

Georgi N Vayssilov

List of Publications by Year in descending order

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151
times ranked

6353
citing authors

#	ARTICLE	IF	CITATIONS
1	Acidic property of YNU-5 zeolite influenced by its unique micropore system. <i>Microporous and Mesoporous Materials</i> , 2022, 330, 111592.	2.2	3
2	Unraveling the Effect of Silanol Defects on the Insertion of Single-Site Mo in the MFI Zeolite Framework. <i>Inorganic Chemistry</i> , 2022, 61, 1418-1425.	1.9	14
3	Dissolution Behavior and Varied Mesoporosity of Zeolites by NH_4F Etching. <i>Chemistry - A European Journal</i> , 2022, 28, e202104339.	1.7	9
4	The relative stability of SCM-14 germanosilicate with different distributions of germanium ions in the absence and presence of structure-directing agents. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 3747-3757.	3.0	3
5	Key Role of CO on Terrace Sites of Metallic Pd Clusters for CO Oxidation. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	5
6	Sodium and Magnesium Ion Location at the Backbone and at the Nucleobase of RNA: <i>Ab Initio</i> Molecular Dynamics in Water Solution. <i>ACS Omega</i> , 2022, 7, 23234-23244.	1.6	3
7	Charting the Atomic C Interaction with Transition Metal Surfaces. <i>ACS Catalysis</i> , 2022, 12, 9256-9269.	5.5	6
8	Infrared spectra of surface nitrates: Revision of the current opinions based on the case study of ceria. <i>Journal of Catalysis</i> , 2021, 394, 245-258.	3.1	53
9	Design of PEG-modified magnetic nanoporous silica based miltefosine delivery system: Experimental and theoretical approaches. <i>Microporous and Mesoporous Materials</i> , 2021, 310, 110664.	2.2	6
10	Catalytic conversion of ethene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route. <i>Journal of Chemical Physics</i> , 2021, 154, 184706.	1.2	4
11	Complex H-bonded silanol network in zeolites revealed by IR and NMR spectroscopy combined with DFT calculations. <i>Journal of Materials Chemistry A</i> , 2021, 9, 27347-27352.	5.2	33
12	Biomimetic CO oxidation below 100°C by a nitrate-containing metal-free microporous system. <i>Nature Communications</i> , 2021, 12, 6033.	5.8	8
13	Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 26702-26709.	7.2	17
14	Defect Formation, T-Atom Substitution and Adsorption of Guest Molecules in MSE-Type Zeolite Framework—DFT Modeling. <i>Molecules</i> , 2021, 26, 7296.	1.7	4
15	Revisiting ceria- NO_x interaction: FTIR studies. <i>Catalysis Today</i> , 2020, 357, 613-620.	2.2	28
16	Influence of the adsorption of CO on the electronic structure of platinum clusters and nanowires deposited on $\text{CeO}_2(111)$ and $\text{Al}_2\text{O}_3(001)$ surfaces. <i>Catalysis Today</i> , 2020, 357, 442-452.	2.2	11
17	Stabilization of Super Electrophilic Pd^{2+} Cations in Small-Pore SSZ-13 Zeolite. <i>Journal of Physical Chemistry C</i> , 2020, 124, 309-321.	1.5	67
18	Preferential location of zirconium dopants in cerium dioxide nanoparticles and the effects of doping on their reducibility: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26568-26582.	1.3	6

