aluminum Oxide Anions (Al₂O₃)_{1â€“6}AlO₂^{â¯}. ChemPhysChem, 2017, 18, 868-872.	1.0	16
43	Dissociative Water Adsorption by Al₃O₄⁺ in the Gas Phase. Journal of Physical Chemistry Letters, 2017, 8, 1272-1277.	2.1	38
44	Ab Initio Prediction of Adsorption Isotherms for Gas Mixtures by Grand Canonical Monte Carlo Simulations on a Lattice of Sites. Journal of Physical Chemistry Letters, 2017, 8, 2713-2718.	2.1	21
45	Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. Crystal Growth and Design, 2017, 17, 1636-1646.	1.4	18
46	O₂ Activation on Ceria Catalystsâ€”The Importance of Substrate Crystallographic Orientation. Angewandte Chemie - International Edition, 2017, 56, 16399-16404.	7.2	106
47	O₂â€Aktivierung an Cerdioxidâ€Katalysatoren â€“ Zur Bedeutung der kristallographischen Orientierung des Substrats. Angewandte Chemie, 2017, 129, 16618-16623.	1.6	21
48	Oxygen Scrambling of CO₂ Adsorbed on CaO(001). Journal of Physical Chemistry C, 2017, 121, 18625-18634.	1.5	12
49	Interactions of Water with the (111) and (100) Surfaces of Ceria. Journal of Physical Chemistry C, 2017, 121, 21571-21578.	1.5	33
50	Toward an Understanding of Selective Alkyne Hydrogenation on Ceria: On the Impact of O Vacancies on H₂ Interaction with CeO₂(111). Journal of the American Chemical Society, 2017, 139, 17608-17616.	6.6	120
51	Oxidative dehydrogenation of methanol at ceria-supported vanadia oligomers. Journal of Catalysis, 2017, 352, 382-387.	3.1	28
52	Ab Initio Adsorption Isotherms for Molecules with Lateral Interactions: CO₂ in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 12789-12799.	1.5	33
53	Gas phase structures and charge localization in small aluminum oxide anions: Infrared photodissociation spectroscopy and electronic structure calculations. Journal of Chemical Physics, 2016, 144, 244305.	1.2	13
54	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. Journal of Catalysis, 2016, 339, 242-255.	3.1	149

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55	BrÃ¸nsted activity of two-dimensional zeolites compared to bulk materials. Faraday Discussions, 2016, 188, 227-234.	1.6	30
56	Accurate adsorption energies for small molecules on oxide surfaces: CH₄/MgO(001) and C₂H₆/MgO(001). Journal of Computational Chemistry, 2016, 37, 2374-2385.	1.5	20
57	Water adsorption and O-defect formation on Fe₂O₃(0001) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 25560-25568.	1.3	91
58	Trapping Aluminum Hydroxide Clusters with Trisilanols during Speciation in Aluminum(III)â€“Water Systems: Reproducible, Large Scale Access to Molecular Aluminate Models. Angewandte Chemie - International Edition, 2016, 55, 12325-12329.	7.2	40
59	Trapping Aluminum Hydroxide Clusters with Trisilanols during Speciation in Aluminum(III)â€“Water Systems: Reproducible, Large Scale Access to Molecular Aluminate Models. Angewandte Chemie, 2016, 128, 12513-12517.	1.6	20
60	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 14047-14056.	6.6	62
61	Hydration Structures of MgO, CaO, and SrO (001) Surfaces. Journal of Physical Chemistry C, 2016, 120, 24762-24769.	1.5	21
62	Abâ€…Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie, 2016, 128, 5321-5323.	1.6	13
63	Abâ€…Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie - International Edition, 2016, 55, 5235-5237.	7.2	100
64	Designing new catalysts: synthesis of new active structures: general discussion. Faraday Discussions, 2016, 188, 131-159.	1.6	4
