Joachim Sauer

List of Publications by Year
in descending order

351 papers	26,550 citations	4103 90 h-index	9865 146 g-index
389 all docs	389 docs citations	389 times ranked	16712 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
152	Vibrations of Silica Supported Vanadia: Variation with Particle Size and Local Surface Structure. Journal of Physical Chemistry C, 2009, 113, 12454-12464.	1.5	34
153	Partial oxidation of methanol on well-ordered V2O5(001)/Au(111) thin films. Physical Chemistry Chemical Physics, 2009, 11, 3290.	1.3	44
154	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
155	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. Topics in Catalysis, 2008, 50, 106-115.	1.3	53
156	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
157	Application of semiempirical longâ€range dispersion corrections to periodic systems in density functional theory. Journal of Computational Chemistry, 2008, 29, 2088-2097.	1.5	294
158	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
159	Formation of one-dimensional molybdenum oxide on Mo(112). Surface Science, 2008, 602, 3338-3342.	0.8	23
160	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
161	Aluminum siting in the framework of silicon rich zeolites. A ZSM-5 study. Studies in Surface Science and Catalysis, 2008, , 781-786.	1.5	4
162	V2O5/SiO2surface inspired, silsesquioxane-derived oxovanadium complexes and their properties. Dalton Transactions, 2008, , 326-331.	1.6	26

#	Article	IF	Citations
163	Gas phase vibrational spectroscopy of mass-selected vanadium oxide anions. Physical Chemistry Chemical Physics, 2008, 10, 3992.	1.3	81
164	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
165	Identification of Conical Structures in Small Aluminum Oxide Clusters: Infrared Spectroscopy of (Al₂O₃)_{1â^'4}(AlO)⁺. Journal of the American Chemical Society, 2008, 130, 15143-15149.	6.6	51
166	Local geometry of AlO4â^' and SiO4 tetrahedra in the silicone rich chabazite. A combined high resolution NMR and QM/MM study. Studies in Surface Science and Catalysis, 2008, , 729-732.	1.5	0
167	Nonuniform temperature dependence of the reactivity of disordered VOx/Î²-Al2O3(001) surfaces: A density functional theory based Monte Carlo study. Journal of Chemical Physics, 2008, 129, 224710.	1.2	5
168	Aluminum Siting in the ZSM-22 and Theta-1 Zeolites Revisited: A QM/MM Study. Collection of Czechoslovak Chemical Communications, 2008, 73, 909-920.	1.0	26
169	Oxygen adsorption on Mo(112) surface studied by ab initio genetic algorithm and experiment. Journal of Chemical Physics, 2007, 126, 234710.	1.2	37
170	Surface Metal-Insulator Transition on a Vanadium Pentoxide (001) Single Crystal. Physical Review Letters, 2007, 99, 226103.	2.9	113
171	Hybrid functionals applied to rare-earth oxides: The example of ceria. Physical Review B, 2007, 75, .	1.1	502
172	Theoretical studies of Cu(i) sites in faujasite and their interaction with carbon monoxide. Physical Chemistry Chemical Physics, 2007, 9, 5446.	1.3	37
173	Activation and isomerization of n-butane on sulfated zirconia model systemsâ€"an integrated study across the materials and pressure gaps. Physical Chemistry Chemical Physics, 2007, 9, 3600-3618.	1.3	25
174	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
175	Oxidative Dehydrogenation of Propane by Monomeric Vanadium Oxide Sites on Silica Support. Journal of Physical Chemistry C, 2007, 111, 6041-6050.	1.5	171
176	Applications of Quantum Chemical Methods in Zeolite Science. Studies in Surface Science and Catalysis, 2007, , 701-XXI.	1.5	16
177	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable Î²-Al2O3(001) Compared to Î±-Al2O3(0001). Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
178	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
179	Structure and Reactivity of Solid Catalysts â€" Quantum Chemical Approach. Studies in Surface Science and Catalysis, 2007, , 19-26.	1.5	2
180	Unexpected Structures of Aluminum Oxide Clusters in the Gas Phase. Angewandte Chemie - International Edition, 2007, 46, 3372-3375.	7.2	113

