Petr Nachtigall

List of Publications by Year
in descending order

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173 papers	9,555 citations	26630 56 h-index	43889 91 g-index
181 all docs	181 docs citations	181 times ranked	8299 citing authors

#	Article	IF	Citations
1	Two-Dimensional Zeolites: Current Status and Perspectives. Chemical Reviews, 2014, 114, 4807-4837.	47.7	625
2	A family of zeolites with controlled pore size prepared using a top-down method. Nature Chemistry, 2013, 5, 628-633.	13.6	355
3	The ADOR mechanism for the synthesis of new zeolites. Chemical Society Reviews, 2015, 44, 7177-7206.	38.1	275
4	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.	2.8	215
5	Postsynthesis Transformation of Three-Dimensional Framework into a Lamellar Zeolite with Modifiable Architecture. Journal of the American Chemical Society, 2011, 133, 6130-6133.	13.7	208
6	Unusual Dirac half-metallicity with intrinsic ferromagnetism in vanadium trihalide monolayers. Journal of Materials Chemistry C, 2016, 4, 2518-2526.	5.5	202
7	Synthesis of â€˜unfeasibleâ€™ zeolites. Nature Chemistry, 2016, 8, 58-62.	13.6	186
8	Comparison of the catalytic activity of MOFs and zeolites in Knoevenagel condensation. Catalysis Science and Technology, 2013, 3, 500-507.	4.1	179
9	New Layered Triazine Framework/Exfoliated 2D Polymer with Superior Sodiumâ€Storage Properties. Advanced Materials, 2018, 30, 1705401.	21.0	177
10	Investigation of the benzene-dimer potential energy surface: DFT/CCSD(T) correction scheme. Journal of Chemical Physics, 2008, 128, 114102.	3.0	172
11	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.	3.0	171
12	Towards operando computational modeling in heterogeneous catalysis. Chemical Society Reviews, 2018, 47, 8307-8348.	38.1	169
13	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. Journal of Physical Chemistry Letters, 2010, 1, 3354-3359.	4.6	166
14	New two-dimensional Mn-based MXenes with room-temperature ferromagnetism and half-metallicity. Journal of Materials Chemistry C, 2016, 4, 11143-11149.	5.5	164
15	Understanding CO₂ Adsorption in CuBTC MOF: Comparing Combined DFTâ€“ab Initio Calculations with Microcalorimetry Experiments. Journal of Physical Chemistry C, 2011, 115, 17925-17933.	3.1	146
16	High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. Journal of Materials Chemistry C, 2016, 4, 6500-6509.	5.5	127
17	Fewâ€Layer Silicene Nanosheets with Superior Lithiumâ€Storage Properties. Advanced Materials, 2018, 30, e1800838.	21.0	126
18	Near-room-temperature Chern insulator and Dirac spin-gapless semiconductor: nickel chloride monolayer. Nanoscale, 2017, 9, 2246-2252.	5.6	120

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19	Synthesis of quinolines via FriedlÃnder reaction catalyzed by CuBTC metalâ€“organic-framework. Dalton Transactions, 2012, 41, 4036.	3.3	118
20	Real-time optical and electronic sensing with a Î²-amino enone linked, triazine-containing 2D covalent organic framework. Nature Communications, 2019, 10, 3228.	12.8	117
21	Calculation of the Siâ€“H bond energies for the monohydride phase of Si(100). Journal of Chemical Physics, 1991, 95, 8652-8654.	3.0	116
22	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.	3.0	112
23	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.	2.8	106
24	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.	2.8	104
25	DFT/CC investigation of physical adsorption on a graphite (0001) surface. Physical Chemistry Chemical Physics, 2010, 12, 6438.	2.8	100
26	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.	2.8	96
27	Structure and Stability of the Waterâ‹¯Graphite Complexes. Journal of Physical Chemistry C, 2009, 113, 8412-8419.	3.1	96
28	Theoretical study of the low-lying triplet and singlet states of tetramethyleneethane: prediction of a triplet below singlet state at the triplet equilibrium geometry. Journal of the American Chemical Society, 1993, 115, 270-271.	13.7	93
29	Controlling the Adsorption Enthalpy of CO₂ in Zeolites by Framework Topology and Composition. ChemSusChem, 2012, 5, 2011-2022.	6.8	93
30	2D Oxide Nanomaterials to Address the Energy Transition and Catalysis. Advanced Materials, 2019, 31, e1801712.	21.0	88
31	Theoretical study of the mechanism of recombinative hydrogen desorption from the monohydride phase of Si(100): The role of defect migration. Journal of Chemical Physics, 1994, 101, 8073-8081.	3.0	87
32	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.	2.6	87
33	The nature of cationic adsorption sites in alkaline zeolitesâ€”single, dual and multiple cation sites. Physical Chemistry Chemical Physics, 2012, 14, 1552-1569.	2.8	87
34	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.	2.6	86
35	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.	2.8	86
36	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.	3.1	86