65	Catalyst design from theory to practice: general discussion. Faraday Discussions, 2016, 188, 279-307.	1.6	2
66	Bridging model and real catalysts: general discussion. Faraday Discussions, 2016, 188, 565-589.	1.6	3
67	Methanol adsorption on monocrystalline ceria surfaces. Journal of Catalysis, 2016, 336, 116-125.	3.1	34
68	CO adsorption on a silica bilayer supported on Ru(0001). Surface Science, 2016, 648, 2-9.	0.8	29
69	Electron stimulated hydroxylation of a metal supported silicate film. Physical Chemistry Chemical Physics, 2016, 18, 3755-3764.	1.3	33
70	Water Interaction with Iron Oxides. Angewandte Chemie - International Edition, 2015, 54, 13942-13946.	7.2	62
71	Accurate Adsorption Thermodynamics of Small Alkanes in Zeolites. Ab initio Theory and Experiment for H-Chabazite. Journal of Physical Chemistry C, 2015, 119, 6128-6137.	1.5	120
72	Water on the MgO(001) Surface: Surface Reconstruction and Ion Solvation. Journal of Physical Chemistry Letters, 2015, 6, 2310-2314.	2.1	34

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73	Ultrathin Ti-Silicate Film on a Ru(0001) Surface. Journal of Physical Chemistry C, 2015, 119, 15443-15448.	1.5	17
74	Surface Structure ofV2O3(0001)Revisited. Physical Review Letters, 2015, 114, 216101.	2.9	30
75	Quantum chemical ab initio prediction of proton exchange barriers between CH4 and different H-zeolites. Journal of Chemical Physics, 2015, 143, 102810.	1.2	38
76	Acidity of two-dimensional zeolites. Physical Chemistry Chemical Physics, 2015, 17, 27873-27882.	1.3	32
77	Regioselectivity of Alâ€“O Bond Hydrolysis during Zeolites Dealumination Unified by BrÃ¸nstedâ€“Evansâ€“Polanyi Relationship. ACS Catalysis, 2015, 5, 11-15.	5.5	73
78	Models in Catalysis. Catalysis Letters, 2015, 145, 109-125.	1.4	130
79	Sites for Methane Activation on Lithiumâ€Doped Magnesium Oxide Surfaces. Angewandte Chemie - International Edition, 2014, 53, 8774-8778.	7.2	152
80	The vibrational spectrum of FeO2+ isomersâ€”Theoretical benchmark and experiment. Journal of Chemical Physics, 2014, 140, 204315.	1.2	20
81	Ultrathin Silica Films: The Atomic Structure of Twoâ€Dimensional Crystals and Glasses. Chemistry - A European Journal, 2014, 20, 9176-9183.	1.7	51
82	Size-Dependent Catalytic Activity of Supported Vanadium Oxide Species: Oxidative Dehydrogenation of Propane. Journal of the American Chemical Society, 2014, 136, 7751-7761.	6.6	126
83	Structure and properties of bimetallic titanium and vanadium oxide clusters. Physical Chemistry Chemical Physics, 2014, 16, 8441.	1.3	13
84	Catalytic Performance of Vanadium MILâ€47 and Linkerâ€Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. ChemPlusChem, 2014, 79, 1183-1197.	1.3	20
85	Catalytically Active Vanadia Species on Silica: Effect of Oxygen and Water. Journal of Physical Chemistry C, 2014, 118, 29159-29163.	1.5	11
86	Support Effect in Oxide Catalysis: Methanol Oxidation on Vanadia/Ceria. Journal of the American Chemical Society, 2014, 136, 14616-14625.	6.6	101
87	Selective oxidation of propene by vanadium oxide monomers supported on silica. Journal of Catalysis, 2014, 317, 75-82.	3.1	45
88	Effect of Anharmonicity on Adsorption Thermodynamics. Journal of Chemical Theory and Computation, 2014, 10, 2479-2487.	2.3	101
89	Interaction of CO with Electron-Rich Defects on MgO(100). Journal of Physical Chemistry C, 2013, 117, 8365-8373.	1.5	9