#	Article	IF	Citations
181	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
182	Gasâ€Phase Infrared Photodissociation Spectroscopy of Tetravanadiumoxo and Oxoâ€“Methoxo Cluster Anions. ChemPhysChem, 2007, 8, 1640-1647.	1.0	27
183	Massâ€selective vibrational spectroscopy of vanadium oxide cluster ions. Mass Spectrometry Reviews, 2007, 26, 542-562.	2.8	192
184	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
185	On the geometrical and electronic structure of an ultra-thin crystalline silica film grown on Mo(112). Surface Science, 2007, 601, 4849-4861.	0.8	48
186	Formation of the cerium orthovanadateCeVO4:DFT+Ustudy. Physical Review B, 2007, 76, .	1.1	61
187	Chapter 25. Zeolite Modelling: Active Sites in Different Framework Structures and in Different Crystallographic Positions. , 2007, , 441-456.		1
188	Isomorphous Substitution in Bimetallic Oxide Clusters. Physical Review Letters, 2006, 96, 233401.	2.9	57
189	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
190	Interaction of SO3 with c-ZrO2(111) films on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 1593.	1.3	12
191	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
192	Interplay between theory and experiment in the quest for silica with reduced dimensionality grown on a Mo(112) surface. Chemical Physics Letters, 2006, 424, 115-119.	1.2	27
193	Formation of one-dimensional crystalline silica on a metal substrate. Surface Science, 2006, 600, L164-L168.	0.8	19
194	Vanadium oxide surfaces and supported vanadium oxide nanoparticles. Topics in Catalysis, 2006, 38, 117-125.	1.3	80
195	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
196	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
197	Thermal Activation of Methane by Tetranuclear [V4O10]+. Angewandte Chemie - International Edition, 2006, 45, 4681-4685.	7.2	236
198	Synthesis and Structure of Ultrathin Aluminosilicate Films. Angewandte Chemie - International Edition, 2006, 45, 7636-7639.	7.2	45

#	Article	IF	Citations
199	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
200	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
201	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
202	Protonated Isobutene in Zeolites:tert-Butyl Cation or Alkoxide?. Angewandte Chemie - International Edition, 2005, 44, 4769-4771.	7.2	109
203	Environmental Effects on Vibrational Proton Dynamics in H5O2+: DFT Study on Crystalline H5O2+ClO4-. ChemInform, 2005, 36, no.	0.1	0
204	Environmental effects on vibrational proton dynamics in H5O2+: DFT study on crystalline H5O2+ClO4â^'. Physical Chemistry Chemical Physics, 2005, 7, 258-263.	1.3	51
205	Reduction of the (001) Surface of Î³-V2O5Compared to Î±-V2O5. Journal of Physical Chemistry B, 2005, 109, 374-380.	1.2	19
206	Vanadium Oxides on Aluminum Oxide Supports. 2. Structure, Vibrational Properties, and Reducibility of V2O5 Clusters on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23532-23542.	1.2	27
207	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23523-23531.	1.2	42
208	Oxidative Activation ofn-Butane on Sulfated Zirconia. Journal of the American Chemical Society, 2005, 127, 16159-16166.	6.6	86
209	Crystal Structure and Vibrational Spectra of AlVO4. A DFT Study. Journal of Physical Chemistry B, 2005, 109, 394-400.	1.2	39
210	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
211	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
212	Hybrid Quantum Mechanics/ Molecular Mechanics Methods and their Application. , 2005, , 241-258.		8
213	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. Physical Review B, 2004, 69, .	1.1	76
214	Gas phase infrared spectroscopy of mono- and divanadium oxide cluster cations. Journal of Chemical Physics, 2004, 120, 6461-6470.	1.2	110
215	Electronic ground states of the V2O4+/0/â^' species from multireference correlation and density functional studies. Journal of Chemical Physics, 2004, 120, 4207-4215.	1.2	47
216	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

