Petr Nachtigall

List of Publications by Year
in descending order

173	9,555	30551 56	49824 91
papers	citations	h-index	g-index

181	181	181	9458
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Flexibilization of Biorefineries: Tuning Lignin Hydrogenation by Hydrogen Partial Pressure. ChemSusChem, 2021, 14, 373-378.	3.6	8
2	Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS₄) nanowires with carriers induces half-metallicity. Journal of Materials Chemistry C, 2021, 9, 3122-3128.	2.7	8
3	Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling. Journal of Materials Chemistry C, 2021, 9, 11132-11141.	2.7	29
4	The Role of Water Loading and Germanium Content in Germanosilicate Hydrolysis. Journal of Physical Chemistry C, 2021, 125, 23744-23757.	1.5	12
5	Mechanism of Zeolite Hydrolysis under Basic Conditions. Chemistry of Materials, 2021, 33, 9202-9212.	3.2	9
6	Two-dimensional tetragonal GaOI and InOI sheets: In-plane anisotropic optical properties and application to photocatalytic water splitting. Catalysis Today, 2020, 340, 178-182.	2.2	20
7	Systematic computational investigation of an Ni3Fe catalyst for the OER. Catalysis Today, 2020, 345, 220-226.	2.2	9
8	Zeolite (In)Stability under Aqueous or Steaming Conditions. Advanced Materials, 2020, 32, e2003264.	11.1	75
9	Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum. ACS Catalysis, 2020, 10, 11057-11068.	5.5	20
10	Synthesis and Postâ€Synthesis Transformation of Germanosilicate Zeolites. Angewandte Chemie, 2020, 132, 19548-19557.	1.6	4
11	Synthesis and Postâ€Synthesis Transformation of Germanosilicate Zeolites. Angewandte Chemie - International Edition, 2020, 59, 19380-19389.	7.2	48
12	2D Oxide Nanomaterials to Address the Energy Transition and Catalysis. Advanced Materials, 2019, 31, e1801712.	11.1	88
13	Real-time optical and electronic sensing with a Î²-amino enone linked, triazine-containing 2D covalent organic framework. Nature Communications, 2019, 10, 3228.	5.8	117
14	MÃ¶ssbauerite as Iron-Only Layered Oxyhydroxide Catalyst for WO₃ Photoanodes. Inorganic Chemistry, 2019, 58, 9655-9662.	1.9	9
15	Structure Determination of the Oxygen Evolution Catalyst MÃ¶ssbauerite. Journal of Physical Chemistry C, 2019, 123, 25157-25165.	1.5	7
16	Fast room temperature lability of aluminosilicate zeolites. Nature Communications, 2019, 10, 4690.	5.8	75
17	The effect of water on the validity of LÃ¶wenstein's rule. Chemical Science, 2019, 10, 5705-5711.	3.7	37
18	Magneto-structural correlations of novel kagomÃ©-type metal organic frameworks. Journal of Materials Chemistry C, 2019, 7, 6692-6697.	2.7	10

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19	The BrÃ¸nsted acidity of three- and two-dimensional zeolites. Microporous and Mesoporous Materials, 2019, 282, 121-132.	2.2	21
20	Control of spintronic and electronic properties of bimetallic and vacancy-ordered vanadium carbide MXenes via surface functionalization. Physical Chemistry Chemical Physics, 2019, 21, 25802-25808.	1.3	22
21	Tuning the Porosity and Photocatalytic Performance of Triazineâ€Based Graphdiyne Polymers through Polymorphism. ChemSusChem, 2019, 12, 194-199.	3.6	39
22	New Layered Triazine Framework/Exfoliated 2D Polymer with Superior Sodiumâ€Storage Properties. Advanced Materials, 2018, 30, 1705401.	11.1	177
23	The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology. Catalysis Today, 2018, 304, 12-21.	2.2	13
24	Pressure-induced chemistry for the 2D to 3D transformation of zeolites. Journal of Materials Chemistry A, 2018, 6, 5255-5259.	5.2	21
