Veronique Van Speybroeck

List of Publications by Year
in descending order

379	23,124	8755 77	14779 131
papers	citations	h-index	g-index

393	393	393	23807
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A general synthesis of azetidines by copper-catalysed photoinduced anti-Baldwin radical cyclization of ynamides. Nature Communications, 2022, 13, 560.	5.8	32
2	A comparative theoretical study on the solvent dependency of anthocyanin extraction profiles. Journal of Molecular Liquids, 2022, 351, 118606.	2.3	5
3	Mechanistic Characterization of Zeolite-Catalyzed Aromatic Electrophilic Substitution at Realistic Operating Conditions. Jacs Au, 2022, 2, 502-514.	3.6	17
4	Atomistic insight in the flexibility and heat transport properties of the stimuli-responsive metalâ€“organic framework MIL-53(Al) for water-adsorption applications using molecular simulations. Faraday Discussions, 2021, 225, 301-323.	1.6	17
5	Identification of vanadium dopant sites in the metalâ€“organic framework DUT-5(Al). Physical Chemistry Chemical Physics, 2021, 23, 7088-7100.	1.3	1
6	Correlating MOF-808 parameters with mixed-matrix membrane (MMM) CO₂ permeation for a more rational MMM development. Journal of Materials Chemistry A, 2021, 9, 12782-12796.	5.2	26
7	Porous organic polymers as metal free heterogeneous organocatalysts. Green Chemistry, 2021, 23, 7361-7434.	4.6	54
8	Access to Biorenewable and CO₂-Based Polycarbonates from Exovinylene Cyclic Carbonates. ACS Sustainable Chemistry and Engineering, 2021, 9, 1714-1728.	3.2	22
9	Unravelling thermal stress due to thermal expansion mismatch in metalâ€“organic frameworks for methane storage. Journal of Materials Chemistry A, 2021, 9, 4898-4906.	5.2	11
10	Crystals springing into action: metalâ€“organic framework CUK-1 as a pressure-driven molecular spring. Chemical Science, 2021, 12, 5682-5687.	3.7	21
11	Texture Formation in Polycrystalline Thin Films of Allâ€Inorganic Lead Halide Perovskite. Advanced Materials, 2021, 33, e2007224.	11.1	18
12	Chlorination of a Zeolitic-Imidazolate Framework Tunes Packing and van der Waals Interaction of Carbon Dioxide for Optimized Adsorptive Separation. Journal of the American Chemical Society, 2021, 143, 4962-4968.	6.6	21
13	Titelbild: Experimental and Theoretical Evidence for the Promotional Effect of Acid Sites on the Diffusion of Alkenes through Smallâ€Pore Zeolites (Angew. Chem. 18/2021). Angewandte Chemie, 2021, 133, 9813-9813.	1.6	1
14	Experimental and Theoretical Evidence for the Promotional Effect of Acid Sites on the Diffusion of Alkenes through Smallâ€Pore Zeolites. Angewandte Chemie, 2021, 133, 10104-10110.	1.6	10
15	Experimental and Theoretical Evidence for the Promotional Effect of Acid Sites on the Diffusion of Alkenes through Smallâ€Pore Zeolites. Angewandte Chemie - International Edition, 2021, 60, 10016-10022.	7.2	39
16	Overview of Nâ€Rich Antennae Investigated in Lanthanideâ€Based Temperature Sensing. Chemistry - A European Journal, 2021, 27, 7214-7230.	1.7	19
17	A Comparative Study on the Photophysical Properties of Anthocyanins and Pyranoanthocyanins. Chemistry - A European Journal, 2021, 27, 5956-5971.	1.7	9
18	Quantifying the Likelihood of Structural Models through a Dynamically Enhanced Powder Xâ€Ray Diffraction Protocol. Angewandte Chemie, 2021, 133, 8995-9004.	1.6	0

