Joachim Sauer

List of Publications by Year
in descending order

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	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. Surface Science Reports, 2007, 62, 219-270.	3.8	1,102
2	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. Chemical Reviews, 2013, 113, 3949-3985.	23.0	849
3	Molecular models in ab initio studies of solids and surfaces: from ionic crystals and semiconductors to catalysts. Chemical Reviews, 1989, 89, 199-255.	23.0	726
4	Theoretical Study of van der Waals Complexes at Surface Sites in Comparison with the Experiment. Chemical Reviews, 1994, 94, 2095-2160.	23.0	704
5	Hybrid functionals applied to rare-earth oxides: The example of ceria. Physical Review B, 2007, 75, .	1.1	502
6	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 50 527 Td (stretchy="false">)</mm	2.9	501
7	Bridging hydrodyl groups in zeolitic catalysts: a computer simulation of their structure, vibrational properties and acidity in protonated faujasites (Hî—‚Y zeolites). Chemical Physics Letters, 1992, 188, 320-325.	1.2	370
8	Acidity Differences between Inorganic Solids Induced by Their Framework Structure. A Combined Quantum Mechanics/Molecular Mechanics ab Initio Study on Zeolites. Journal of the American Chemical Society, 1998, 120, 1556-1570.	6.6	359
9	Molecular mechanics potential for silica and zeolite catalysts based on ab initio calculations. 1. Dense and microporous silica. The Journal of Physical Chemistry, 1994, 98, 1238-1244.	2.9	317
10	Application of semiempirical longâ€rrange dispersion corrections to periodic systems in density functional theory. Journal of Computational Chemistry, 2008, 29, 2088-2097.	1.5	294
11	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
12	Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting. Science, 2021, 374, 454-459.	6.0	281
13	23Na NMR Spectroscopy of Solids: Interpretation of Quadrupole Interaction Parameters and Chemical Shifts. The Journal of Physical Chemistry, 1994, 98, 1544-1551.	2.9	277
14	Interaction of methanol with Broensted acid sites of zeolite catalysts: an ab initio study. Journal of the American Chemical Society, 1995, 117, 3780-3789.	6.6	267
15	Vibrational spectra of alumina- and silica-supported vanadia revisited: An experimental and theoretical model catalyst study. Journal of Catalysis, 2004, 226, 88-100.	3.1	258
16	Thermal Activation of Methane by Tetranuclear [V4O10]+. Angewandte Chemie - International Edition, 2006, 45, 4681-4685.	7.2	236
17	Aluminum Siting in Siliconâ€Rich Zeolite Frameworks: A Combined Highâ€Resolution ²⁷Alâ€…NMR Spectroscopy and Quantum Mechanicsâ€‰/â€‰Molecular Mechanics Study of ZSMâ€5. Angewandte Chemie - International Edition, 2007, 46, 7286-7289.	7.2	234
18	Treating dispersion effects in extended systems by hybrid MP2:DFT calculationsâ€”protonation of isobutene in zeolite ferrierite. Physical Chemistry Chemical Physics, 2006, 8, 3955-3965.	1.3	232

#	Article	IF	Citations
19	Predicting Absolute and Site Specific Acidities for Zeolite Catalysts by a Combined Quantum Mechanics/Interatomic Potential Function Approachâ€. Journal of Physical Chemistry B, 1997, 101, 10035-10050.	1.2	227
20	Ab Initio Study of Hydrogen Adsorption in MOF-5. Journal of the American Chemical Society, 2009, 131, 4143-4150.	6.6	225
21	Combining quantum mechanics and interatomic potential functions inab initio studies of extended systems. Journal of Computational Chemistry, 2000, 21, 1470-1493.	1.5	221
22	Coordination and siting of Cu+ ions in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 1999, 1, 2019-2026.	1.3	215