25	New catalytic materials for energy and chemistry in transition. Chemical Society Reviews, 2018, 47, 8066-8071.	18.7	27
26	Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite. Journal of Physical Chemistry C, 2018, 122, 26088-26095.	1.5	13
27	Towards operando computational modeling in heterogeneous catalysis. Chemical Society Reviews, 2018, 47, 8307-8348.	18.7	169
28	Fluorescent Sulphurâ€and Nitrogenâ€Containing Porous Polymers with Tuneable Donorâ€“Acceptor Domains for Lightâ€Driven Hydrogen Evolution. Chemistry - A European Journal, 2018, 24, 11916-11921.	1.7	38
29	Fewâ€Layer Silicene Nanosheets with Superior Lithiumâ€Storage Properties. Advanced Materials, 2018, 30, e1800838.	11.1	126
30	Near-room-temperature Chern insulator and Dirac spin-gapless semiconductor: nickel chloride monolayer. Nanoscale, 2017, 9, 2246-2252.	2.8	120
31	Assemblyâ€“Disassemblyâ€“Organizationâ€“Reassembly Synthesis of Zeolites Based on cfi-Type Layers. Chemistry of Materials, 2017, 29, 5605-5611.	3.2	60
32	Theoretical investigation of CO catalytic oxidation by a Feâ€“PtSe₂ monolayer. RSC Advances, 2017, 7, 19630-19638.	1.7	10
33	The Influence of Water on the Performance of Molybdenum Carbide Catalysts in Hydrodeoxygenation Reactions: A Combined Theoretical and Experimental Study. ChemCatChem, 2017, 9, 1985-1991.	1.8	29
34	Twinned Growth of Metalâ€Free, Triazineâ€Based Photocatalyst Films as Mixedâ€Dimensional (2D/3D) van der Waals Heterostructures. Advanced Materials, 2017, 29, 1703399.	11.1	59
35	Tailored Band Gaps in Sulfurâ€and Nitrogenâ€Containing Porous Donorâ€“Acceptor Polymers. Chemistry - A European Journal, 2017, 23, 13023-13027.	1.7	35
36	Exploring the stability and reactivity of Ni2P and Mo2C catalysts using ab initio atomistic thermodynamics and conceptual DFT approaches. Biomass Conversion and Biorefinery, 2017, 7, 377-383.	2.9	3

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37	Manipulation with Zeolitic Layers Toward New Porous Materials. Advanced Science Letters, 2017, 23, 5955-5957.	0.2	0
38	Metalâ€“Organic Frameworks Mâ€MOFâ€74 and Mâ€MILâ€100: Comparison of Textural, Acidic, and Catalytic Properties. ChemPlusChem, 2016, 81, 828-835.	1.3	28
39	Direct hydrodeoxygenation of phenol over carbon-supported Ru catalysts: A computational study. Journal of Molecular Catalysis A, 2016, 423, 300-307.	4.8	20
40	The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports. Catalysis Today, 2016, 277, 108-117.	2.2	2
41	The surface stability and equilibrium crystal morphology of Ni₂P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach. CrystEngComm, 2016, 18, 3808-3818.	1.3	17
42	Combined PDF and Rietveld studies of ADORable zeolites and the disordered intermediate IPC-1P. Dalton Transactions, 2016, 45, 14124-14130.	1.6	9
43	New two-dimensional Mn-based MXenes with room-temperature ferromagnetism and half-metallicity. Journal of Materials Chemistry C, 2016, 4, 11143-11149.	2.7	164
44	The effect of the zeolite pore size on the Lewis acid strength of extra-framework cations. Physical Chemistry Chemical Physics, 2016, 18, 18063-18073.	1.3	9
45	High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. Journal of Materials Chemistry C, 2016, 4, 6500-6509.	2.7	127
46	Unusual Dirac half-metallicity with intrinsic ferromagnetism in vanadium trihalide monolayers. Journal of Materials Chemistry C, 2016, 4, 2518-2526.	2.7	202
47	Understanding the Structure of Cationic Sites in Alkali Metal-Grafted USY Zeolites. Journal of Physical Chemistry C, 2016, 120, 4954-4960.	1.5	11
48	Palladium clusters on graphene support: An ab initio study. Chemical Physics Letters, 2016, 646, 56-63.	1.2	5