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19	Quantifying the Likelihood of Structural Models through a Dynamically Enhanced Powder Xâ€Ray Diffraction Protocol. Angewandte Chemie - International Edition, 2021, 60, 8913-8922.	7.2	11
20	Coordination and activation of nitrous oxide by iron zeolites. Nature Catalysis, 2021, 4, 332-340.	16.1	49
21	High-rate nanofluidic energy absorption in porous zeolitic frameworks. Nature Materials, 2021, 20, 1015-1023.	13.3	52
22	Frontispiece: Overview of Nâ€Rich Antennae Investigated in Lanthanideâ€Based Temperature Sensing. Chemistry - A European Journal, 2021, 27, .	1.7	0
23	Non-food applications of natural dyes extracted from agro-food residues: A critical review. Journal of Cleaner Production, 2021, 301, 126920.	4.6	40
24	Towards modeling spatiotemporal processes in metalâ€“organic frameworks. Trends in Chemistry, 2021, 3, 605-619.	4.4	31
25	Large-Scale Molecular Dynamics Simulations Reveal New Insights Into the Phase Transition Mechanisms in MIL-53(Al). Frontiers in Chemistry, 2021, 9, 718920.	1.8	15
26	Mobility and Reactivity of Cu⁺ Species in Cu-CHA Catalysts under NH₃-SCR-NOx Reaction Conditions: Insights from AIMD Simulations. Jacs Au, 2021, 1, 1778-1787.	3.6	27
27	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
28	Dynamic evolution of catalytic active sites within zeolite catalysis. , 2021, , .		0
29	Interfacial study of clathrates confined in reversed silica pores. Journal of Materials Chemistry A, 2021, 9, 21835-21844.	5.2	8
30	Acidity effect on benzene methylation kinetics over substituted H-MeAlPO-5 catalysts. Journal of Catalysis, 2021, 404, 594-606.	3.1	10
31	Elucidation of the pre-nucleation phase directing metal-organic framework formation. Cell Reports Physical Science, 2021, 2, 100680.	2.8	11
32	RÃ¼cktitelbild: BrÃ¸nsted Acid Catalyzed Tandem Defunctionalization of Biorenewable Ferulic acid and Derivates into Bioâ€Catechol (Angew. Chem. 8/2020). Angewandte Chemie, 2020, 132, 3364-3364.	1.6	0
33	The potential of anthocyanins from blueberries as a natural dye for cotton: A combined experimental and theoretical study. Dyes and Pigments, 2020, 176, 108180.	2.0	73
34	BrÃ¸nsted Acid Catalyzed Tandem Defunctionalization of Biorenewable Ferulic acid and Derivates into Bioâ€Catechol. Angewandte Chemie, 2020, 132, 3087-3092.	1.6	11
35	BrÃ¸nsted Acid Catalyzed Tandem Defunctionalization of Biorenewable Ferulic acid and Derivates into Bioâ€Catechol. Angewandte Chemie - International Edition, 2020, 59, 3063-3068.	7.2	31
36	Structural and Photophysical Properties of Various Polypyridyl Ligands: A Combined Experimental and Computational Study. ChemPhysChem, 2020, 21, 2489-2505.	1.0	5

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37	Mechanistic Insight into the Framework Methylation of H-ZSM-5 for Varying Methanol Loadings and Si/Al Ratios Using First-Principles Molecular Dynamics Simulations. ACS Catalysis, 2020, 10, 8904-8915.	5.5	36
38	Shape-selective Câ€“H activation of aromatics to biarylic compounds using molecular palladium in zeolites. Nature Catalysis, 2020, 3, 1002-1009.	16.1	41
39	Strongly Reducing (Diarylamino)benzene-Based Covalent Organic Framework for Metal-Free Visible Light Photocatalytic H₂O₂ Generation. Journal of the American Chemical Society, 2020, 142, 20107-20116.	6.6	239
40	Theoretical and Spectroscopic Evidence of the Dynamic Nature of Copper Active Sites in Cu-CHA Catalysts under Selective Catalytic Reduction (NH₃â€“SCRâ€“NO_x) Conditions. Journal of Physical Chemistry Letters, 2020, 11, 10060-10066.	2.1	27
41	Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts. Nature Materials, 2020, 19, 1081-1087.	13.3	52
42	Structural and Photophysical Properties of Various Polypyridyl Ligands: A Combined Experimental and Computational Study. ChemPhysChem, 2020, 21, 2488-2488.	1.0	0
43	Cationâ‹¯Ï€ Interactions Accelerate the Living Cationic Ring-Opening Polymerization of Unsaturated 2-Alkyl-2-oxazolines. Macromolecules, 2020, 53, 3832-3846.	2.2	4
44	Nâ€“Rich Porous Polymer with Isolated Tb³⁺â€“Ions Displays Unique Temperature Dependent Behavior through the Absence of Thermal Quenching. Chemistry - A European Journal, 2020, 26, 15596-15604.	1.7	4
45	Light Olefin Diffusion during the MTO Process on H-SAPO-34: A Complex Interplay of Molecular Factors. Journal of the American Chemical Society, 2020, 142, 6007-6017.	6.6	92
46	Charting the Metal-Dependent High-Pressure Stability of Bimetallic UiO-66 Materials. , 2020, 2, 438-445.		21
47	Elucidating the promotional effect of a covalent triazine framework in aerobic oxidation. Applied Catalysis B: Environmental, 2020, 269, 118769.	10.8	17
48	Engineering a Highly Defective Stable UiO-66 with Tunable Lewis- BrÃ¸nsted Acidity: The Role of the Hemilabile Linker. Journal of the American Chemical Society, 2020, 142, 3174-3183.	6.6	156
49	Ab initio enhanced sampling kinetic study on MTO ethene methylation reaction. Journal of Catalysis, 2020, 388, 38-51.	3.1	24
50	Optical Properties of Isolated and Covalent Organic Framework-Embedded Ruthenium Complexes. Journal of Physical Chemistry A, 2019, 123, 6854-6867.	1.1	7
51	Thermal unequilibrium of strained black CsPbI ₃ thin films. Science, 2019, 365, 679-684.	6.0	444
52	Insight into the Role of Water on the Methylation of Hexamethylbenzene in Hâ€“SAPOâ€“34 from First Principle Molecular Dynamics Simulations. ChemCatChem, 2019, 11, 3993-4010.	1.8	17
53	Thermal Engineering of Metalâ€“Organic Frameworks for Adsorption Applications: A Molecular Simulation Perspective. ACS Applied Materials & Interfaces, 2019, 11, 38697-38707.	4.0	56
54	Unraveling the thermodynamic criteria for size-dependent spontaneous phase separation in soft porous crystals. Nature Communications, 2019, 10, 4842.	5.8	47