23	The Atomic Structure of a Metalâ€Supported Vitreous Thin Silica Film. Angewandte Chemie - International Edition, 2012, 51, 404-407.	7.2	207
24	Molecular Mechanics Potential for Silica and Zeolite Catalysts Based on ab Initio Calculations. 2. Aluminosilicates. The Journal of Physical Chemistry, 1995, 99, 9536-9550.	2.9	203
25	Structure and reactivity of silica and zeolite catalysts by a combined quantum mechanics[ndash]shell-model potential approach based on DFT. Faraday Discussions, 1997, 106, 41-62.	1.6	203
26	Growth and Structure of Crystalline Silica Sheet on Ru(0001). Physical Review Letters, 2010, 105, 146104.	2.9	198
27	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
28	Massâ€selective vibrational spectroscopy of vanadium oxide cluster ions. Mass Spectrometry Reviews, 2007, 26, 542-562.	2.8	192
29	Role of Ceria in Oxidative Dehydrogenation on Supported Vanadia Catalysts. Journal of the American Chemical Society, 2010, 132, 2345-2349.	6.6	191
30	Oxidation of Methanol to Formaldehyde on Supported Vanadium Oxide Catalysts Compared to Gas Phase Molecules. Journal of the American Chemical Society, 2005, 127, 10861-10868.	6.6	187
31	Interaction of Water with BrÃ¸nsted Acidic Sites of Zeolite Catalysts. Ab Initio Study of 1:1 and 2:1 Surface Complexes. The Journal of Physical Chemistry, 1996, 100, 6199-6211.	2.9	183
32	Activation of Methane by Oligomeric (Al₂O₃)_x⁺ (x=3,4,5): The Role of Oxygenâ€Centered Radicals in Thermal Hydrogenâ€Atom Abstraction. Angewandte Chemie - International Edition, 2008, 47, 1946-1950.	7.2	183
33	Combiningab initio techniques with analytical potential functions for structure predictions of large systems: Method and application to crystalline silica polymorphs. Journal of Computational Chemistry, 1997, 18, 463-477.	1.5	181
34	Oxidative Dehydrogenation of Propane by Monomeric Vanadium Oxide Sites on Silica Support. Journal of Physical Chemistry C, 2007, 111, 6041-6050.	1.5	171
35	The Surface Structure of Sulfated Zirconia:â€‰ Periodic ab Initio Study of Sulfuric Acid Adsorbed on ZrO2(101) and ZrO2(001). Journal of the American Chemical Society, 1998, 120, 13503-13512.	6.6	168
36	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

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37	Sites for Methane Activation on Lithiumâ€Doped Magnesium Oxide Surfaces. Angewandte Chemie - International Edition, 2014, 53, 8774-8778.	7.2	152
38	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. Journal of Catalysis, 2016, 339, 242-255.	3.1	149
39	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
40	Finding transition structures in extended systems: A strategy based on a combined quantum mechanicsâ€“empirical valence bond approach. Journal of Chemical Physics, 2000, 112, 6983-6996.	1.2	142
41	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
42	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
43	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
44	Potential Functions for Silica and Zeolite Catalysts Based on ab Initio Calculations. 3. A Shell Model Ion Pair Potential for Silica and Aluminosilicatesâ€. The Journal of Physical Chemistry, 1996, 100, 11043-11049.	2.9	135
45	(V2O5)n Gas-Phase Clusters (n = 1â^'12) Compared to V2O5 Crystal:â€‰ DFT Calculations. Journal of Physical Chemistry A, 2001, 105, 8588-8598.	1.1	135
46	Siting of Al and bridging hydroxyl groups in ZSM-5: A computer simulation study. Zeolites, 1992, 12, 20-23.	0.9	132
47	Proton Mobility in Chabazite, Faujasite, and ZSM-5 Zeolite Catalysts. Comparison Based on ab Initio Calculations. Journal of Physical Chemistry B, 2001, 105, 1603-1613.	1.2	132
48	Models in Catalysis. Catalysis Letters, 2015, 145, 109-125.	1.4	130