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37	Adsorption of CO2 in FAU zeolites: Effect of zeolite composition. Catalysis Today, 2014, 227, 50-56.	4.4	80
38	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.	2.6	79
39	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.	2.6	77
40	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.	3.1	75
41	Combined DFT/CC and IR spectroscopic studies on carbon dioxide adsorption on the zeolite H-FER. Energy and Environmental Science, 2009, 2, 1187.	30.8	75
42	Combined volumetric, infrared spectroscopic and theoretical investigation of CO2 adsorption on Na-A zeolite. Microporous and Mesoporous Materials, 2011, 146, 97-105.	4.4	75
43	Fast room temperature lability of aluminosilicate zeolites. Nature Communications, 2019, 10, 4690.	12.8	75
44	Zeolite (In)Stability under Aqueous or Steaming Conditions. Advanced Materials, 2020, 32, e2003264.	21.0	75
45	The vibrational dynamics of carbon monoxide in a confined spaceâ€"CO in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 4849-4852.	2.8	74
46	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.	2.8	73
47	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.	2.6	72
48	Si adatom binding and diffusion on the Si(100) surface: Comparison of ab initio, semiempirical and empirical potential results. Journal of Chemical Physics, 1995, 102, 1044-1056.	3.0	71
49	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.	2.5	71
50	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.	2.5	69
51	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.	2.6	69
52	Accurate Description of Argon and Water Adsorption on Surfaces of Graphene-Based Carbon Allotropes. Journal of Physical Chemistry A, 2011, 115, 11387-11393.	2.5	68
53	Theoretical study of the low-lying triplet and singlet states of diradicals. 1. Tetramethyleneethane. Journal of the American Chemical Society, 1992, 114, 4743-4747.	13.7	65
54	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.	3.1	63

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55	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.	2.8	62
56	Assemblyâ€“Disassemblyâ€“Organizationâ€“Reassembly Synthesis of Zeolites Based on cfi-Type Layers. Chemistry of Materials, 2017, 29, 5605-5611.	6.7	60
57	Twinned Growth of Metalâ€Free, Triazineâ€Based Photocatalyst Films as Mixedâ€Dimensional (2D/3D) van der Waals Heterostructures. Advanced Materials, 2017, 29, 1703399.	21.0	59
58	Coordination of alkali metal ions in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 2003, 5, 3311-3317.	2.8	58
59	FTIR spectroscopic and computational studies on hydrogen adsorption on the zeolite Liâ€“FER. Physical Chemistry Chemical Physics, 2006, 8, 2286-2292.	2.8	57
60	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.	3.7	54
61	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. ChemPhysChem, 2012, 13, 488-495.	2.1	53
62	Ab initio calculation of the energy of recombinative hydrogen desorption from the monohydride phase of silicon (100). The Journal of Physical Chemistry, 1993, 97, 11666-11672.	2.9	51
63	Computational Study of Extraframework Cu+Sites in Ferrierite:Â Structure, Coordination, and Photoluminescence Spectra. Journal of Physical Chemistry B, 2001, 105, 3510-3517.	2.6	49
64	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.	2.8	49
65	Investigation of the Benzeneâ€“Naphthalene and Naphthaleneâ€“Naphthalene Potential Energy Surfaces: DFT/CCSD(T) Correction Scheme. ChemPhysChem, 2008, 9, 1702-1708.	2.1	48
66	Adsorption of Propane and Propylene on CuBTC Metalâ€“Organic Framework: Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2013, 117, 11159-11167.	3.1	48
67	Synthesis and Postâ€Synthesis Transformation of Germanosilicate Zeolites. Angewandte Chemie - International Edition, 2020, 59, 19380-19389.	13.8	48
68	Adsorptive desulfurization with CPO-27/MOF-74: an experimental and computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 10759-10766.	2.8	47
69	Barriers for hydrogen atom diffusion on the Si(100)â€2Ã—1 surface. Journal of Chemical Physics, 1995, 102, 8249-8254.	3.0	45
70	Carbon monoxide adsorption on low-silica zeolitesâ€”from single to dual and to multiple cation sites. Physical Chemistry Chemical Physics, 2007, 9, 4657.	2.8	44
71	Periodic density functional and FTIR spectroscopic studies on CO adsorption on the zeolite Na-FER. Microporous and Mesoporous Materials, 2007, 106, 162-173.	4.4	44
72	Theoretical investigation of site-specific characteristics of CO adsorption complexes in the Li+-FER zeolite. Applied Catalysis A: General, 2006, 307, 118-127.	4.3	43