90	Accurate adsorption energies of small molecules on oxide surfaces: COâ€“MgO(001). Physical Chemistry Chemical Physics, 2013, 15, 16481.	1.3	64

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91	Quantum Chemical Free Energies: Structure Optimization and Vibrational Frequencies in Normal Modes. Journal of Chemical Theory and Computation, 2013, 9, 5038-5045.	2.3	53
92	Titration of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Ce</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math> in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 687 Td (stretchy="false">)</mml:mo> 2061.	2.9	55
93	Adsorption, Activation, and Dissociation of Oxygen on Doped Oxides. Angewandte Chemie - International Edition, 2013, 52, 11385-11387.	7.2	76
94	Stability and migration barriers of small vanadium oxide clusters on the CeO2(111) surface studied by density functional theory. Faraday Discussions, 2013, 162, 233.	1.6	25
95	Interaction of Probe Molecules with Bridging Hydroxyls of Two-Dimensional Zeolites: A Surface Science Approach. Journal of Physical Chemistry C, 2013, 117, 13547-13556.	1.5	67
96	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. Chemical Reviews, 2013, 113, 3949-3985.	23.0	849
97	Introduction: Surface Chemistry of Oxides. Chemical Reviews, 2013, 113, 3859-3862.	23.0	47
98	Oligomeric Vanadium Oxide Species Supported on the CeO₂(111) Surface: Structure and Reactivity Studied by Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 5274-5285.	1.5	60
99	Atomic Structure of an Ultrathin Fe-Silicate Film Grown on a Metal: AÂMonolayer of Clay?. Journal of the American Chemical Society, 2013, 135, 19222-19228.	6.6	35
100	Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100). Physical Review Letters, 2013, 111, 045502.	2.9	104
101	Thermal Methane Activation by a Binary Vâ€“Nb Transitionâ€Metal Oxide Cluster Cation: A Further Example for the Crucial Role of Oxygenâ€Centered Radicals. Chemistry - A European Journal, 2013, 19, 11496-11501.	1.7	29
102	Structural variability in transition metal oxide clusters: gas phase vibrational spectroscopy of V3O6â€“8+. Physical Chemistry Chemical Physics, 2012, 14, 9377.	1.3	55
103	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. Journal of Chemical Physics, 2012, 137, 014701.	1.2	43
104	Partial oxidation of ethanol on vanadia catalysts on supporting oxides with different redox properties compared to propane. Journal of Catalysis, 2012, 296, 120-131.	3.1	138
105	Kinetic study of the reaction of vanadium and vanadiumâ€“titanium oxide cluster anions with SO2. Physical Chemistry Chemical Physics, 2012, 14, 14344.	1.3	28
106	Thin silica films on Ru(0001): monolayer, bilayer and three-dimensional networks of [SiO4] tetrahedra. Physical Chemistry Chemical Physics, 2012, 14, 11344.	1.3	106
107	Structure determination of neutral MgO clustersâ€”hexagonal nanotubes and cages. Physical Chemistry Chemical Physics, 2012, 14, 2849.	1.3	100
108	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metalâ€“Organic Frameworks: The Effect of Lateral Interactions for Methane/CPO-27-Mg. Journal of the American Chemical Society, 2012, 134, 18354-18365.	6.6	90

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109	Stabilizing Gold Adatoms by Thiophenyl Derivatives: A Possible Route toward Metal Redispersion. Journal of the American Chemical Society, 2012, 134, 11161-11167.	6.6	16