49	A High-Resolution17O and29Si NMR Study of Zeolite Siliceous Ferrierite and ab Initio Calculations of NMR Parameters. Journal of the American Chemical Society, 2000, 122, 4948-4958.	6.6	129
50	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
51	A hybrid MP2/planewave-DFT scheme for large chemical systems: proton jumps in zeolites. Chemical Physics Letters, 2004, 387, 388-394.	1.2	125
52	Proton NMR chemical shift and intrinsic acidity of hydroxyl groups. Ab initio calculations on catalytically active sites and gas-phase molecules. Journal of the American Chemical Society, 1993, 115, 7833-7838.	6.6	124
53	Coordination, Structure, and Vibrational Spectra of Titanium in Silicates and Zeolites in Comparison with Related Molecules. An ab Initio Study. The Journal of Physical Chemistry, 1996, 100, 5025-5034.	2.9	123
54	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

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55	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
56	Effect of Alâ^'Siâ^'Al and Alâ^'Siâ^'Siâ^'Al Pairs in the ZSM-5 Zeolite Framework on the ²⁷Al NMR Spectra. A Combined High-Resolution ²⁷Al NMR and DFT/MM Study. Journal of Physical Chemistry C, 2009, 113, 1447-1458.	1.5	121
57	Computational Elucidation of the Transition State Shape Selectivity Phenomenon. Journal of the American Chemical Society, 2004, 126, 936-947.	6.6	120
58	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
59	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
60	Structure and reactivity of V2O5: bulk solid, nanosized clusters, species supported on silica and alumina, cluster cations and anions. Dalton Transactions, 2004, , 3116-3121.	1.6	119
61	The infrared spectrum of the Oâ‹¯Hâ‹¯O fragment of H[sub 5]O[sub 2][sup +]: Ab initio classical molecular dynamics and quantum 4D model calculations. Journal of Chemical Physics, 2001, 114, 240.	1.2	118
62	Polyhedral Vanadium Oxide Cages: Infrared Spectra of Cluster Anions and Size-Induced d Electron Localization. Angewandte Chemie - International Edition, 2005, 44, 3122-3125.	7.2	116
63	Surface Metal-Insulator Transition on a Vanadium Pentoxide (001) Single Crystal. Physical Review Letters, 2007, 99, 226103.	2.9	113
64	Unexpected Structures of Aluminum Oxide Clusters in the Gas Phase. Angewandte Chemie - International Edition, 2007, 46, 3372-3375.	7.2	113
65	Acidic sites in heterogeneous catalysis: structure, properties and activity. Journal of Molecular Catalysis, 1989, 54, 312-323.	1.2	112
66	Gas-Phase Vanadium Oxide Anions:Â Structure and Detachment Energies from Density Functional Calculations. Journal of Physical Chemistry A, 2000, 104, 10913-10922.	1.1	110
67	Gas phase infrared spectroscopy of mono- and divanadium oxide cluster cations. Journal of Chemical Physics, 2004, 120, 6461-6470.	1.2	110
68	Gas-Phase Oxidation of Propane and 1-Butene with [V3O7]+: Experiment and Theory in Concert. Angewandte Chemie - International Edition, 2006, 45, 4677-4681.	7.2	110
69	Coordination of Cu+Ions to Zeolite Frameworks Strongly Enhances Their Ability To Bind NO2. An ab Initio Density Functional Study. Journal of the American Chemical Society, 1998, 120, 1545-1551.	6.6	109
70	Protonated Isobutene in Zeolites:tert-Butyl Cation or Alkoxide?. Angewandte Chemie - International Edition, 2005, 44, 4769-4771.	7.2	109
71	Probing the Electronic Structure of Early Transition-Metal Oxide Clusters:â€‰ Polyhedral Cages of (V₂O₅)_n⁻ (n = 2â^'4) and (M₂O₅)₂⁻ (M = Nb, Ta). Journal of the American Chemical Society, 2007, 129, 13270-13276.	6.6	109
72	Molecular structure of orthosilicic acid, silanol, and H3SiOH.cntdot.AlH3 complex: models of surface hydroxyls in silica and zeolites. The Journal of Physical Chemistry, 1987, 91, 2315-2319.	2.9	108