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73	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.	2.6	42
74	Calculations of the site specific stretching frequencies of CO adsorbed on Li+/ZSM-5. Physical Chemistry Chemical Physics, 2004, 6, 5580-5587.	2.8	41
75	Hydrogen adsorption on the zeolite Ca-A: DFT and FT-IR investigation. Chemical Physics Letters, 2009, 477, 139-143.	2.6	40
76	Tuning the Porosity and Photocatalytic Performance of Triazineâ€Based Graphdiyne Polymers through Polymorphism. ChemSusChem, 2019, 12, 194-199.	6.8	39
77	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.	3.3	38
78	The effect of water on the validity of LÃ¶wenstein's rule. Chemical Science, 2019, 10, 5705-5711.	7.4	37
79	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.	5.3	36
80	On the site-specificity of polycarbonyl complexes in Cu/zeolites: combined experimental and DFT study. Physical Chemistry Chemical Physics, 2006, 8, 5535-5542.	2.8	35
81	Tailored Band Gaps in Sulfurâ€and Nitrogenâ€Containing Porous Donorâ€“Acceptor Polymers. Chemistry - A European Journal, 2017, 23, 13023-13027.	3.3	35
82	On the Existence of CuI Pairs in ZSM-5â€”A Computational Study. Chemistry - A European Journal, 2002, 8, 2099.	3.3	33
83	Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL. Catalysis Today, 2013, 204, 15-21.	4.4	33
84	Theoretical investigation of the FriedlÃnder reaction catalysed by CuBTC: Concerted effect of the adjacent Cu2+ sites. Catalysis Today, 2013, 204, 101-107.	4.4	33
85	Theoretical investigation of layered zeolites with MWW topology: MCM-22P vs. MCM-56. Dalton Transactions, 2014, 43, 10443-10450.	3.3	33
86	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.	2.6	32
87	From Doubleâ€Fourâ€Ring Germanosilicates to New Zeolites: In Silico Investigation. ChemPhysChem, 2014, 15, 2972-2976.	2.1	31
88	The ADOR synthesis of new zeolites: In silico investigation. Catalysis Today, 2015, 243, 32-38.	4.4	30
89	Adsorption of pentane isomers on metal-organic frameworks Cu-BTC and Fe-BTC. Catalysis Today, 2015, 243, 69-75.	4.4	30
90	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.	2.8	29