110	Fast atom diffraction during grazing scattering from a MgO(001) surface. Surface Science, 2012, 606, 161-173.	0.8	39
111	The structure of epitaxial V2O3 films and their surfaces: A medium energy ion scattering study. Surface Science, 2012, 606, 1716-1727.	0.8	16
112	Modeling Zeolites with Metalâ€Supported Twoâ€Dimensional Aluminosilicate Films. Angewandte Chemie - International Edition, 2012, 51, 6005-6008.	7.2	96
113	The Atomic Structure of a Metalâ€Supported Vitreous Thin Silica Film. Angewandte Chemie - International Edition, 2012, 51, 404-407.	7.2	207
114	Structures and vibrational spectroscopy of partially reduced gas-phase cerium oxide clusters. Physical Chemistry Chemical Physics, 2011, 13, 19393.	1.3	50
115	Adsorption and Diffusion of Fructose in Zeolite HZSM-5: Selection of Models and Methods for Computational Studies. Journal of Physical Chemistry C, 2011, 115, 21785-21790.	1.5	30
116	Interaction Between Gold Atoms and Thio-Aryl Ligands on the Au(111) Surface. Journal of Physical Chemistry C, 2011, 115, 24871-24879.	1.5	11
117	Structural Analysis of Silica-Supported Molybdena Based on X-ray Spectroscopy: Quantum Theory and Experiment. Journal of Physical Chemistry C, 2011, 115, 15449-15458.	1.5	28
118	Structures of the Ordered Water Monolayer on MgO(001). Journal of Physical Chemistry C, 2011, 115, 6764-6774.	1.5	88
119	Periodic Density Functional Theory Study of VO_n Species Supported on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2011, 115, 7399-7410.	1.5	61
120	Electron Distribution in Partially Reduced Mixed Metal Oxide Systems: Infrared Spectroscopy of Ce_mV_nO_o⁺ Gas-Phase Clusters. Journal of Physical Chemistry A, 2011, 115, 11187-11192.	1.1	42
121	Heats of Adsorption of CO and CO₂ in Metalâ€“Organic Frameworks: Quantum Mechanical Study of CPO-27-M (M = Mg, Ni, Zn). Journal of Physical Chemistry C, 2011, 115, 21777-21784.	1.5	122
122	Electron Localization in Defective Ceria Films: A Study with Scanning-Tunneling Microscopy and Density-Functional Theory. Physical Review Letters, 2011, 106, 246801.	2.9	158
123	Methanol Adsorption on V2O3(0001). Topics in Catalysis, 2011, 54, 669-684.	1.3	18
124	Structural Diversity and Flexibility of MgO Gasâ€Phase Clusters. Angewandte Chemie - International Edition, 2011, 50, 1716-1719.	7.2	67
125	Pyrazolateâ€Based Cobalt(II)â€Containing Metalâ€“Organic Frameworks in Heterogeneous Catalytic Oxidation Reactions: Elucidating the Role of Entatic States for Biomimetic Oxidation Processes. Chemistry - A European Journal, 2011, 17, 8671-8695.	1.7	138
126	Reactions of H₂, CH₄, C₂H₆, and C₃H₈ with [(MgO)_n]⁺ Clusters Studied by Density Functional Theory. ChemCatChem, 2010, 2, 819-826.	1.8	51

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127	Activation of Câ€“H bonds mediated by Moî€,Mo moieties in heterobimetallic Zn/O/Moclusters. Dalton Transactions, 2010, 39, 103-106.	1.6	19
128	Modeling environmental effects on charge density distributions in polar organometallics: Validation of embedded cluster models for the methyl lithium crystal. Journal of Computational Chemistry, 2010, 31, 2568-2576.	1.5	12
129	Preferential Activation of Primary Cï£¿H Bonds in the Reactions of Small Alkanes with the Diatomic MgO^{+.} Cation. Chemistry - A European Journal, 2010, 16, 4110-4119.	1.7	38
130	The tertâ€‹Butyl Cation in Hâ€Zeolites: Deprotonation to Isobutene and Conversion into Surface Alkoxides. Angewandte Chemie - International Edition, 2010, 49, 4678-4680.	7.2	97