49	Synthesis of â€˜unfeasibleâ€™ zeolites. Nature Chemistry, 2016, 8, 58-62.	6.6	186
50	The ADOR synthesis of new zeolites: In silico investigation. Catalysis Today, 2015, 243, 32-38.	2.2	30
51	Adsorption of pentane isomers on metal-organic frameworks Cu-BTC and Fe-BTC. Catalysis Today, 2015, 243, 69-75.	2.2	30
52	Theoretical and experimental study of CO adsorption on Ca-FER zeolite. Catalysis Today, 2015, 243, 53-61.	2.2	11
53	Adsorptive desulfurization with CPO-27/MOF-74: an experimental and computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 10759-10766.	1.3	47
54	The ADOR mechanism for the synthesis of new zeolites. Chemical Society Reviews, 2015, 44, 7177-7206.	18.7	275

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55	Unexpected Photoreactivity in a NO₂-Functionalized Aluminum-MOF. Journal of Physical Chemistry C, 2015, 119, 26401-26408.	1.5	9
56	Accurate Ab Initio Description of Adsorption on Coordinatively Unsaturated Cu2+ and Fe3+ Sites in MOFs. Journal of Chemical Theory and Computation, 2015, 11, 230-238.	2.3	36
57	Accurate ab initio Description of Adsorption on Coordinatively Unsaturated Sites in Metalâ€“Organic Frameworks. , 2015, , 175-206.		3
58	From Doubleâ€Fourâ€Ring Germanosilicates to New Zeolites: In Silico Investigation. ChemPhysChem, 2014, 15, 2972-2976.	1.0	31
59	Two-Dimensional Zeolites: Current Status and Perspectives. Chemical Reviews, 2014, 114, 4807-4837.	23.0	625
60	Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. Catalysis Today, 2014, 227, 2-8.	2.2	25
61	Measuring the BrÃ¸nsted acid strength of zeolites â€“ does it correlate with the Oâ€“H frequency shift probed by a weak base?. Physical Chemistry Chemical Physics, 2014, 16, 10129-10141.	1.3	62
62	Theoretical investigation of layered zeolites with MWW topology: MCM-22P vs. MCM-56. Dalton Transactions, 2014, 43, 10443-10450.	1.6	33
63	Catalysis by Dynamically Formed Defects in a Metalâ€“Organic Framework Structure: Knoevenagel Reaction Catalyzed by Copper Benzeneâ€1,3,5â€tricarboxylate. ChemCatChem, 2014, 6, 2821-2824.	1.8	54
64	Layered inorganic solids. Dalton Transactions, 2014, 43, 10274.	1.6	11
65	Adsorption of CO2 in FAU zeolites: Effect of zeolite composition. Catalysis Today, 2014, 227, 50-56.	2.2	80
66	Computational Investigation of the Lewis Acidity in Three-Dimensional and Corresponding Two-Dimensional Zeolites: UTL vs IPC-1P. Journal of Physical Chemistry A, 2014, 118, 7526-7534.	1.1	16
67	CO2 Adsorption in Porous Materials. , 2013, , 535-558.		1
68	Comparison of the catalytic activity of MOFs and zeolites in Knoevenagel condensation. Catalysis Science and Technology, 2013, 3, 500-507.	2.1	179
69	Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL. Catalysis Today, 2013, 204, 15-21.	2.2	33
70	UTL zeolite and the way beyond. Microporous and Mesoporous Materials, 2013, 182, 229-238.	2.2	18
71	Theoretical investigation of the FriedlÃnder reaction catalysed by CuBTC: Concerted effect of the adjacent Cu2+ sites. Catalysis Today, 2013, 204, 101-107.	2.2	33
72	Adsorption of Propane and Propylene on CuBTC Metalâ€“Organic Framework: Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2013, 117, 11159-11167.	1.5	48

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73	A family of zeolites with controlled pore size prepared using a top-down method. Nature Chemistry, 2013, 5, 628-633.	6.6	355
74	Intramolecular Hydroalkoxylation of Nonâ€Activated Cï£¾C Bonds Catalysed by Zeolites: An Experimental and Theoretical Study. ChemSusChem, 2013, 6, 1021-1030.	3.6	10
