Georgi N Vayssilov

List of Publications by Year
in descending order

146	5,607	109137	85405
papers	citations	35 h-index	71 g-index

151	151	151	6353
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. Nature Materials, 2011, 10, 310-315.	13.3	748
2	Characterization of oxide surfaces and zeolites by carbon monoxide as an IR probe molecule. Advances in Catalysis, 2002, , 307-511.	0.1	450
3	Structural and Physicochemical Features of Titanium Silicalites. Catalysis Reviews - Science and Engineering, 1997, 39, 209-251.	5.7	294
4	Reassignment of the Vibrational Spectra of Carbonates, Formates, and Related Surface Species on Ceria: A Combined Density Functional and Infrared Spectroscopy Investigation. Journal of Physical Chemistry C, 2011, 115, 23435-23454.	1.5	294
5	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. Journal of Materials Chemistry, 2010, 20, 10535.	6.7	192
6	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	2.2	160
7	One-pot synthesis of silanol-free nanosized MFIÂzeolite. Nature Materials, 2017, 16, 1010-1015.	13.3	135
8	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO_x Adsorbers. Angewandte Chemie - International Edition, 2018, 57, 16672-16677.	7.2	129
9	Defects in MOFs: A Thorough Characterization. ChemPhysChem, 2012, 13, 2025-2029.	1.0	121
10	Structure and Bonding of a Site-Isolated Transition Metal Complex:Â Rhodium Dicarbonyl in Highly Dealuminated Zeolite Y. Journal of the American Chemical Society, 2000, 122, 8056-8066.	6.6	116
11	Can the state of platinum species be unambiguously determined by the stretching frequency of an adsorbed CO probe molecule?. Physical Chemistry Chemical Physics, 2016, 18, 22108-22121.	1.3	113
12	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. Journal of Physical Chemistry C, 2012, 116, 12103-12113.	1.5	108
13	Oxidation of Supported Rhodium Clusters by Support Hydroxy Groups. Angewandte Chemie - International Edition, 2003, 42, 1391-1394.	7.2	107
14	Effects of deposited Pt particles on the reducibility of CeO2(111). Physical Chemistry Chemical Physics, 2011, 13, 11384.	1.3	89
15	Catalytic Activity of Titanium Silicalitesâ€"a DFT Study. Journal of Catalysis, 1998, 175, 170-174.	3.1	87
16	Elastic Polarizable Environment Cluster Embedding Approach for Covalent Oxides and Zeolites Based on a Density Functional Method. Journal of Physical Chemistry B, 2003, 107, 2228-2241.	1.2	73
17	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. Angewandte Chemie - International Edition, 2014, 53, 13371-13375.	7.2	73
18	Stabilization of Super Electrophilic Pd⁺² Cations in Small-Pore SSZ-13 Zeolite. Journal of Physical Chemistry C, 2020, 124, 309-321.	1.5	67