131	Infrared spectroscopic characterization of the oxidative dehydrogenation of propane by V4O10+. International Journal of Mass Spectrometry, 2010, 297, 102-106.	0.7	29
132	Imaging of individual adatoms on oxide surfaces by dynamic force microscopy. Physical Review B, 2010, 81, .	1.1	4
133	Growth and Structure of Crystalline Silica Sheet on Ru(0001). Physical Review Letters, 2010, 105, 146104.	2.9	198
134	Thickness-Dependent Hydroxylation of MgO(001) Thin Films. Journal of Physical Chemistry C, 2010, 114, 18207-18214.	1.5	57
135	Role of Ceria in Oxidative Dehydrogenation on Supported Vanadia Catalysts. Journal of the American Chemical Society, 2010, 132, 2345-2349.	6.6	191
136	Vanadia Aggregates on an Ultrathin Aluminum Oxide Film on NiAl(110). Journal of Physical Chemistry C, 2010, 114, 4983-4994.	1.5	20
137	Oxidation of Methanol to Formaldehyde on Silica-Supported Molybdena: Density Functional Theory Study on Models of Mononuclear Sites. Journal of Physical Chemistry C, 2010, 114, 2967-2979.	1.5	38
138	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
139	Accurate quantum chemical energies for the interaction of hydrocarbons with oxide surfaces: CH4/MgO(001). Physical Chemistry Chemical Physics, 2010, 12, 14330.	1.3	122
140	Density-Functional Calculations of the Structure of Near-Surface Oxygen Vacancies and Electron Localization on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 207 Td (stretchy="false">)</mm	2.9	501
141	The [(Al₂O₃)₂]^{â˜’} Anion Cluster: Electron Localizationâ€“Delocalization Isomerism. ChemPhysChem, 2009, 10, 2410-2413.	1.0	27
142	Formaldehyde Formation on Vanadium Oxide Surfaces V₂O₃(0001) and V₂O₅(001): How does the Stable Methoxy Intermediate Form?. Angewandte Chemie - International Edition, 2009, 48, 3695-3698.	7.2	70
143	Resolving the Atomic Structure of Vanadia Monolayer Catalysts: Monomers, Trimers, and Oligomers on Ceria. Angewandte Chemie - International Edition, 2009, 48, 8006-8009.	7.2	138
144	Vanadium Oxides Supported on a Thin Silica Film Grown on Mo(112): Insights from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 8336-8342.	1.5	17

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145	Quantum Chemical Modeling of Zeolite-Catalyzed Methylation Reactions: Toward Chemical Accuracy for Barriers. Journal of the American Chemical Society, 2009, 131, 816-825.	6.6	288
146	Vanadia and Water Coadsorption on Tetragonal Zirconia Surfaces. Journal of Physical Chemistry C, 2009, 113, 18191-18203.	1.5	17
147	Oxidative Dehydrogenation of Hydrocarbons by V3O7+ Compared to Other Vanadium Oxide Species. Journal of Physical Chemistry A, 2009, 113, 11586-11594.	1.1	55
148	Aluminium siting in the ZSM-5 framework by combination of high resolution 27Al NMR and DFT/MM calculations. Physical Chemistry Chemical Physics, 2009, 11, 1237-1247.	1.3	196
149	Point defects in CaF2 and CeO2 investigated by the periodic electrostatic embedded cluster method. Journal of Chemical Physics, 2009, 130, 174710.	1.2	88
150	Ab Initio Study of Hydrogen Adsorption in MOF-5. Journal of the American Chemical Society, 2009, 131, 4143-4150.	6.6	225
151	Protonation of water clusters in the cavities of acidic zeolites: (H2O)nÂ·H-chabazite, n = 1â€“4. Physical Chemistry Chemical Physics, 2009, 11, 1702.	1.3	64
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