#	Article	IF	Citations
217	Catalytic dehydrogenation of ethane over mononuclear Cr(III) surface sites on silica. part I. Câ€”H activation by Ïƒâ€bond metathesis. Journal of Physical Organic Chemistry, 2004, 17, 990-1006.	0.9	44
218	A hybrid MP2/planewave-DFT scheme for large chemical systems: proton jumps in zeolites. Chemical Physics Letters, 2004, 387, 388-394.	1.2	125
219	Methane activation by silica-supported Zr(iv) hydrides: the dihydride [(î€,SiO)2ZrH2] is much faster than the monohydride [(î€,SiO)3ZrH]. Chemical Communications, 2004, , 1729-1731.	2.2	35
220	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
221	Ion Chemistry of OV(OCH3)3in the Gas Phase:Â Molecular Cations and Anions and Their Primary Fragmentations. Inorganic Chemistry, 2004, 43, 1976-1985.	1.9	31
222	Computational Elucidation of the Transition State Shape Selectivity Phenomenon. Journal of the American Chemical Society, 2004, 126, 936-947.	6.6	120
223	Surface Structure of Hydroxylated and Sulfated Zirconia. A Periodic Density-Functional Studyâ€. Journal of Physical Chemistry B, 2004, 108, 14652-14662.	1.2	82
224	Electron hole formation in acidic zeolite catalysts. Journal of Chemical Physics, 2004, 121, 6034-6041.	1.2	49
225	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
226	Bond Dissociation Energies and Structures of CuNO+ and Cu(NO)2+.. ChemInform, 2003, 34, no.	0.1	0
227	Electronic States of Fe2S-/0/+. ChemInform, 2003, 34, no.	0.1	0
228	Stable Mechanistically-Relevant Aromatic-Based Carbenium Ions in Zeolite Catalysts. Journal of the American Chemical Society, 2003, 125, 2136-2141.	6.6	95
229	Electronic States of Fe2S-/0/+. Collection of Czechoslovak Chemical Communications, 2003, 68, 405-422.	1.0	4
230	Relative stability of alkoxides and carbocations in zeolites. QM/MM embedding and QM calculations applying periodic boundary conditions. Studies in Surface Science and Catalysis, 2002, 142, 643-649.	1.5	3
231	Bond Dissociation Energies and Structures of CuNO+and Cu(NO)2+. Inorganic Chemistry, 2002, 41, 5882-5890.	1.9	46
232	The electronic states of Fe2S2âˆ’/0/+/2+. Journal of Chemical Physics, 2002, 116, 617-628.	1.2	44
233	Structure and thermochemistry of Fe2S2âˆ’/0/+gas phase clusters and their fragments. B3LYP calculations. Physical Chemistry Chemical Physics, 2002, 4, 5234-5243.	1.3	47
234	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

#	Article	IF	Citations
235	On the Existence of CuI Pairs in ZSM-5â€"A Computational Study. Chemistry - A European Journal, 2002, 8, 2099.	1.7	33
236	Confirmation of Î£ and Î£ ground states of Fe2 and Fe2â^' by CASSCF/MRCI. Chemical Physics Letters, 2002, 358, 442-448.	1.2	45
237	Structure and Thermochemistry of Fe₂S₂^{â€‰0/+} Gas Phase Clusters and Their Fragments. B3LYP Calculations.. ChemInform, 2002, 33, 2-2.	0.1	0
238	(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
239	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
240	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
241	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
242	Vibrational spectra of the methanol tetramer in the OH stretch region. Two cyclic isomers and concerted proton tunneling. Journal of Chemical Physics, 2001, 114, 2623-2628.	1.2	36
243	Ab Initio Simulation of Cu-Species in Zeolites: Siting, Coordination, UV-Vis Spectra and Reactivity. , 2001, , 221-234.		6
244	Combining quantum mechanics and interatomic potential functions inab initio studies of extended systems. Journal of Computational Chemistry, 2000, 21, 1470-1493.	1.5	221
245	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
246	Electronic structure and magnetic coupling in sodium electro sodalite: All-electron density functional calculations. Journal of Chemical Physics, 2000, 113, 5466.	1.2	11
247	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
248	On the interpretation of the experimental Raman spectrum of Î²-eucryptite LiAlSiO4 from atomistic computer modeling. Journal of Non-Crystalline Solids, 2000, 274, 264-270.	1.5	13
249	HISTORY OF SCIENCE:Before the Fall of the Wall. Science, 2000, 287, 1210-1211.	6.0	0
250	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
251	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
252	Combined Quantum Mechanics:Â Interatomic Potential Function Investigation of rac-meso Configurational Stability and Rotational Transition in Zirconocene-Based Zieglerâ^'Natta Catalysts. Journal of Physical Chemistry A, 2000, 104, 10932-10938.	1.1	30