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73	1H NMR Chemical Shifts of Ammonia, Methanol, and Water Molecules Interacting with Broensted Acid Sites of Zeolite Catalysts: Ab-Initio Calculations. The Journal of Physical Chemistry, 1994, 98, 3083-3085.	2.9	108
74	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
75	O₂ Activation on Ceria Catalystsâ€"The Importance of Substrate Crystallographic Orientation. Angewandte Chemie - International Edition, 2017, 56, 16399-16404.	7.2	106
76	Heterogeneity of BrÃ¸nsted Acidic Sites in Faujasite Type Zeolites due to Aluminum Content and Framework Structure. Journal of Physical Chemistry B, 1998, 102, 6397-6404.	1.2	105
77	Coordination of Cu+ and Cu2+ ions in ZSM-5 in the vicinity of two framework Al atoms. Physical Chemistry Chemical Physics, 2001, 3, 1552-1559.	1.3	104
78	Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100). Physical Review Letters, 2013, 111, 045502.	2.9	104
79	Support Effect in Oxide Catalysis: Methanol Oxidation on Vanadia/Ceria. Journal of the American Chemical Society, 2014, 136, 14616-14625.	6.6	101
80	Effect of Anharmonicity on Adsorption Thermodynamics. Journal of Chemical Theory and Computation, 2014, 10, 2479-2487.	2.3	101
81	Ab initio molecular dynamics simulation of methanol adsorbed in chabazite. Chemical Physics Letters, 1997, 266, 397-402.	1.2	100
82	Structure determination of neutral MgO clustersâ€"hexagonal nanotubes and cages. Physical Chemistry Chemical Physics, 2012, 14, 2849.	1.3	100
83	Abâ€...Initio Calculation of Rate Constants for Moleculeâ€"Surface Reactions with Chemical Accuracy. Angewandte Chemie - International Edition, 2016, 55, 5235-5237.	7.2	100
84	Water in Interaction with Acid Sites in H-ZSM-5 Zeolite Does Not Form Hydroxonium Ions. A Comparison between Neutron Scattering Results and ab Initio Calculations. The Journal of Physical Chemistry, 1996, 100, 19545-19550.	2.9	99
85	A High-Resolution17O NMR Study of Siliceous Zeolite Faujasite. Journal of the American Chemical Society, 1998, 120, 3510-3511.	6.6	97
86	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
87	Adsorption of NH3and H2O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. Journal of Physical Chemistry B, 2005, 109, 3539-3545.	1.2	96
88	Modeling Zeolites with Metalâ€Supported Twoâ€Dimensional Aluminosilicate Films. Angewandte Chemie - International Edition, 2012, 51, 6005-6008.	7.2	96
89	Stable Mechanistically-Relevant Aromatic-Based Carbenium Ions in Zeolite Catalysts. Journal of the American Chemical Society, 2003, 125, 2136-2141.	6.6	95
90	Stabilities of C3â€"C5 alkoxide species inside H-FER zeolite: a hybrid QM/MM study. Journal of Catalysis, 2005, 231, 393-404.	3.1	91

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91	Water adsorption and O-defect formation on Fe₂O₃(0001) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 25560-25568.	1.3	91
92	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
93	Oxidative dehydrogenation of propane: Differences between N2O and O2 in the reoxidation of reduced vanadia sites and consequences for selectivity. Journal of Catalysis, 2008, 256, 84-94.	3.1	88
94	Point defects in CaF2 and CeO2 investigated by the periodic electrostatic embedded cluster method. Journal of Chemical Physics, 2009, 130, 174710.	1.2	88
95	Structures of the Ordered Water Monolayer on MgO(001). Journal of Physical Chemistry C, 2011, 115, 6764-6774.	1.5	88
96	29Si NMR Chemical Shifts of Silicate Species:Â Ab Initio Study of Environment and Structure Effects. Journal of the American Chemical Society, 1996, 118, 13015-13020.	6.6	87