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19	Tamoxifen Delivery System Based on PEGylated Magnetic MCM-41 Silica. <i>Molecules</i> , 2020, 25, 5129.	1.7	8
20	Paraquat adsorption on NaY zeolite at various Si/Al ratios: A combined experimental and computational study. <i>Materials Chemistry and Physics</i> , 2019, 238, 121824.	2.0	25
21	Verapamil delivery systems on the basis of mesoporous ZSM-5/KIT-6 and ZSM-5/SBA-15 polymer nanocomposites as a potential tool to overcome MDR in cancer cells. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2019, 142, 460-472.	2.0	8
22	Characterization and temperature evolution of iron-containing species in HZSM-5 zeolite prepared from different iron sources. <i>Journal of Porous Materials</i> , 2019, 26, 1227-1240.	1.3	10
23	Hydrophobic Tungsten-Containing MFI-Type Zeolite Films for Exhaust Gas Detection. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 12914-12919.	4.0	16
24	Subsurface Carbon: A General Feature of Noble Metals. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1744-1748.	7.2	31
25	Subsurface Carbon: A General Feature of Noble Metals. <i>Angewandte Chemie</i> , 2019, 131, 1758-1762.	1.6	6
26	Modified mesoporous silica nanoparticles coated by polymer complex as novel curcumin delivery carriers. <i>Journal of Drug Delivery Science and Technology</i> , 2019, 49, 700-712.	1.4	27
27	Optimization and in-vitro/in-vivo evaluation of doxorubicin-loaded chitosan-alginate nanoparticles using a melanoma mouse model. <i>International Journal of Pharmaceutics</i> , 2019, 556, 1-8.	2.6	50
28	Room-Temperature Ethene Hydrogenation Activity of Transition-Metal-Free HY Zeolites. <i>ACS Catalysis</i> , 2019, 9, 839-847.	5.5	12
29	Interaction of Na ⁺ , K ⁺ , Mg ²⁺ and Ca ²⁺ counter cations with RNA. <i>Metallomics</i> , 2018, 10, 659-678.	1.0	42
30	Computational elucidation of the reaction mechanism for synthesis of pyrrolidinedione derivatives via Nef-type rearrangement – cyclization reaction. <i>RSC Advances</i> , 2018, 8, 3178-3188.	1.7	4
31	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Small-Pore Zeolite SSZ-13: High Capacity and High Efficiency Low-Temperature CO and Passive NO _x Adsorbers (<i>Angew. Chem.</i> 51/2018). <i>Angewandte Chemie</i> , 2018, 130, 17152-17152.	1.6	1
32	Structure and reducibility of yttrium-doped cerium dioxide nanoparticles and (111) surface. <i>RSC Advances</i> , 2018, 8, 33728-33741.	1.7	5
33	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Small-Pore Zeolite SSZ-13: High Capacity and High Efficiency Low-Temperature CO and Passive NO _x Adsorbers. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 16672-16677.	7.2	129
34	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Small-Pore Zeolite SSZ-13: High Capacity and High Efficiency Low-Temperature CO and Passive NO _x Adsorbers. <i>Angewandte Chemie</i> , 2018, 130, 16914-16919.	1.6	34
35	Species formed during NO adsorption and NO ⁻ +O ₂ co-adsorption on ceria: A combined FTIR and DFT study. <i>Molecular Catalysis</i> , 2018, 451, 114-124.	1.0	30
36	Amino-modified KIT-6 mesoporous silica/polymer composites for quercetin delivery: Experimental and theoretical approaches. <i>Microporous and Mesoporous Materials</i> , 2018, 270, 40-47.	2.2	18