75	The Effect of Synthesis Conditions and Nature of Heteroelement on Acidic Properties of Isomorphously Substituted UTL Zeolites. Advanced Porous Materials, 2013, 1, 103-113.	0.3	11
76	Synthesis of quinolines via FriedlÃnder reaction catalyzed by CuBTC metalâ€“organic-framework. Dalton Transactions, 2012, 41, 4036.	1.6	118
77	Reply to the â€˜Comment on â€œThe nature of cationic adsorption sites in alkaline zeolitesâ€”single, dual and multiple cation sitesâ€• by O. Cairon, Phys. Chem. Chem. Phys., 2012, 14, DOI: 10.1039/c2cp40963a. Physical Chemistry Chemical Physics, 2012, 14, 10353.	1.3	3
78	The nature of cationic adsorption sites in alkaline zeolitesâ€”single, dual and multiple cation sites. Physical Chemistry Chemical Physics, 2012, 14, 1552-1569.	1.3	87
79	Control of CO2adsorption heats by the Al distribution in FER zeolites. Physical Chemistry Chemical Physics, 2012, 14, 1117-1120.	1.3	28
80	Controlling the Adsorption Enthalpy of CO₂ in Zeolites by Framework Topology and Composition. ChemSusChem, 2012, 5, 2011-2022.	3.6	93
81	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. ChemPhysChem, 2012, 13, 488-495.	1.0	53
82	Combined Experimental and Theoretical Investigations of Heterogeneous Dual Cation Sites in Cu,M-FER Zeolites. Journal of Physical Chemistry C, 2011, 115, 13312-13321.	1.5	20
83	Understanding CO₂ Adsorption in CuBTC MOF: Comparing Combined DFTâ€“ab Initio Calculations with Microcalorimetry Experiments. Journal of Physical Chemistry C, 2011, 115, 17925-17933.	1.5	146
84	Accurate Description of Argon and Water Adsorption on Surfaces of Graphene-Based Carbon Allotropes. Journal of Physical Chemistry A, 2011, 115, 11387-11393.	1.1	68
85	Accurate Prediction of Methane Adsorption in a Metalâ€“Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation. Journal of Physical Chemistry C, 2011, 115, 23074-23080.	1.5	86
86	Combined volumetric, infrared spectroscopic and theoretical investigation of CO2 adsorption on Na-A zeolite. Microporous and Mesoporous Materials, 2011, 146, 97-105.	2.2	75
87	Postsynthesis Transformation of Three-Dimensional Framework into a Lamellar Zeolite with Modifiable Architecture. Journal of the American Chemical Society, 2011, 133, 6130-6133.	6.6	208
88	Variableâ€Temperature IR Spectroscopic and Theoretical Studies on CO₂ Adsorbed in Zeolite Kâ€FER. ChemPhysChem, 2011, 12, 1435-1443.	1.0	26
89	Vibrational dynamics of adsorbed CO2: Separability of the CO2 asymmetric stretching mode. Collection of Czechoslovak Chemical Communications, 2011, 76, 669-682.	1.0	1
90	Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER. Physical Chemistry Chemical Physics, 2010, 12, 1497.	1.3	49

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91	Themed Issue on characterization of adsorbed species. Physical Chemistry Chemical Physics, 2010, 12, 6307.	1.3	10
92	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. Journal of Physical Chemistry Letters, 2010, 1, 3354-3359.	2.1	166
93	DFT/CC investigation of physical adsorption on a graphite (0001) surface. Physical Chemistry Chemical Physics, 2010, 12, 6438.	1.3	100
94	Experimental and theoretical determination of adsorption heats of CO2 over alkali metal exchanged ferrierites with different Si/Al ratio. Physical Chemistry Chemical Physics, 2010, 12, 6413.	1.3	86
95	Computational and Variableâ€Temperature Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on Zeolite Caâ€A. ChemPhysChem, 2009, 10, 1058-1065.	1.0	14
96	Hydrogen adsorption on the zeolite Ca-A: DFT and FT-IR investigation. Chemical Physics Letters, 2009, 477, 139-143.	1.2	40