97	Understanding the Nature of Water Bound to Solid Acid Surfaces. Ab Initio Simulation on HSAPO-34. Journal of the American Chemical Society, 1998, 120, 8512-8516.	6.6	87
98	Coordination Change of Cu+ Sites in ZSM-5 on Excitation in the Triplet State:â€‰ Understanding of the Photoluminescence Spectra. Journal of Physical Chemistry B, 2000, 104, 1738-1745.	1.2	87
99	Nature of the Cu+âˆ’NO Bond in the Gas Phase and at Different Types of Cu+Sites in Zeolite Catalysts. Journal of Physical Chemistry B, 2004, 108, 13674-13682.	1.2	86
100	Oxidative Activation ofn-Butane on Sulfated Zirconia. Journal of the American Chemical Society, 2005, 127, 16159-16166.	6.6	86
101	The effect of hydration on structure and location of Ti-sites in Ti-silicalite catalysts. A computational study. Physical Chemistry Chemical Physics, 2000, 2, 2195-2204.	1.3	85
102	Surface Structure of Hydroxylated and Sulfated Zirconia. A Periodic Density-Functional Studyâ€. Journal of Physical Chemistry B, 2004, 108, 14652-14662.	1.2	82
103	Gas phase vibrational spectroscopy of mass-selected vanadium oxide anions. Physical Chemistry Chemical Physics, 2008, 10, 3992.	1.3	81
104	Vanadium oxide surfaces and supported vanadium oxide nanoparticles. Topics in Catalysis, 2006, 38, 117-125.	1.3	80
105	Ab initio molecular dynamics simulation of methanol interacting with acidic zeolites of different framework structure. Microporous and Mesoporous Materials, 2000, 35-36, 379-385.	2.2	77
106	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. Physical Review B, 2004, 69, .	1.1	76
107	Adsorption, Activation, and Dissociation of Oxygen on Doped Oxides. Angewandte Chemie - International Edition, 2013, 52, 11385-11387.	7.2	76
108	Degradation of Ionized OV(OCH3)3in the Gas Phase. From the Neutral Compound All the Way down to the Quasi-terminal Fragments VO+and VOH+â€. Inorganic Chemistry, 2006, 45, 6235-6245.	1.9	75

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109	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
110	Bonding ability of surface sites on silica and their effect on hydrogen bonds. A quantum-chemical and statistical thermodynamic treatment. The Journal of Physical Chemistry, 1981, 85, 4061-4067.	2.9	72
111	A comparison between plane wave and Gaussian-type orbital basis sets for hydrogen bonded systems: Formic acid as a test case. Journal of Chemical Physics, 2007, 127, 154102.	1.2	72
112	Minimal basis set MINI-1 ? powerful tool for calculating of molecular interactions. I. Neutral complexes. Theoretica Chimica Acta, 1984, 65, 279-290.	0.9	71
113	Translational proton motion in zeolite H-ZSM-5. Energy barriers and jump rates from DFT calculations. Physical Chemistry Chemical Physics, 2002, 4, 5207-5216.	1.3	71
114	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
115	Ab Initio Calculations for Moleculeâ€“Surface Interactions with Chemical Accuracy. Accounts of Chemical Research, 2019, 52, 3502-3510.	7.6	70
116	The acidity of surface silanol groups. A theoretical estimate based on ab initio calculations on a model surface. Chemical Physics Letters, 1994, 218, 333-337.	1.2	69
117	Formation of hydronium ions on BrÃ¸nsted sites in zeolitic catalysts: a quantum-chemical ab initio study. Chemical Physics Letters, 1990, 173, 26-32.	1.2	68
118	Gas-Phase Infrared Spectrum of the Protonated Water Dimer: Molecular Dynamics Simulation and Accuracy of the Potential Energy Surface. ChemPhysChem, 2005, 6, 1706-1710.	1.0	68
119	Gas phase acidities and molecular geometries of H3SiOH, H3COH, and H2O. Journal of Chemical Physics, 1990, 93, 2575-2583.	1.2	67
120	Structural Diversity and Flexibility of MgO Gasâ€Phase Clusters. Angewandte Chemie - International Edition, 2011, 50, 1716-1719.	7.2	67