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91	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.	4.4	29
92	Theoretical investigation of dinitrosyl complexes in Cu-zeolites as intermediates in deNOx process. Physical Chemistry Chemical Physics, 2009, 11, 1447.	2.8	29
93	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.	3.7	29
94	Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling. Journal of Materials Chemistry C, 2021, 9, 11132-11141.	5.5	29
95	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.	2.6	28
96	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.	2.8	28
97	Control of CO2adsorption heats by the Al distribution in FER zeolites. Physical Chemistry Chemical Physics, 2012, 14, 1117-1120.	2.8	28
98	Metalâ€“Organic Frameworks Mâ€MOFâ€74 and Mâ€MILâ€100: Comparison of Textural, Acidic, and Catalytic Properties. ChemPlusChem, 2016, 81, 828-835.	2.8	28
99	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.	2.6	27
100	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.	2.6	27
101	New catalytic materials for energy and chemistry in transition. Chemical Society Reviews, 2018, 47, 8066-8071.	38.1	27
102	Investigation of a hybrid TCSCF-DFT procedure. Theoretical Chemistry Accounts, 1998, 99, 135-140.	1.4	26
103	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.	1.8	26
104	Variableâ€Temperature IR Spectroscopic and Theoretical Studies on CO₂ Adsorbed in Zeolite Kâ€FER. ChemPhysChem, 2011, 12, 1435-1443.	2.1	26
105	Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. Catalysis Today, 2014, 227, 2-8.	4.4	25
106	Theoretical study of the low-lying triplet and singlet states of diradicals. 2. Cyclopentadienyltrimethylenemethane. Journal of the American Chemical Society, 1992, 114, 4747-4752.	13.7	23
107	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.	3.0	22
108	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.	3.1	22

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109	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.	3.1	22
110	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.	2.8	22
111	Structure and Hydrogen Bonding of Different Isomers of 2-AminopyridineÂ·NH3Studied by IR/R2PI Spectroscopy. Journal of Physical Chemistry A, 2004, 108, 3338-3343.	2.5	21
112	Characterization of the Cu+ sites in MFI zeolites: combined computational and experimental study. Catalysis Today, 2005, 100, 385-389.	4.4	21
113	Pressure-induced chemistry for the 2D to 3D transformation of zeolites. Journal of Materials Chemistry A, 2018, 6, 5255-5259.	10.3	21
114	The BrÃ¸nsted acidity of three- and two-dimensional zeolites. Microporous and Mesoporous Materials, 2019, 282, 121-132.	4.4	21
115	Correlation Between Catalytic Activity and Metal Cation Coordination: NO Decomposition Over Cu/Zeolites. ChemCatChem, 2009, 1, 449-453.	3.7	20
116	Combined Experimental and Theoretical Investigations of Heterogeneous Dual Cation Sites in Cu,M-FER Zeolites. Journal of Physical Chemistry C, 2011, 115, 13312-13321.	3.1	20
117	Direct hydrodeoxygenation of phenol over carbon-supported Ru catalysts: A computational study. Journal of Molecular Catalysis A, 2016, 423, 300-307.	4.8	20
118	Two-dimensional tetragonal GaOI and InOI sheets: In-plane anisotropic optical properties and application to photocatalytic water splitting. Catalysis Today, 2020, 340, 178-182.	4.4	20
119	Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum. ACS Catalysis, 2020, 10, 11057-11068.	11.2	20
120	Characterization of Ag+ Sites in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 2001, 3, 4791-4795.	2.8	18
121	A density functional study of EPR hyperfine coupling of vanadocene(IV) complexes. Chemical Physics, 2004, 305, 291-298.	1.9	18
122	UTL zeolite and the way beyond. Microporous and Mesoporous Materials, 2013, 182, 229-238.	4.4	18
123	Comment on â€˜â€˜Temperature programmed desorption of molecular hydrogen from a Si(100)â€2Ã—1 surface: Theory and experimentâ€™â€™ [J. Chem. Phys. 99, 7038 (1993)]. Journal of Chemical Physics, 1994, 101, 2648-2649.	3.0	17
124	The surface stability and equilibrium crystal morphology of Ni₂P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach. CrystEngComm, 2016, 18, 3808-3818.	2.6	17
125	Topological study of the chemisorption behavior of carbon monoxide on the Ni(112) and Cu(112) surfaces. Surface Science, 1987, 181, 413-435.	1.9	16
126	Applications of Quantum Chemical Methods in Zeolite Science. Studies in Surface Science and Catalysis, 2007, , 701-XXI.	1.5	16