97	Correlation Between Catalytic Activity and Metal Cation Coordination: NO Decomposition Over Cu/Zeolites. ChemCatChem, 2009, 1, 449-453.	1.8	20
98	Localization and Coordination of Mg²⁺Cations in Ferrierite: Combined FTIR Spectroscopic and Computation Investigation of CO Adsorption Complexes. Journal of Physical Chemistry C, 2009, 113, 11066-11076.	1.5	22
99	Adsorption of CO₂ on Sodium-Exchanged Ferrierites: The Bridged CO₂ Complexes Formed between Two Extraframework Cations. Journal of Physical Chemistry C, 2009, 113, 2928-2935.	1.5	75
100	Structure and Stability of the Waterâ"Graphite Complexes. Journal of Physical Chemistry C, 2009, 113, 8412-8419.	1.5	96
101	Combined DFT/CC and IR spectroscopic studies on carbon dioxide adsorption on the zeolite H-FER. Energy and Environmental Science, 2009, 2, 1187.	15.6	75
102	Theoretical investigation of dinitrosyl complexes in Cu-zeolites as intermediates in deNOx process. Physical Chemistry Chemical Physics, 2009, 11, 1447.	1.3	29
103	Computational and FTIR spectroscopic studies on carbon monoxide and dinitrogen adsorption on a high-silica H-FER zeolite. Physical Chemistry Chemical Physics, 2009, 11, 791-802.	1.3	73
104	Investigation of the Benzeneâ€"Naphthalene and Naphthaleneâ€"Naphthalene Potential Energy Surfaces: DFT/CCSD(T) Correction Scheme. ChemPhysChem, 2008, 9, 1702-1708.	1.0	48
105	Stable Triazenes Derived from 2â€Alkylaminonaphthalenes and 5â€Nitrobenzo[c]â€1,2â€thiazoleâ€3â€diazonium Hydrogensulfate. European Journal of Organic Chemistry, 2008, 2008, 3272-3278.	1.2	8
106	Investigation of the benzene-dimer potential energy surface: DFT/CCSD(T) correction scheme. Journal of Chemical Physics, 2008, 128, 114102.	1.2	172
107	Interaction of acetonitrile with Na-zeolites: adsorption modes and vibrational dynamics in the zeolite channels and cavities. Physical Chemistry Chemical Physics, 2008, 10, 4189.	1.3	11
108	Computational and Fourier Transform Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on the Zeolites Na-ZSM-5 and K-ZSM-5:â€‰ Evidence of Dual-Cation Sites. Journal of Physical Chemistry C, 2008, 112, 4658-4666.	1.5	63

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109	Combined TPD and theoretical investigation of CO desorption from Cu-K-FER zeolite. Studies in Surface Science and Catalysis, 2008, , 893-896.	1.5	3
110	Evidence of heterogeneous dual cation sites in zeolites by combined IR and DFT investigation. Studies in Surface Science and Catalysis, 2008, , 1005-1008.	1.5	8
111	Applications of Quantum Chemical Methods in Zeolite Science. Studies in Surface Science and Catalysis, 2007, , 701-XXI.	1.5	16
112	Carbon monoxide adsorption on low-silica zeolitesâ€"from single to dual and to multiple cation sites. Physical Chemistry Chemical Physics, 2007, 9, 4657.	1.3	44
113	FTIR Study of CO Interactions with Li⁺Ions in Micro- and Mesoporous Matrices:â€‰Coordination and Localization of Li⁺Ions. Journal of Physical Chemistry C, 2007, 111, 11353-11362.	1.5	22
114	Coordination Compounds Based on 1,2,3,4-Tetrahydro-isoquinoline-3-carboxylic Acid. Molecules, 2007, 12, 1064-1079.	1.7	4
115	Periodic density functional and FTIR spectroscopic studies on CO adsorption on the zeolite Na-FER. Microporous and Mesoporous Materials, 2007, 106, 162-173.	2.2	44
116	Thermodynamics of reversible gas adsorption on alkali-metal exchanged zeolitesâ€"the interplay of infrared spectroscopy and theoretical calculations. Physical Chemistry Chemical Physics, 2007, 9, 1421-1437.	1.3	96
117	On the site-specificity of polycarbonyl complexes in Cu/zeolites: combined experimental and DFT study. Physical Chemistry Chemical Physics, 2006, 8, 5535-5542.	1.3	35