#	Article	IF	Citations
253	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
254	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
255	Absolute acidities and site specific properties of zeolite catalysts modelled by advanced computational chemistry technology. Chemical Physics Letters, 1999, 308, 147-154.	1.2	27
256	Quantum anharmonic frequencies of the Oâ‹¯ Hâ‹¯ O fragment of the H5O2+ ion: a model three-dimensional study. Chemical Physics Letters, 1999, 312, 591-597.	1.2	34
257	Acidic Catalysis by Zeolites: Ab Initio Modeling of Transition Structures. ACS Symposium Series, 1999, , 358-367.	0.5	27
258	Sodium doped sodium sodalite: magnetic coupling between F centers and hyperfine interactions with framework atoms. Physical Chemistry Chemical Physics, 1999, 1, 4505.	1.3	13
259	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
260	Influence of Ti Substitution on the ²⁹Si NMR Spectra of Silicalite. A Computational Study. Zeitschrift Fur Physikalische Chemie, 1999, 209, 21-32.	1.4	17
261	A CASSCF/ACPF study of spectroscopic properties of FeS and FeSâ¯ and the photoelectron spectrum of FeSâ¯. Chemical Physics Letters, 1998, 294, 37-44.	1.2	37
262	The Th1 and Th2 cytokines IFN-Î³ and IL-4 antagonize the inhibition of monocyte IL-1 receptor antagonist by glucocorticoids: involvement of IL-1. European Journal of Immunology, 1998, 28, 2075-2085.	1.6	17
263	A High-Resolution17O NMR Study of Siliceous Zeolite Faujasite. Journal of the American Chemical Society, 1998, 120, 3510-3511.	6.6	97
264	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
265	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
266	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
267	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
268	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
269	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
270	Comparing the Acidities of Microporous Aluminosilicate and Silico-Aluminophosphate Catalysts: A Combined Quantum Mechanics-Interatomic Potential Function Study. Collection of Czechoslovak Chemical Communications, 1998, 63, 1394-1408.	1.0	42

#	Article	IF	Citations
271	Ab initio molecular dynamics simulation of H5 O2+ and H7 O3+ gas phase clusters based on density functional theory. Molecular Physics, 1997, 91, 963-975.	0.8	9
272	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
273	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
274	Ab initio predictions of zeolite structures and 29Si NMR chemical shifts. Solid State Nuclear Magnetic Resonance, 1997, 9, 155-164.	1.5	48
275	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
276	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
277	Ab initio molecular dynamics simulation of methanol adsorbed in chabazite. Chemical Physics Letters, 1997, 266, 397-402.	1.2	100
278	Formic acid tetramers: structure isomers in the gas phase. Chemical Physics Letters, 1997, 267, 111-115.	1.2	29
279	Ab initio molecular dynamics simulation of H5O+2 and H7O+3 gas phase clusters based on density functional theory. Molecular Physics, 1997, 91, 963-975.	0.8	29
280	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
281	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
282	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
283	Probing Catalysts with Water. Science, 1996, 271, 774-775.	6.0	32
284	Optimized molecular integration schemes for density functional theory ab initio molecular dynamics simulations. Chemical Physics Letters, 1996, 255, 187-194.	1.2	17
285	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
286	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
287	Ab initio study of the interaction of methanol with BrÃ¸nsted acid sites of zeolites. Studies in Surface Science and Catalysis, 1995, 98, 242-243.	1.5	0
288	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