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19	Interaction of Methanol with Alkali Metal Exchanged Molecular Sieves. 2. Density Functional Study. Journal of Physical Chemistry B, 2000, 104, 8614-8623.	1.2	63
20	Density Functional Studies of Alkali-Exchanged Zeolites: Basicity and Core-Level Shifts of Framework Oxygen Atoms. Journal of Catalysis, 1999, 186, 423-432.	3.1	59
21	Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters:â€‰ An Embedded Cluster Density Functional Study of Models M₆(M = Rh, Ir, or Au). Journal of Physical Chemistry C, 2007, 111, 12340-12351.	1.5	57
22	Density Functional Studies of Alkali-Exchanged Zeolites. Cation Location at Six-Rings of Different Aluminum Content. Journal of Physical Chemistry B, 1999, 103, 7920-7928.	1.2	55
23	Infrared spectra of surface nitrates: Revision of the current opinions based on the case study of ceria. Journal of Catalysis, 2021, 394, 245-258.	3.1	53
24	Influence of Alkali and Alkaline Earth Cations on the BrÃ¸nsted Acidity of Zeolites. Journal of Physical Chemistry B, 2001, 105, 4277-4284.	1.2	51
25	Reverse hydrogen spillover in supported subnanosize clusters of the metals of groups 8 to 11. A computational model study. Physical Chemistry Chemical Physics, 2005, 7, 4019.	1.3	51
26	Comparison of All Sites for Ti Substitution in Zeolite TS-1 by an Accurate Embedded-Cluster Method. Journal of Physical Chemistry B, 2005, 109, 24304-24310.	1.2	50
27	The syn-Oriented 2-OH Provides a Favorable Proton Transfer Geometry in 1,2-Diol Monoester Aminolysis:Â Implications for the Ribosome Mechanism. Journal of the American Chemical Society, 2006, 128, 4964-4965.	6.6	50
28	Stabilization of Small Platinum Nanoparticles on Ptâ€“CeO₂Thin Film Electrocatalysts During Methanol Oxidation. Journal of Physical Chemistry C, 2016, 120, 19723-19736.	1.5	50
29	Optimization and in-vitro/in-vivo evaluation of doxorubicin-loaded chitosan-alginate nanoparticles using a melanoma mouse model. International Journal of Pharmaceutics, 2019, 556, 1-8.	2.6	50
30	FTIR and density functional study of NO interaction with reduced ceria: Identification of N3â˜ and NO2â˜ as new intermediates in NO conversion. Applied Catalysis B: Environmental, 2015, 176-177, 107-119.	10.8	43
31	Structural properties of metalâ€organic frameworks within the densityâ€functional based tightâ€binding method. Physica Status Solidi (B): Basic Research, 2012, 249, 335-342.	0.7	42
32	Interaction of Na⁺, K⁺, Mg²⁺ and Ca²⁺ counter cations with RNA. Metallomics, 2018, 10, 659-678.	1.0	42
33	Density Functional Modeling of the Interactions of Platinum Clusters with CeO₂ Nanoparticles of Different Size. Journal of Physical Chemistry C, 2011, 115, 16081-16086.	1.5	40
34	The structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling. Physical Chemistry Chemical Physics, 2015, 17, 14551-14560.	1.3	37
35	The cluster Ir4 and its interaction with a hydrogen impurity. A density functional study. Physical Chemistry Chemical Physics, 2005, 7, 2656.	1.3	36
36	Effects of the Aluminum Content of a Zeolite Framework:â€‰ A DFT/MM Hybrid Approach Based on Cluster Models Embedded in an Elastic Polarizable Environment. Journal of Chemical Theory and Computation, 2005, 1, 459-471.	2.3	36

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37	New method for preparation of delivery systems of poorly soluble drugs on the basis of functionalized mesoporous MCM-41 nanoparticles. Microporous and Mesoporous Materials, 2014, 198, 247-255.	2.2	35
38	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO_x Adsorbers. Angewandte Chemie, 2018, 130, 16914-16919.	1.6	34
39	A New Interpretation of the IR Bands of Supported Rh(I) Monocarbonyl Complexes. Journal of the American Chemical Society, 2002, 124, 3783-3786.	6.6	33
40	Complex H-bonded silanol network in zeolites revealed by IR and NMR spectroscopy combined with DFT calculations. Journal of Materials Chemistry A, 2021, 9, 27347-27352.	5.2	33
41	Effect of Si/Al Ratio and Rh Precursor Used on the Synthesis of HY Zeolite-Supported Rhodium Carbonyl Hydride Complexes. Journal of Physical Chemistry C, 2015, 119, 17166-17181.	1.5	32
42	Predicting adsorption enthalpies on silicalite and HZSMâ€5: A benchmark study on DFT strategies addressing dispersion interactions. Journal of Computational Chemistry, 2014, 35, 809-819.	1.5	31
43	Subsurface Carbon: A General Feature of Noble Metals. Angewandte Chemie - International Edition, 2019, 58, 1744-1748.	7.2	31
44	Density functional modeling of reverse hydrogen spillover on zeolite-supported tetrairidium clusters. Chemical Physics Letters, 2007, 444, 215-219.	1.2	30
45	Species formed during NO adsorption and NOâ€¯+â€¯O 2 co-adsorption on ceria: A combined FTIR and DFT study. Molecular Catalysis, 2018, 451, 114-124.	1.0	30
46	Heterolytic dissociation and recombination of H2 over Zn,H-ZSM-5 zeolitesâ€”A density functional model study. Journal of Molecular Catalysis A, 2006, 256, 149-155.	4.8	29
47	A Combined Pulsed Electron Paramagnetic Resonance Spectroscopic and DFT Analysis of the ¹³CO₂ and ¹³CO Adsorption on the Metalâ€“Organic Framework Cu_{2.97}Zn_{0.03}(btc)₂. Journal of Physical Chemistry C, 2013, 117, 8231-8240.	1.5	28
48	Revisiting ceria-NOx interaction: FTIR studies. Catalysis Today, 2020, 357, 613-620.	2.2	28
49	Regio- and Stereoselective [2+2] Photodimerization of 3-Substituted 2-Alkoxy-2-oxo-2H-1,2-benzoxaphosphorines. Molecules, 2002, 7, 420-432.	1.7	28
50	Saturation of Small Supported Metal Clusters by Adsorbed Hydrogen. A Computational Study on Tetrahedral Models of Rh₄, Ir₄, and Pt₄. Journal of Physical Chemistry C, 2010, 114, 8500-8506.	1.5	27
51	Modified mesoporous silica nanoparticles coated by polymer complex as novel curcumin delivery carriers. Journal of Drug Delivery Science and Technology, 2019, 49, 700-712.	1.4	27
52	Free and Zeolite-Supported Hexarhodium Clusters with Light Impurity Atoms. Journal of Physical Chemistry B, 2004, 108, 180-192.	1.2	26
53	Framework Stability of Heteroatom-Substituted Forms of Extra-Large-Pore Ge-Silicate Molecular Sieves: The Case of ITQ-44. Chemistry of Materials, 2012, 24, 2509-2518.	3.2	26
54	Synthesis, Modeling, and Catalytic Properties of HY Zeolite-Supported Rhodium Dinitrosyl Complexes. ACS Catalysis, 2017, 7, 5965-5982.	5.5	26