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37	Decomposition behavior of platinum clusters supported on ceria and γ -alumina in the presence of carbon monoxide. <i>Catalysis Science and Technology</i> , 2017, 7, 734-742.	2.1	12
38	Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21514-21521.	1.3	3
39	Elucidation of the higher coking resistance of small versus large nickel nanoparticles in methane dry reforming via computational modeling. <i>Catalysis Science and Technology</i> , 2017, 7, 3339-3347.	2.1	15
40	Synthesis, Modeling, and Catalytic Properties of HY Zeolite-Supported Rhodium Dinitrosyl Complexes. <i>ACS Catalysis</i> , 2017, 7, 5965-5982.	5.5	26
41	One-pot synthesis of silanol-free nanosized MFI Zeolite. <i>Nature Materials</i> , 2017, 16, 1010-1015.	13.3	135
42	Ethene hydrogenation on zeolite-supported rhodium clusters. A mechanistic study by density functional and microkinetic modeling. <i>Applied Catalysis A: General</i> , 2017, 543, 201-208.	2.2	4
43	Partial Oxidation of Activated Aromatics on Molecular Sieve Catalysts. , 2017, , 493-496.		0
44	Experimental and theoretical study of quercetin complexes formed on pure silica and Zn-modified mesoporous MCM-41 and SBA-16 materials. <i>Microporous and Mesoporous Materials</i> , 2016, 228, 256-265.	2.2	21
45	Stabilization of Small Platinum Nanoparticles on Pt/CeO ₂ Thin Film Electrocatalysts During Methanol Oxidation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19723-19736.	1.5	50
46	Can the state of platinum species be unambiguously determined by the stretching frequency of an adsorbed CO probe molecule?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22108-22121.	1.3	113
47	Adsorption and transformations of ethene on hydrogenated rhodium clusters in faujasite-type zeolite. A computational study. <i>Catalysis Science and Technology</i> , 2016, 6, 1726-1736.	2.1	5
48	Hydrogen Adsorption on Small Zeolite-Supported Rhodium Clusters. A Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1121-1129.	1.5	13
49	Formation of N ₃ ⁺ during interaction of NO with reduced ceria. <i>Chemical Communications</i> , 2015, 51, 5668-5671.	2.2	12
50	Relative stability and reducibility of CeO ₂ and Rh/CeO ₂ species on the surface and in the cavities of γ -Al ₂ O ₃ : a periodic DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22389-22401.	1.3	6
51	Effect of Si/Al Ratio and Rh Precursor Used on the Synthesis of HY Zeolite-Supported Rhodium Carbonyl Hydride Complexes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17166-17181.	1.5	32
52	Inhibition of Palm Oil Oxidation by Zeolite Nanocrystals. <i>Journal of Agricultural and Food Chemistry</i> , 2015, 63, 4655-4663.	2.4	10
53	Hydrogen Atom Transfer from Water or Alcohols Activated by Presolvated Electrons. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 986-992.	2.1	7
54	The structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14551-14560.	1.3	37

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55	FTIR and density functional study of NO interaction with reduced ceria: Identification of N3 ⁺ and NO2 ⁺ as new intermediates in NO conversion. <i>Applied Catalysis B: Environmental</i> , 2015, 176-177, 107-119.	10.8	43
56	Theoretical and Experimental Local Reactivity Parameters of 3-Substituted Coumarin Derivatives. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11062-11073.	1.1	5
57	Predicting adsorption enthalpies on silicalite and HZSM-5: A benchmark study on DFT strategies addressing dispersion interactions. <i>Journal of Computational Chemistry</i> , 2014, 35, 809-819.	1.5	31
58	Effect of Si/Al Ratio on the Nature and Reactivity of HY Zeolite-Supported Rhodium Dicarbonyl Complexes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26772-26788.	1.5	16
59	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 13371-13375.	7.2	73
60	New method for preparation of delivery systems of poorly soluble drugs on the basis of functionalized mesoporous MCM-41 nanoparticles. <i>Microporous and Mesoporous Materials</i> , 2014, 198, 247-255.	2.2	35
61	Ab Initio Molecular Dynamics of Na ⁺ and Mg ²⁺ Counterions at the Backbone of RNA in Water Solution. <i>ACS Chemical Biology</i> , 2013, 8, 1576-1589.	1.6	16
62	A Combined Pulsed Electron Paramagnetic Resonance Spectroscopic and DFT Analysis of the ¹³ C ₂ and ¹³ C Adsorption on the Metal-Organic Framework Cu _{2.97} Zn _{0.03} (btc) ₂ . <i>Journal of Physical Chemistry C</i> , 2013, 117, 8231-8240.	1.5	28
63	Framework Stability of Heteroatom-Substituted Forms of Extra-Large-Pore Ge-Silicate Molecular Sieves: The Case of ITQ-44. <i>Chemistry of Materials</i> , 2012, 24, 2509-2518.	3.2	26
64	Precise Identification of the Infrared Bands of the Polycarbonyl Complexes on Ni-MOR Zeolite by ¹² C ₁₆ and ¹³ C ₁₈ Co-adsorption and Computational Modeling. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22823-22831.	1.5	15
65	Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5879.	1.3	18
66	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. <i>Journal of Physical Chemistry C</i> , 2012, 116, 12103-12113.	1.5	108
67	Structural properties of metal-organic frameworks within the density-functional based tight-binding method. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 335-342.	0.7	42
68	Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. <i>Soft Materials</i> , 2012, 10, 216-234.	0.8	3
69	Bayesian approach to electron correlation in density functional theory. <i>Annalen Der Physik</i> , 2012, 524, 822-825.	0.9	1
70	Defects in MOFs: A Thorough Characterization. <i>ChemPhysChem</i> , 2012, 13, 2025-2029.	1.0	121
71	Computational Modeling of Coordination Chemistry of Transition Metal Cations in Zeolites and in Metal-organic Frameworks. <i>Current Physical Chemistry</i> , 2012, 2, 189-199.	0.1	4
72	Interaction of ethene and ethyne with bare and hydrogenated Ir ₄ clusters. A density functional study. <i>Catalysis Science and Technology</i> , 2011, 1, 958.	2.1	11