#	Article	IF	Citations
289	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
290	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
291	Inhibition of Interleukin-2-Mediated Lymphocyte Activation in Patients with Cushingâ€™s Syndrome: A Comparison with Hypocortisolemic Patients. Neuroendocrinology, 1994, 59, 144-151.	1.2	20
292	Structure and reactivity of zeolite catalysts: Atomistic modelling using ab initio techniques. Studies in Surface Science and Catalysis, 1994, , 2039-2057.	1.5	40
293	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
294	Ab initio calculations of the structure and properties of disiloxane. The effect of electron correlation and basis set extension. Chemical Physics Letters, 1994, 226, 405-412.	1.2	51
295	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
296	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
297	Theoretical Study of van der Waals Complexes at Surface Sites in Comparison with the Experiment. Chemical Reviews, 1994, 94, 2095-2160.	23.0	704
298	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
299	Starting from first principles. Nature, 1993, 363, 493-494.	13.7	21
300	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
301	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
302	PROTON TRANSFER FROM ACIDIC SITES TO WATER, METHANOL AND AMMONIA. A COMPARATIVE AB INITIO STUDY. , 1993, , 679-686.		3
303	Siting of Al and bridging hydroxyl groups in ZSM-5: A computer simulation study. Zeolites, 1992, 12, 20-23.	0.9	132
304	Relative propensity of methanol and silanol towards hydrogen bond formation. Chemical Physics Letters, 1992, 191, 537-547.	1.2	34
305	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
306	Ab initiocalculation of nuclear motion corrections to the geometries of water, methanol and silanol. Molecular Physics, 1991, 73, 335-348.	0.8	9

#	Article	IF	Citations
307	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
308	The beryllium atomâ€"water molecule interaction A many-body perturbation theory study. Chemical Physics Letters, 1990, 174, 19-24.	1.2	8
309	Gas phase acidities and molecular geometries of H3SiOH, H3COH, and H2O. Journal of Chemical Physics, 1990, 93, 2575-2583.	1.2	67
310	Quantum Chemical Studies of Zeolite Acidity. Studies in Surface Science and Catalysis, 1989, 52, 73-90.	1.5	5
311	Nonempirical direct SCF calculations on sodalite and double six-ring models of SiO2 and AlPO4 minerals: H24Si24O60, H12Si12O30, H12Al6P6O30. Chemical Physics Letters, 1989, 164, 199-204.	1.2	27
312	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
313	The HF-AlF3 gas-phase complex: An ab initio molecular orbital study. Chemical Physics Letters, 1989, 156, 125-128.	1.2	12
314	Acidic sites in heterogeneous catalysis: structure, properties and activity. Journal of Molecular Catalysis, 1989, 54, 312-323.	1.2	112
315	Theoretical interpretation of 29Si NMR chemical shifts of aluminosilicates. Computational and Theoretical Chemistry, 1989, 183, 223-232.	1.5	8
316	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
317	Internal silanols in zeolites - inferences from quantum chemical calculations. Catalysis Today, 1988, 3, 485-492.	2.2	26
318	Vibrational properties of surface hydroxyls: Nonempirical model calculations including anharmonicities. Collection of Czechoslovak Chemical Communications, 1988, 53, 2191-2202.	1.0	36
319	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
320	Applicability of the supermolecule MP2 approach to intermolecular interactions: He2 and Ne2. Chemical Physics Letters, 1987, 134, 553-559.	1.2	26
321	The H2Oî—¸Mg van der waals complex â€" a theoretical study. Chemical Physics, 1987, 113, 201-209.	0.9	3
322	Charge differences between silicon atoms in aluminosilicates and their relation to 29Si NMR chemical shifts. A quantum-chemical study. Computational and Theoretical Chemistry, 1986, 139, 113-124.	1.5	14
323	Wechselwirkung von Ethen mit Na⁺â€‰ionen in der Gasphase und in Zeolithen: Abâ€initioâ€Berechnung des Schwingungsspektrums. Zeitschrift FÃ¼r Chemie, 1985, 25, 254-255.	0.0	1
324	Transferability test of epen/2-type potential functions based on quantum-chemical interaction energies (QPEN). Chemical Physics Letters, 1984, 107, 530-534.	1.2	10