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55	Dynamic Interplay between Defective UiOâ€66 and Protic Solvents in Activated Processes. Chemistry - A European Journal, 2019, 25, 15315-15325.	1.7	13
56	A Supramolecular View on the Cooperative Role of BrÃ¸nsted and Lewis Acid Sites in Zeolites for Methanol Conversion. Journal of the American Chemical Society, 2019, 141, 14823-14842.	6.6	80
57	Unraveling the thermodynamic conditions for negative gas adsorption in soft porous crystals. Communications Physics, 2019, 2, .	2.0	9
58	Ethene Dimerization on Zeolite-Hosted Ni Ions: Reversible Mobilization of the Active Site. ACS Catalysis, 2019, 9, 5645-5650.	5.5	54
59	A Switchable Domino Process for the Construction of Novel CO₂â€Sourced Sulfurâ€Containing Building Blocks and Polymers. Angewandte Chemie - International Edition, 2019, 58, 11768-11773.	7.2	26
60	Collective action of water molecules in zeolite dealumination. Catalysis Science and Technology, 2019, 9, 3721-3725.	2.1	43
61	Effect of Zeolite Topology and Reactor Configuration on the Direct Conversion of CO₂ to Light Olefins and Aromatics. ACS Catalysis, 2019, 9, 6320-6334.	5.5	144
62	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. Matter, 2019, 1, 219-234.	5.0	170
63	Modeling the Structural and Thermal Properties of Loaded Metalâ€“Organic Frameworks. An Interplay of Quantum and Anharmonic Fluctuations. Journal of Chemical Theory and Computation, 2019, 15, 3237-3249.	2.3	22
64	Electronic properties of heterogenized Ru(<scp>ii</scp>) polypyridyl photoredox complexes on covalent triazine frameworks. Journal of Materials Chemistry A, 2019, 7, 8433-8442.	5.2	6
65	On the importance of anharmonicities and nuclear quantum effects in modelling the structural properties and thermal expansion of MOF-5. Journal of Chemical Physics, 2019, 150, 094503.	1.2	16
66	Active Role of Methanol in Post-Synthetic Linker Exchange in the Metalâ€“Organic Framework UiO-66. Chemistry of Materials, 2019, 31, 1359-1369.	3.2	43
67	Immobilization of Ir(I) complex on covalent triazine frameworks for C H borylation reactions: A combined experimental and computational study. Journal of Catalysis, 2019, 371, 135-143.	3.1	37
68	Modeling Gas Adsorption in Flexible Metalâ€“Organic Frameworks via Hybrid Monte Carlo/Molecular Dynamics Schemes. Advanced Theory and Simulations, 2019, 2, 1800177.	1.3	40
69	The impact of lattice vibrations on the macroscopic breathing behavior of MIL-53(Al). Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 529-545.	0.4	22
70	Frontiers in Modeling Metalâ€“Organic Frameworks. Advanced Theory and Simulations, 2019, 2, 1900196.	1.3	3
71	Pillared-layered metalâ€“organic frameworks for mechanical energy storage applications. Journal of Materials Chemistry A, 2019, 7, 22663-22674.	5.2	34
72	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220