118	FTIR spectroscopic and computational studies on hydrogen adsorption on the zeolite Liâ€"FER. Physical Chemistry Chemical Physics, 2006, 8, 2286-2292.	1.3	57
119	The vibrational dynamics of carbon monoxide in a confined spaceâ€"CO in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 4849-4852.	1.3	74
120	Single and Dual Cation Sites in Zeolites:Â Theoretical Calculations and FTIR Spectroscopic Studies on CO Adsorption on K-FER. Journal of Physical Chemistry B, 2006, 110, 22542-22550.	1.2	79
121	Combined Theoretical and FTIR Spectroscopic Studies on Hydrogen Adsorption on the Zeolites Naâ^'FER and Kâ^'FER. Journal of Physical Chemistry B, 2006, 110, 395-402.	1.2	72
122	Theoretical investigation of site-specific characteristics of CO adsorption complexes in the Li+-FER zeolite. Applied Catalysis A: General, 2006, 307, 118-127.	2.2	43
123	A simple correlation between average Tâ€"Oâ€"T angles and 27Al NMR chemical shifts does not hold in high-silica zeolites. Microporous and Mesoporous Materials, 2005, 85, 279-283.	2.2	29
124	Characterization of the Cu+ sites in MFI zeolites: combined computational and experimental study. Catalysis Today, 2005, 100, 385-389.	2.2	21
125	Theoretical Investigation of CO Interaction with Copper Sites in Zeolites:Â Periodic DFT and Hybrid Quantum Mechanical/Interatomic Potential Function Study. Journal of Physical Chemistry B, 2005, 109, 9631-9638.	1.2	77
126	Synthesis, characterization and structural investigation of the first vanadocene(IV) carboxylic acid complexes prepared from the vanadocene dichloride. Journal of Organometallic Chemistry, 2004, 689, 1180-1187.	0.8	26

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127	A density functional study of EPR hyperfine coupling of vanadocene(IV) complexes. Chemical Physics, 2004, 305, 291-298.	0.9	18
128	Calculations of the site specific stretching frequencies of CO adsorbed on Li+/ZSM-5. Physical Chemistry Chemical Physics, 2004, 6, 5580-5587.	1.3	41
129	Structure and Hydrogen Bonding of Different Isomers of 2-AminopyridineÂ·NH3Studied by IR/R2PI Spectroscopy. Journal of Physical Chemistry A, 2004, 108, 3338-3343.	1.1	21
130	Localization of Cu+sites and framework Al positions in high-silica zeolites: Combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2004, 6, 2003-2007.	1.3	29
131	Nature of the Cu+â^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
132	Structure and hydrogen bonding of 2-aminopyridineÂ·(H2O)n(nâ€‰=â€‰1, 2) studied by infrared ion depletion spectroscopy. Physical Chemistry Chemical Physics, 2004, 6, 515-521.	1.3	28
133	Pyrrole as a Probe Molecule for Characterization of Basic Sites in ZSM-5:Â A Combined FTIR Spectroscopy and Computational Study. Journal of Physical Chemistry B, 2004, 108, 16012-16022.	1.2	32
134	Theoretical investigation of the vibrational dynamics of Ag+CO solvated in the Ne matrix. Chemical Physics Letters, 2003, 375, 54-58.	1.2	3
135	Calculations of Site-Specific CO Stretching Frequencies for Copper Carbonyls with the â€œNear Spectroscopic Accuracyâ€•â€‰ CO Interaction with Cu+/MFI. Journal of Physical Chemistry A, 2003, 107, 10381-10388.	1.1	71
136	Characterization of the Cu+Sites in High-Silica Zeolites Interacting with the CO Molecule:Â Combined Computational and Experimental Study. Journal of Physical Chemistry B, 2003, 107, 2327-2332.	1.2	69
137	Coordination of alkali metal ions in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 2003, 5, 3311-3317.	1.3	58