#	Article	IF	Citations
325	Quantum chemical studies on zeolites and silica. International Journal of Quantum Chemistry, 1984, 26, 793-822.	1.0	62
326	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
327	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
328	Transferable analytical potential based on nonempirical quantum chemical calculations (QPEN) for water-silica interactions. The Journal of Physical Chemistry, 1984, 88, 6375-6383.	2.9	31
329	Molecular structure of orthosilicic acid and importance of (p-d)Ï€ bonding. An ab initio molecular orbital study. Chemical Physics Letters, 1983, 97, 275-278.	1.2	35
330	Interaction of ethene, 2-methylpropene, and benzene with the sodium(1+) ion. 1. Quantum chemical study of gas-phase complexes. The Journal of Physical Chemistry, 1982, 86, 1327-1332.	2.9	17
331	Relative Stability of á—'Alâ€"Oâ€"Al á—• Linkages in Zeolites. A Nonempirical Molecular Orbital Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1982, 37, 277-279.	0.7	12
332	INDO/S calculations on simple silicon compounds and some silicon organic molecules. Collection of Czechoslovak Chemical Communications, 1982, 47, 1149-1168.	1.0	14
333	Interaction of ethene, 2-methylpropene and benzene with the Na+ ion. II. Quantum chemical study of sorption complexes in faujasites. Zeolites, 1982, 2, 114-120.	0.9	35
334	BasizitÃt von Disiloxan: Nichtempirische Berechnung der Protonierungsenergie. Zeitschrift FÃ¼r Chemie, 1982, 22, 60-61.	0.0	3
335	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
336	THE ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF THIONITROSO COMPOUNDSâ€"A QUANTUM CHEMICAL STUDY. Phosphorous and Sulfur and the Related Elements, 1981, 11, 325-334.	0.2	22
337	Quantum chemical investigation of interaction sites in zeolites and silica. The Journal of Physical Chemistry, 1980, 84, 3318-3326.	2.9	61
338	Molecular and electronic structure of disiloxane, an ab initio MO study. Chemical Physics Letters, 1979, 65, 587-591.	1.2	44
339	Opening of 3-membered rings to 4Ï€-electron systems. Tetrahedron, 1979, 35, 2109-2112.	1.0	11
340	Sydnon-Äthylene. II. Elektronische Wechselwirkungen in 4-Styryl-sydnonen. Journal FÃ¼r Praktische Chemie, 1978, 320, 71-80.	0.2	6
341	Sydnon-Äthylene. III. Chemische Reaktionen elektronisch angeregter 4-Styryl-sydnone. Journal FÃ¼r Praktische Chemie, 1978, 320, 81-90.	0.2	11
342	Isomers of weak Ï€-Ï€-complexes predicted by CT energy calculations. TCNE complexes with stilbene and analogs. Advances in Molecular Relaxation and Interaction Processes, 1978, 12, 1-11.	0.6	0

#	Article	IF	Citations
343	Orbital energies in open shell systems. Journal of Chemical Physics, 1978, 69, 495.	1.2	11
344	Effective semi-empirical excited state calculations using morokuma's EHP method. Chemical Physics Letters, 1978, 55, 119-124.	1.2	3
345	Interactions of open-shell systems, RHF molecular potential equations. Chemical Physics Letters, 1977, 46, 438-441.	1.2	0
346	Zeitschrift FÃ¼r Chemie, 1977, 17, 30-30.	0.0	3
347	Charge-transfer-Anregungsenergien von TetracyanÄthylen-MolekÃ¼lkomplexen phenylsubstituierter Ã„thylene und substituierter trans-Stilbene. Journal FÃ¼r Praktische Chemie, 1976, 318, 618-626.	0.2	9
348	Konsequenzen des Koopmansschen Theorems in den Restricted Hartree Fock Methoden fÃ¼r open-shell-Systeme. Theoretica Chimica Acta, 1975, 40, 129-141.	0.9	13
349	Restricted Hartree-Fock-Berechnungen von open-shell-Systemen mittels halbempirischer MO-LCAO-SCF-Verfahren. Collection of Czechoslovak Chemical Communications, 1974, 39, 1235-1245.	1.0	11
350	Ï€â€Elektronenberechnungen an substituierten Sydnonen. Zeitschrift FÃ¼r Chemie, 1973, 13, 434-435.	0.0	8
351	Gas Phase Mechanism of Oâ€¢â¯/Ni2+â€mediated Methane Conversion to Formaldehyde. Angewandte Chemie, 0, , .	1.6	0