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55	Dinitrogen as probe molecule of alkali-exchanged zeolites. Journal of Molecular Catalysis A, 2000, 162, 135-145.	4.8	25
56	Density Functional Study of Hydrogen Adsorption on Tetrairidium Supported on Hydroxylated and Dehydroxylated Zeolite Surfaces. Journal of Physical Chemistry C, 2007, 111, 14484-14492.	1.5	25
57	Paraquat adsorption on NaY zeolite at various Si/Al ratios: A combined experimental and computational study. Materials Chemistry and Physics, 2019, 238, 121824.	2.0	25
58	Transition metal clusters and supported species with metalâ€“carbon bonds from first-principles quantum chemistry. Journal of Organometallic Chemistry, 2004, 689, 4384-4394.	0.8	24
59	Theoretical investigation of ethane dehydrogenation on cationic Zn species in ZSM-5 zeolitesâ€”The second Al center in vicinity of the cation is essential for the accomplishment of the complete catalytic cycle. Catalysis Today, 2010, 152, 78-87.	2.2	22
60	Structure, stability, electronic and magnetic properties of Ni4 clusters containing impurity atoms. Physical Chemistry Chemical Physics, 2006, 8, 1282.	1.3	21
61	First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region To Minimize Boundary Effects on the Quantum Region. Journal of Chemical Theory and Computation, 2007, 3, 2290-2300.	2.3	21
62	Experimental and theoretical study of quercetin complexes formed on pure silica and Zn-modified mesoporous MCM-41 and SBA-16 materials. Microporous and Mesoporous Materials, 2016, 228, 256-265.	2.2	21
63	Density Functional Study of Hydrogen Bond Formation between Methanol and Organic Molecules Containing Cl, F, NH₂, OH, and COOH Functional Groups. Journal of Physical Chemistry A, 2011, 115, 14054-14068.	1.1	19
64	Hydrogen Adsorption on Zeolite-Supported Tetrairidium Clusters. Thermodynamic Modeling from Density Functional Calculations. Journal of Physical Chemistry C, 2008, 112, 18572-18577.	1.5	18
65	Catalytic Role of Vicinal OH in Ester Aminolysis: Proton Shuttle versus Hydrogen Bond Stabilization. Journal of Organic Chemistry, 2010, 75, 6782-6792.	1.7	18
66	Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. Physical Chemistry Chemical Physics, 2012, 14, 5879.	1.3	18
67	Amino-modified KIT-6 mesoporous silica/polymer composites for quercetin delivery: Experimental and theoretical approaches. Microporous and Mesoporous Materials, 2018, 270, 40-47.	2.2	18
68	Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism. Angewandte Chemie - International Edition, 2021, 60, 26702-26709.	7.2	17
69	Theoretical study of the o-OH participation in catechol ester ammonolysis. Organic and Biomolecular Chemistry, 2005, 3, 737.	1.5	16
70	Effect of the size of the quantum region in a hybrid embedded-cluster scheme for zeolite systems. Chemical Physics, 2009, 363, 33-41.	0.9	16
71	Ab Initio Molecular Dynamics of Na+and Mg2+Countercations at the Backbone of RNA in Water Solution. ACS Chemical Biology, 2013, 8, 1576-1589.	1.6	16
72	Effect of Si/Al Ratio on the Nature and Reactivity of HY Zeolite-Supported Rhodium Dicarbonyl Complexes. Journal of Physical Chemistry C, 2014, 118, 26772-26788.	1.5	16