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73	Effects of deposited Pt particles on the reducibility of CeO ₂ (111). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11384.	1.3	89
74	Density Functional Study of Hydrogen Bond Formation between Methanol and Organic Molecules Containing Cl, F, NH ₂ , OH, and COOH Functional Groups. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14054-14068.	1.1	19
75	Density Functional Modeling of the Interactions of Platinum Clusters with CeO ₂ Nanoparticles of Different Size. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16081-16086.	1.5	40
76	Computational evaluation of the capability of transition metal exchanged zeolites for complete purification of hydrogen for fuel cell applications: the cheapest performs the best. <i>Energy and Environmental Science</i> , 2011, 4, 1879.	15.6	5
77	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. <i>Nature Materials</i> , 2011, 10, 310-315.	13.3	748
78	Determination of the optimal position of adjacent proton-donor centers for the activation or inhibition of peptide bond formation – A computational model study. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 30, 10-14.	1.3	1
79	Reassignment of the Vibrational Spectra of Carbonates, Formates, and Related Surface Species on Ceria: A Combined Density Functional and Infrared Spectroscopy Investigation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23435-23454.	1.5	294
80	Impurity Atoms on Small Transition Metal Clusters. Insights from Density Functional Model Studies. <i>Topics in Catalysis</i> , 2011, 54, 363-377.	1.3	8
81	Coordination state of Cu ⁺ ions in Cu-[Al]MCM-41. <i>Applied Catalysis B: Environmental</i> , 2011, 106, 186-186.	10.8	8
82	Enhanced reactivity of carbonyl compounds on MgO surface: A computational study. <i>Journal of Molecular Catalysis A</i> , 2011, 342-343, 67-73.	4.8	3
83	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. <i>Chemical Communications</i> , 2010, 46, 5936.	2.2	160
84	Hierarchical approach to conformational search and selection of computational method in modeling the mechanism of ester ammonolysis. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 246-255.	1.3	5
85	Theoretical investigation of ethane dehydrogenation on cationic Zn species in ZSM-5 zeolites – The second Al center in vicinity of the cation is essential for the accomplishment of the complete catalytic cycle. <i>Catalysis Today</i> , 2010, 152, 78-87.	2.2	22
86	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. <i>Journal of Materials Chemistry</i> , 2010, 20, 10535.	6.7	192
87	Catalytic Role of Vicinal OH in Ester Aminolysis: Proton Shuttle versus Hydrogen Bond Stabilization. <i>Journal of Organic Chemistry</i> , 2010, 75, 6782-6792.	1.7	18
88	Saturation of Small Supported Metal Clusters by Adsorbed Hydrogen. A Computational Study on Tetrahedral Models of Rh ₄ , Ir ₄ , and Pt ₄ . <i>Journal of Physical Chemistry C</i> , 2010, 114, 8500-8506.	1.5	27
89	Redox behavior of small metal clusters with respect to hydrogen. The effect of the cluster charge from density functional results. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11015.	1.3	6
90	Computational Modelling of Nanoporous Materials. , 2009, , 211-238.		4