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127	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.	2.5	16
128	Computational and Variableâ€Temperature Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on Zeolite Caâ€A. ChemPhysChem, 2009, 10, 1058-1065.	2.1	14
129	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.	3.0	13
130	The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology. Catalysis Today, 2018, 304, 12-21.	4.4	13
131	Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite. Journal of Physical Chemistry C, 2018, 122, 26088-26095.	3.1	13
132	The Role of Water Loading and Germanium Content in Germanosilicate Hydrolysis. Journal of Physical Chemistry C, 2021, 125, 23744-23757.	3.1	12
133	Interaction of acetonitrile with Na-zeolites: adsorption modes and vibrational dynamics in the zeolite channels and cavities. Physical Chemistry Chemical Physics, 2008, 10, 4189.	2.8	11
134	Layered inorganic solids. Dalton Transactions, 2014, 43, 10274.	3.3	11
135	Theoretical and experimental study of CO adsorption on Ca-FER zeolite. Catalysis Today, 2015, 243, 53-61.	4.4	11
136	Understanding the Structure of Cationic Sites in Alkali Metal-Grafted USY Zeolites. Journal of Physical Chemistry C, 2016, 120, 4954-4960.	3.1	11
137	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
138	Themed Issue on characterization of adsorbed species. Physical Chemistry Chemical Physics, 2010, 12, 6307.	2.8	10
139	Intramolecular Hydroalkoxylation of Nonâ€Activated Cï£¾C Bonds Catalysed by Zeolites: An Experimental and Theoretical Study. ChemSusChem, 2013, 6, 1021-1030.	6.8	10
140	Theoretical investigation of CO catalytic oxidation by a Feâ€“PtSe₂ monolayer. RSC Advances, 2017, 7, 19630-19638.	3.6	10
141	Magneto-structural correlations of novel kagomÃ©-type metal organic frameworks. Journal of Materials Chemistry C, 2019, 7, 6692-6697.	5.5	10
142	Unexpected Photoreactivity in a NO₂-Functionalized Aluminum-MOF. Journal of Physical Chemistry C, 2015, 119, 26401-26408.	3.1	9
143	Combined PDF and Rietveld studies of ADORable zeolites and the disordered intermediate IPC-1P. Dalton Transactions, 2016, 45, 14124-14130.	3.3	9
144	The effect of the zeolite pore size on the Lewis acid strength of extra-framework cations. Physical Chemistry Chemical Physics, 2016, 18, 18063-18073.	2.8	9

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145	MÃ¶ssbauerite as Iron-Only Layered Oxyhydroxide Catalyst for WO₃ Photoanodes. Inorganic Chemistry, 2019, 58, 9655-9662.	4.0	9
146	Systematic computational investigation of an Ni3Fe catalyst for the OER. Catalysis Today, 2020, 345, 220-226.	4.4	9
147	Mechanism of Zeolite Hydrolysis under Basic Conditions. Chemistry of Materials, 2021, 33, 9202-9212.	6.7	9
148	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.	2.4	8
149	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
150	Flexibilization of Biorefineries: Tuning Lignin Hydrogenation by Hydrogen Partial Pressure. ChemSusChem, 2021, 14, 373-378.	6.8	8
151	Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS₄) nanowires with carriers induces half-metallicity. Journal of Materials Chemistry C, 2021, 9, 3122-3128.	5.5	8
152	Topological study of the chemisorption behavior of carbon monoxide on the Pt(112) surface. Chemical Physics, 1988, 119, 289-295.	1.9	7
153	Structure Determination of the Oxygen Evolution Catalyst MÃ¶ssbauerite. Journal of Physical Chemistry C, 2019, 123, 25157-25165.	3.1	7
154	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
155	Ab Initio Simulation of Cu-Species in Zeolites: Siting, Coordination, UV-Vis Spectra and Reactivity. , 2001, , 221-234.		6
156	Palladium clusters on graphene support: An ab initio study. Chemical Physics Letters, 2016, 646, 56-63.	2.6	5
157	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
158	Coordination Compounds Based on 1,2,3,4-Tetrahydro-isoquinoline-3-carboxylic Acid. Molecules, 2007, 12, 1064-1079.	3.8	4
159	Synthesis and Postâ€Synthesis Transformation of Germanosilicate Zeolites. Angewandte Chemie, 2020, 132, 19548-19557.	2.0	4
160	Topological study of light sensitive photocathodes based on the Sb(NaKCs) system. Applied Surface Science, 1986, 25, 167-178.	6.1	3
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