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73	Hydrophobic Tungsten-Containing MFI-Type Zeolite Films for Exhaust Gas Detection. ACS Applied Materials & Interfaces, 2019, 11, 12914-12919.	4.0	16
74	Para-selective alkylation of toluene with methanol over ZSM-5 zeolitesA kinetic model. Applied Catalysis A: General, 1993, 94, 117-130.	2.2	15
75	Precise Identification of the Infrared Bands of the Polycarbonyl Complexes on Niâ€“MOR Zeolite by12C16Oâ€“13C18O Coadsorption and Computational Modeling. Journal of Physical Chemistry C, 2012, 116, 22823-22831.	1.5	15
76	Elucidation of the higher coking resistance of small versus large nickel nanoparticles in methane dry reforming via computational modeling. Catalysis Science and Technology, 2017, 7, 3339-3347.	2.1	15
77	Unraveling the Effect of Silanol Defects on the Insertion of Single-Site Mo in the MFI Zeolite Framework. Inorganic Chemistry, 2022, 61, 1418-1425.	1.9	14
78	Quantum chemical model study of the acyl migration in 2â€²(3â€²)-formylnucleosides. International Journal of Quantum Chemistry, 2006, 106, 1346-1356.	1.0	13
79	Unusual Carbonylâ^'Nitrosyl Complexes of Rh2+in Rhâ^'ZSM-5:â€‰ A Combined FTIR Spectroscopy and Computational Study. Journal of Physical Chemistry C, 2007, 111, 10412-10418.	1.5	13
80	Hydrogen Adsorption on Small Zeolite-Supported Rhodium Clusters. A Density Functional Study. Journal of Physical Chemistry C, 2015, 119, 1121-1129.	1.5	13
81	Determination of the basicity of alkali-exchanged molecular sieves. Physical Chemistry Chemical Physics, 2002, 4, 146-148.	1.3	12
82	Formation of N₃^{â^'} during interaction of NO with reduced ceria. Chemical Communications, 2015, 51, 5668-5671.	2.2	12
83	Decomposition behavior of platinum clusters supported on ceria and Î³-alumina in the presence of carbon monoxide. Catalysis Science and Technology, 2017, 7, 734-742.	2.1	12
84	Room-Temperature Ethene Hydrogenation Activity of Transition-Metal-Free HY Zeolites. ACS Catalysis, 2019, 9, 839-847.	5.5	12
85	Theoretical investigation of Zn-containing species in pores of ZSM-5 zeolites. Studies in Surface Science and Catalysis, 2005, , 593-600.	1.5	11
86	Interaction of ethene and ethyne with bare and hydrogenated Ir4 clusters. A density functional study. Catalysis Science and Technology, 2011, 1, 958.	2.1	11
87	Influence of the adsorption of CO on the electronic structure of platinum clusters and nanowires deposited on CeO2(111) and Î³-Al2O3(001) surfaces. Catalysis Today, 2020, 357, 442-452.	2.2	11
88	Influence of Single Impurity Atoms on the Structure, Electronic, and Magnetic Properties of Ni5 Clusters. Journal of Physical Chemistry A, 2007, 111, 2067-2076.	1.1	10
89	Density functional study of Ni6 clusters containing impurity atoms. Chemical Physics, 2008, 348, 61-68.	0.9	10
90	Inhibition of Palm Oil Oxidation by Zeolite Nanocrystals. Journal of Agricultural and Food Chemistry, 2015, 63, 4655-4663.	2.4	10