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91	Effect of the size of the quantum region in a hybrid embedded-cluster scheme for zeolite systems. <i>Chemical Physics</i> , 2009, 363, 33-41.	0.9	16
92	Density functional study of Ni ₆ clusters containing impurity atoms. <i>Chemical Physics</i> , 2008, 348, 61-68.	0.9	10
93	Hydrogen Adsorption on Zeolite-Supported Tetrairidium Clusters. Thermodynamic Modeling from Density Functional Calculations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18572-18577.	1.5	18
94	CO Coordination at XNi ₄ Clusters with Impurities X = H, C, O. A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8523-8528.	1.1	3
95	Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters: An Embedded Cluster Density Functional Study of Models M ₆ (M = Rh, Ir, or Au). <i>Journal of Physical Chemistry C</i> , 2007, 111, 12340-12351.	1.5	57
96	Influence of Single Impurity Atoms on the Structure, Electronic, and Magnetic Properties of Ni ₅ Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2067-2076.	1.1	10
97	Density Functional Study of Hydrogen Adsorption on Tetrairidium Supported on Hydroxylated and Dehydroxylated Zeolite Surfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14484-14492.	1.5	25
98	Unusual Carbonyl-Nitrosyl Complexes of Rh ₂ in Rh-ZSM-5: A Combined FTIR Spectroscopy and Computational Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10412-10418.	1.5	13
99	First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region To Minimize Boundary Effects on the Quantum Region. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2290-2300.	2.3	21
100	Density functional modeling of reverse hydrogen spillover on zeolite-supported tetrairidium clusters. <i>Chemical Physics Letters</i> , 2007, 444, 215-219.	1.2	30
101	Preface: Third Humboldt Conference on Computational Chemistry. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1651-1652.	1.0	0
102	Influence of BH ₃ and alkaline cation released from the reduction agent on a tandem reduction/acylation reaction-A computational study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1814-1825.	1.0	1
103	Structure, stability, electronic and magnetic properties of Ni ₄ clusters containing impurity atoms. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1282.	1.3	21
104	The syn-Oriented 2-OH Provides a Favorable Proton Transfer Geometry in 1,2-Diol Monoester Aminolysis: Implications for the Ribosome Mechanism. <i>Journal of the American Chemical Society</i> , 2006, 128, 4964-4965.	6.6	50
105	Quantum chemical model study of the acyl migration in 2-(3)-formyl nucleosides. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1346-1356.	1.0	13
106	Heterolytic dissociation and recombination of H ₂ over Zn,H-ZSM-5 zeolites: A density functional model study. <i>Journal of Molecular Catalysis A</i> , 2006, 256, 149-155.	4.8	29
107	Theoretical elucidation of the regioselectivity in a tandem 1,4-hydride addition/acylation of diethylphosphonocoumarin. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 177-187.	1.5	6
108	Theoretical investigation of Zn-containing species in pores of ZSM-5 zeolites. <i>Studies in Surface Science and Catalysis</i> , 2005, , 593-600.	1.5	11

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109	The cluster Ir ₄ and its interaction with a hydrogen impurity. A density functional study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2656.	1.3	36
110	Comparison of All Sites for Ti Substitution in Zeolite TS-1 by an Accurate Embedded-Cluster Method. <i>Journal of Physical Chemistry B</i> , 2005, 109, 24304-24310.	1.2	50
111	Reverse hydrogen spillover in supported subnanosize clusters of the metals of groups 8 to 11. A computational model study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 4019.	1.3	51
112	Effects of the Aluminum Content of a Zeolite Framework: A DFT/MM Hybrid Approach Based on Cluster Models Embedded in an Elastic Polarizable Environment. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 459-471.	2.3	36
113	Theoretical study of the o-OH participation in catechol ester ammonolysis. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 737.	1.5	16
114	Transition metal clusters and supported species with metal-carbon bonds from first-principles quantum chemistry. <i>Journal of Organometallic Chemistry</i> , 2004, 689, 4384-4394.	0.8	24
115	Theoretical Investigation of the Coordination of N ₂ Ligands to the Cluster Ni ₃ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 6127-6144.	1.1	7
116	Free and Zeolite-Supported Hexarhodium Clusters with Light Impurity Atoms. <i>Journal of Physical Chemistry B</i> , 2004, 108, 180-192.	1.2	26
117	Supported metal species and adsorption complexes on metal oxides and in zeolites: Density functional cluster model studies. <i>Theoretical and Computational Chemistry</i> , 2004, , 367-450.	0.2	5
118	Oxidation of Supported Rhodium Clusters by Support Hydroxy Groups. <i>Angewandte Chemie</i> , 2003, 115, 1429-1432.	1.6	7
119	Oxidation of Supported Rhodium Clusters by Support Hydroxy Groups. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 1391-1394.	7.2	107
120	Elastic Polarizable Environment Cluster Embedding Approach for Covalent Oxides and Zeolites Based on a Density Functional Method. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2228-2241.	1.2	73
121	Characterization of oxide surfaces and zeolites by carbon monoxide as an IR probe molecule. <i>Advances in Catalysis</i> , 2002, , 307-511.	0.1	450
122	A New Interpretation of the IR Bands of Supported Rh(I) Monocarbonyl Complexes. <i>Journal of the American Chemical Society</i> , 2002, 124, 3783-3786.	6.6	33
123	Determination of the basicity of alkali-exchanged molecular sieves. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 146-148.	1.3	12
124	Regio- and Stereoselective [2+2] Photodimerization of 3-Substituted 2-Alkoxy-2-oxo-2H-1,2-benzoxaphosphorines. <i>Molecules</i> , 2002, 7, 420-432.	1.7	28
125	Influence of Alkali and Alkaline Earth Cations on the Brønsted Acidity of Zeolites. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4277-4284.	1.2	51
126	Dinitrogen as probe molecule of alkali-exchanged zeolites. <i>Journal of Molecular Catalysis A</i> , 2000, 162, 135-145.	4.8	25