121	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
122	Comparison of a combined quantum mechanics/interatomic potential function approach with its periodic quantum-mechanical limit: Proton siting and ammonia adsorption in zeolite chabazite. Journal of Chemical Physics, 1998, 109, 10379-10389.	1.2	66
123	BrÃ¸nsted sites in zeolitic catalysts. An ab initio study of local geometries and of the barrier for proton jumps between neighbouring sites. Chemical Physics Letters, 1989, 164, 193-198.	1.2	64
124	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
125	Accurate adsorption energies of small molecules on oxide surfaces: COâ€“MgO(001). Physical Chemistry Chemical Physics, 2013, 15, 16481.	1.3	64
126	The vibrational frequency of the donor OH group in the H-bonded dimers of water, methanol and silanol. Ab initio calculations including anharmonicities. Chemical Physics Letters, 1995, 238, 243-252.	1.2	63

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127	Quantum chemical studies on zeolites and silica. International Journal of Quantum Chemistry, 1984, 26, 793-822.	1.0	62
128	Water Interaction with Iron Oxides. Angewandte Chemie - International Edition, 2015, 54, 13942-13946.	7.2	62
129	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
130	Quantum chemical investigation of interaction sites in zeolites and silica. The Journal of Physical Chemistry, 1980, 84, 3318-3326.	2.9	61
131	Formation of the cerium orthovanadateCeVO4:DFT+Ustudy. Physical Review B, 2007, 76, .	1.1	61
132	Oxidative conversion of C1â€“C3 alkanes by vanadium oxide catalysts. DFT results and their accuracy. International Journal of Quantum Chemistry, 2008, 108, 2223-2229.	1.0	61
133	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
134	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
135	Preferred stability of aluminum-oxygen-silicon-oxygen-aluminum linkages in high-silica zeolite catalysts: theoretical predictions contrary to Dempsey's rule. The Journal of Physical Chemistry, 1993, 97, 6579-6581.	2.9	59
136	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
137	Combining ab initio techniques with analytical potential functions. A study of zeolite-adsorbate interactions for NH3 on H-faujasite. Journal of Molecular Catalysis A, 1997, 119, 19-33.	4.8	57
138	Isomorphous Substitution in Bimetallic Oxide Clusters. Physical Review Letters, 2006, 96, 233401.	2.9	57
139	Thickness-Dependent Hydroxylation of MgO(001) Thin Films. Journal of Physical Chemistry C, 2010, 114, 18207-18214.	1.5	57
140	The minimal basis set MINI-1?powerful tool for calculating intermolecular interactions. II. Ionic complexes. Theoretica Chimica Acta, 1984, 65, 291-302.	0.9	56
141	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
142	Physisorption and Chemisorption of Hydrocarbons in H-FAU Using QM-Pot(MP2//B3LYP) Calculations. Journal of Physical Chemistry C, 2008, 112, 11796-11812.	1.5	55
143	Oxidative Dehydrogenation of Hydrocarbons by V3O7+ Compared to Other Vanadium Oxide Species. Journal of Physical Chemistry A, 2009, 113, 11586-11594.	1.1	55
144	Structural variability in transition metal oxide clusters: gas phase vibrational spectroscopy of V3O6â€“8+. Physical Chemistry Chemical Physics, 2012, 14, 9377.	1.3	55

#	Article	IF	Citations
145	[illegible] 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></mm 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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 727 Td (stretchy="fa 2061	2.9	55
146	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. Topics in Catalysis, 2008, 50, 106-115.	1.3	53
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