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91	Characterization and temperature evolution of iron-containing species in HZSM-5 zeolite prepared from different iron sources. Journal of Porous Materials, 2019, 26, 1227-1240.	1.3	10
92	Catalytic oxidation of anisole over titanium silicalite-1. Chemical Engineering and Technology, 1997, 20, 333-337.	0.9	9
93	Dissolution Behavior and Varied Mesoporosity of Zeolites by NH₄F Etching. Chemistry - A European Journal, 2022, 28, e202104339.	1.7	9
94	Energy transfer in adsorbed molecule-solid surface vibration interactions. Surface Science, 1991, 255, 355-360.	0.8	8
95	Impurity Atoms on Small Transition Metal Clusters. Insights from Density Functional Model Studies. Topics in Catalysis, 2011, 54, 363-377.	1.3	8
96	Coordination state of Cu+ ions in Cu-[Al]MCM-41. Applied Catalysis B: Environmental, 2011, 106, 186-186.	10.8	8
97	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. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 142, 460-472.	2.0	8
98	Tamoxifen Delivery System Based on PEGylated Magnetic MCM-41 Silica. Molecules, 2020, 25, 5129.	1.7	8
99	Biomimetic CO oxidation below â˜'100â€‰Â°C by a nitrate-containing metal-free microporous system. Nature Communications, 2021, 12, 6033.	5.8	8
100	Quantum Brownian motion and classical diffusion. Chemical Physics Letters, 1992, 195, 423-426.	1.2	7
101	Oxidation of Supported Rhodium Clusters by Support Hydroxy Groups. Angewandte Chemie, 2003, 115, 1429-1432.	1.6	7
102	Theoretical Investigation of the Coordination of N2Ligands to the Cluster Ni3. Journal of Physical Chemistry A, 2004, 108, 6127-6144.	1.1	7
103	Hydrogen Atom Transfer from Water or Alcohols Activated by Presolvated Electrons. Journal of Physical Chemistry Letters, 2015, 6, 986-992.	2.1	7
104	Theoretical elucidation of the regioselectivity in a tandem 1,4-hydride addition/acylation of diethylphosphonocoumarin. Computational and Theoretical Chemistry, 2006, 759, 177-187.	1.5	6
105	Redox behavior of small metal clusters with respect to hydrogen. The effect of the cluster charge from density functional results. Physical Chemistry Chemical Physics, 2010, 12, 11015.	1.3	6
106	Relative stability and reducibility of CeO2 and Rh/CeO2 species on the surface and in the cavities of Î³-Al2O3: a periodic DFT study. Physical Chemistry Chemical Physics, 2015, 17, 22389-22401.	1.3	6
107	Subsurface Carbon: A General Feature of Noble Metals. Angewandte Chemie, 2019, 131, 1758-1762.	1.6	6
108	Preferential location of zirconium dopants in cerium dioxide nanoparticles and the effects of doping on their reducibility: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 26568-26582.	1.3	6

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109	Design of PEG-modified magnetic nanoporous silica based miltefosine delivery system: Experimental and theoretical approaches. Microporous and Mesoporous Materials, 2021, 310, 110664.	2.2	6
110	Charting the Atomic C Interaction with Transition Metal Surfaces. ACS Catalysis, 2022, 12, 9256-9269.	5.5	6
111	Temperature dependence of the rate constant for dissociation of absorbed molecules. Chemical Physics Letters, 1992, 188, 497-500.	1.2	5
112	Influence of the solid surface vibrations on the rate constants of surface reactions. Advances in Colloid and Interface Science, 1993, 43, 51-85.	7.0	5
113	Theoretical models for description of the gas-solid surface vibrational interactions. Advances in Colloid and Interface Science, 1995, 57, 123-159.	7.0	5
114	Supported metal species and adsorption complexes on metal oxides and in zeolites: Density functional cluster model studies. Theoretical and Computational Chemistry, 2004, , 367-450.	0.2	5
115	Hierarchical approach to conformational search and selection of computational method in modeling the mechanism of ester ammonolysis. Journal of Molecular Graphics and Modelling, 2010, 29, 246-255.	1.3	5
116	Computational evaluation of the capability of transition metal exchanged zeolites for complete purification of hydrogen for fuel cell applications: the cheapest performs the best. Energy and Environmental Science, 2011, 4, 1879.	15.6	5
117	Theoretical and Experimental Local Reactivity Parameters of 3-Substituted Coumarin Derivatives. Journal of Physical Chemistry A, 2014, 118, 11062-11073.	1.1	5
118	Adsorption and transformations of ethene on hydrogenated rhodium clusters in faujasite-type zeolite. A computational study. Catalysis Science and Technology, 2016, 6, 1726-1736.	2.1	5
119	Structure and reducibility of yttrium-doped cerium dioxide nanoparticles and (111) surface. RSC Advances, 2018, 8, 33728-33741.	1.7	5
120	Key Role of aâ€Top CO on Terrace Sites of Metallic Pd Clusters for CO Oxidation. Chemistry - A European Journal, 2022, 28, .	1.7	5
121	Memory effect on preexponential factor of rate constant for dissociation of adsorbed molecules. The Journal of Physical Chemistry, 1992, 96, 3452-3454.	2.9	4
122	Computational Modelling of Nanoporous Materials. , 2009, , 211-238.		4
123	Ethene hydrogenation on zeolite-supported rhodium clusters. A mechanistic study by density functional and microkinetic modeling. Applied Catalysis A: General, 2017, 543, 201-208.	2.2	4
124	Computational elucidation of the reaction mechanism for synthesis of pyrrolidinedione derivatives via Nef-type rearrangement â€“ cyclization reaction. RSC Advances, 2018, 8, 3178-3188.	1.7	4
125	Catalytic conversion of ethene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route. Journal of Chemical Physics, 2021, 154, 184706.	1.2	4
126	Computational Modeling of Coordination Chemistry of Transition Metal Cations in Zeolites and in Metal-organic Frameworks. Current Physical Chemistry, 2012, 2, 189-199.	0.1	4