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127	Structure and Bonding of a Site-Isolated Transition Metal Complex: A Rhodium Dicarbonyl in Highly Dealuminated Zeolite Y. <i>Journal of the American Chemical Society</i> , 2000, 122, 8056-8066.	6.6	116
128	Interaction of Methanol with Alkali Metal Exchanged Molecular Sieves. 2. Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8614-8623.	1.2	63
129	Density Functional Studies of Alkali-Exchanged Zeolites: Basicity and Core-Level Shifts of Framework Oxygen Atoms. <i>Journal of Catalysis</i> , 1999, 186, 423-432.	3.1	59
130	Density Functional Studies of Alkali-Exchanged Zeolites. Cation Location at Six-Rings of Different Aluminum Content. <i>Journal of Physical Chemistry B</i> , 1999, 103, 7920-7928.	1.2	55
131	Catalytic Activity of Titanium Silicalites – a DFT Study. <i>Journal of Catalysis</i> , 1998, 175, 170-174.	3.1	87
132	Theoretical Modelling of Propane Partial Oxidation over Titanium Silicalites. , 1998, , 439-445.		0
133	Liquid phase oxidation of alkylaromatic hydrocarbons over titanium silicalites. <i>Studies in Surface Science and Catalysis</i> , 1997, 110, 909-918.	1.5	1
134	Structural and Physicochemical Features of Titanium Silicalites. <i>Catalysis Reviews - Science and Engineering</i> , 1997, 39, 209-251.	5.7	294
135	Catalytic oxidation of anisole over titanium silicalite-1. <i>Chemical Engineering and Technology</i> , 1997, 20, 333-337.	0.9	9
136	Theoretical models for description of the gas-solid surface vibrational interactions. <i>Advances in Colloid and Interface Science</i> , 1995, 57, 123-159.	7.0	5
137	Influence of the solid surface vibrations on the rate constants of surface reactions. <i>Advances in Colloid and Interface Science</i> , 1993, 43, 51-85.	7.0	5
138	Structure and catalytic transformations of lower hydrocarbons on single-crystal surfaces of transition metals. <i>Advances in Colloid and Interface Science</i> , 1993, 47, 25-57.	7.0	3
139	Para-selective alkylation of toluene with methanol over ZSM-5 zeolites A kinetic model. <i>Applied Catalysis A: General</i> , 1993, 94, 117-130.	2.2	15
140	Effect of vibrational interaction on the rate of dissociation of adsorbed molecules: ethene on a nickel surface. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 2049.	1.7	1
141	Memory effect on preexponential factor of rate constant for dissociation of adsorbed molecules. <i>The Journal of Physical Chemistry</i> , 1992, 96, 3452-3454.	2.9	4
142	Interaction between surface phonons and bond vibrations of molecules adsorbed perpendicular to a solid surface. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 1627.	1.7	1
143	Temperature dependence of the rate constant for dissociation of adsorbed molecules. <i>Chemical Physics Letters</i> , 1992, 188, 497-500.	1.2	5
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