138	Theoretical Study of Pyrrole Interaction with Alkali Metal Exchanged Zeolites: Investigation of the Reliability of Cluster and Periodic Models. Collection of Czechoslovak Chemical Communications, 2003, 68, 1848-1860.	1.0	7
139	Theoretical investigation of the effect of the rare gas matrices on the vibrational spectra of solvated molecular ions: Cu+CO. Journal of Chemical Physics, 2002, 117, 9298-9305.	1.2	22
140	On the Existence of CuI Pairs in ZSM-5â€”A Computational Study. Chemistry - A European Journal, 2002, 8, 2099.	1.7	33
141	Concerted Use of Slab and Cluster Models in an ab Initio Study of Hydrogen Desorption from the Si(100) Surface. Journal of Physical Chemistry B, 2001, 105, 4031-4038.	1.2	42
142	Characterization of Ag+ Sites in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 2001, 3, 4791-4795.	1.3	18
143	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
144	RI-MP2 calculations with extended basis setsÃ¢â‚¬â€a promising tool for study of H-bonded and stacked DNA base pairs. Physical Chemistry Chemical Physics, 2001, 3, 4578-4582.	1.3	106

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145	Computational Study of Extraframework Cu+Sites in Ferrierite:Â Structure, Coordination, and Photoluminescence Spectra. Journal of Physical Chemistry B, 2001, 105, 3510-3517.	1.2	49
146	State-Specific Brillouinâ^'Wigner Multireference Coupled Cluster Study of the Singletâ^'Triplet Separation in the Tetramethyleneethane Diradical. Journal of Physical Chemistry A, 2001, 105, 1354-1356.	1.1	69
147	Nonadiabatic interactions between the ground and low-lying excited electronic states: Vibronic states of the Clâ€“HCl complex. Journal of Chemical Physics, 2001, 115, 5974-5983.	1.2	13
148	Ab Initio Simulation of Cu-Species in Zeolites: Siting, Coordination, UV-Vis Spectra and Reactivity. , 2001, , 221-234.		6
149	The calculation of the vibrational states of SO2 in the Cì*f*1B2 electronic state up to the SO(3Î£â^')+O(3P) dissociation limit. Chemical Physics Letters, 2000, 318, 607-613.	1.2	28
150	Absorption and resonance emission spectra of SO2(Xì*f*1A1/Cì*f*1B2) calculated from ab initio potential energy and transition dipole moment surfaces. Chemical Physics Letters, 2000, 329, 503-510.	1.2	27
151	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
152	Investigation of the potential energy surfaces for the ground Xì*f*1A1 and excited Cì*f*1B2 electronic states of SO2. Chemical Physics Letters, 1999, 303, 441-446.	1.2	27
153	Assessment of the single-root multireference Brillouinâ€“Wigner coupled- cluster method:â€‰Testâ€‰calculationsâ€‰onâ€‰CH2,â€‰SiH2,â€‰andâ€‰twistedâ€‰ethylene. Journal of Chemical Physics, 1999, 10275-10282.	1.2	17
154	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
155	Investigation of a hybrid TCSCF-DFT procedure. Theoretical Chemistry Accounts, 1998, 99, 135-140.	0.5	26
156	Reliability of DFT Methods for Description of Cu Sites and Their Interaction with NO in Zeolites. Collection of Czechoslovak Chemical Communications, 1998, 63, 1202-1212.	1.0	5
157	Water Photolysis in Rare Gas Environment: The CASPT2 Excited State H2O(A)-Ar Potential. Collection of Czechoslovak Chemical Communications, 1998, 63, 1321-1328.	1.0	1
158	Investigation of the reliability of density functional methods: Reaction and activation energies for Siâ€“Si bond cleavage and H2 elimination from silanes. Journal of Chemical Physics, 1996, 104, 148-158.	1.2	112
159	Barriers for hydrogen atom diffusion on the Si(100)â€2Ã—1 surface. Journal of Chemical Physics, 1995, 102, 8249-8254.	1.2	45
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