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127	Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism. Angewandte Chemie, 0, , .	1.6	4
128	Defect Formation, T-Atom Substitution and Adsorption of Guest Molecules in MSE-Type Zeolite Frameworkâ€"DFT Modeling. Molecules, 2021, 26, 7296.	1.7	4
129	Structure and catalytic transformations of lower hydrocarbons on single-crystal surfaces of transition metals. Advances in Colloid and Interface Science, 1993, 47, 25-57.	7.0	3
130	CO Coordination at XNi₄Clusters with Impurities X = H, C, O. A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 8523-8528.	1.1	3
131	Enhanced reactivity of carbonyl compounds on MgO surface: A computational study. Journal of Molecular Catalysis A, 2011, 342-343, 67-73.	4.8	3
132	Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. Soft Materials, 2012, 10, 216-234.	0.8	3
133	Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling. Physical Chemistry Chemical Physics, 2017, 19, 21514-21521.	1.3	3
134	Acidic property of YNU-5 zeolite influenced by its unique micropore system. Microporous and Mesoporous Materials, 2022, 330, 111592.	2.2	3
135	The relative stability of SCM-14 germanosilicate with different distributions of germanium ions in the absence and presence of structure-directing agents. Inorganic Chemistry Frontiers, 2022, 9, 3747-3757.	3.0	3
136	Sodium and Magnesium Ion Location at the Backbone and at the Nucleobase of RNA: Ab Initio Molecular Dynamics in Water Solution. ACS Omega, 2022, 7, 23234-23244.	1.6	3
137	Interaction between surface phonons and bond vibrations of molecules adsorbed perpendicular to a solid surface. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1627.	1.7	1
138	Effect of vibrational interaction on the rate of dissociation of adsorbed molecules: ethene on a nickel surface. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2049.	1.7	1
139	Liquid phase oxidation of alkylaromatic hydrocarbons over titanium silicalites. Studies in Surface Science and Catalysis, 1997, 110, 909-918.	1.5	1
140	Influence of BH3and alkaline cation released from the reduction agent on a tandem reduction/acylation reaction-A computational study. International Journal of Quantum Chemistry, 2007, 107, 1814-1825.	1.0	1
141	Determination of the optimal position of adjacent proton-donor centers for the activation or inhibition of peptide bond formation â€“ A computational model study. Journal of Molecular Graphics and Modelling, 2011, 30, 10-14.	1.3	1
142	Bayesian approach to electron correlation in density functional theory. Annalen Der Physik, 2012, 524, 822-825.	0.9	1
143	RÃ¼cktitelbild: Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO_x Adsorbers (Angew. Chem. 51/2018). Angewandte Chemie, 2018, 130, 17152-17152.	1.6	1
144	Preface: Third Humboldt Conference on Computational Chemistry. International Journal of Quantum Chemistry, 2007, 107, 1651-1652.	1.0	0

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145	Theoretical Modelling of Propane Partial Oxidation over Titanium Silicalites. , 1998, , 439-445.		0
146	Partial Oxidation of Activated Aromatics on Molecular Sieve Catalysts. , 2017, , 493-496.		0