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73	Understanding BrÃ¸nsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 338-338.	1.0	0
74	Exploring Lanthanide Doping in UiO-66: A Combined Experimental and Computational Study of the Electronic Structure. Inorganic Chemistry, 2018, 57, 5463-5474.	1.9	51
75	The Importance of Cell Shape Sampling To Accurately Predict Flexibility in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2018, 14, 1186-1197.	2.3	13
76	Extension of the QuickFF force field protocol for an improved accuracy of structural, vibrational, mechanical and thermal properties of metalâ€“organic frameworks. Journal of Computational Chemistry, 2018, 39, 999-1011.	1.5	59
77	On the intrinsic dynamic nature of the rigid UiO-66 metalâ€“organic framework. Chemical Science, 2018, 9, 2723-2732.	3.7	41
78	Formation of Fluorinated Amido Esters through Unexpected C3â^'C4 Bond Fission in 4â€Trifluoromethylâ€3â€oxoâ€²â€lactams. Chemistry - an Asian Journal, 2018, 13, 421-431.	1.7	4
79	Thermodynamic insight into stimuli-responsive behaviour of soft porous crystals. Nature Communications, 2018, 9, 204.	5.8	104
80	Elucidating the Vibrational Fingerprint of the Flexible Metalâ€“Organic Framework MIL-53(Al) Using a Combined Experimental/Computational Approach. Journal of Physical Chemistry C, 2018, 122, 2734-2746.	1.5	70
81	Theoretical insight into the regioselective ring-expansions of bicyclic aziridinium ions. Organic and Biomolecular Chemistry, 2018, 16, 796-806.	1.5	16
82	Use of 3-Hydroxy-4-(trifluoromethyl)azetidin-2-ones as Building Blocks for the Preparation of Trifluoromethyl-Containing Aminopropanes, 1,3-Oxazinan-2-ones, Aziridines, and 1,4-Dioxan-2-ones. Synthesis, 2018, 50, 1439-1456.	1.2	11
83	Influence of a Confined Methanol Solvent on the Reactivity of Active Sites in UiOâ€66. ChemPhysChem, 2018, 19, 420-429.	1.0	17
84	Understanding BrÃ¸nstedâ€Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 341-358.	1.0	21
85	Reliably Modeling the Mechanical Stability of Rigid and Flexible Metalâ€“Organic Frameworks. Accounts of Chemical Research, 2018, 51, 138-148.	7.6	88
86	Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. Journal of Chemical Theory and Computation, 2018, 14, 6359-6369.	2.3	12
87	Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. Nature Communications, 2018, 9, 4899.	5.8	90
88	Protocol for Identifying Accurate Collective Variables in Enhanced Molecular Dynamics Simulations for the Description of Structural Transformations in Flexible Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2018, 14, 5511-5526.	2.3	19
89	How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. ACS Catalysis, 2018, 8, 9579-9595.	5.5	70
90	Structureâ€“performance descriptors and the role of Lewis acidity in the methanol-to-propylene process. Nature Chemistry, 2018, 10, 804-812.	6.6	221

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91	Entropy Contributions to Transition State Modeling. , 2018, , 189-228.		5
92	The Remarkable Amphoteric Nature of Defective UiOâ€66 in Catalytic Reactions. ChemCatChem, 2017, 9, 2203-2210.	1.8	46
93	Design of a thermally controlled sequence of triazolinedione-based click and transclick reactions. Chemical Science, 2017, 8, 3098-3108.	3.7	45
94	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation ofn-Butane in BrÃ¸nsted Acidic Zeolites. ACS Catalysis, 2017, 7, 2685-2697.	5.5	42
95	Mechanical properties of a gallium fumarate metalâ€“organic framework: a joint experimental-modelling exploration. Journal of Materials Chemistry A, 2017, 5, 11047-11054.	5.2	27
96	Alternating Copolymer of Double Four Ring Silicate and Dimethyl Silicone Monomerâ€“PSSâ€1. Chemistry - A European Journal, 2017, 23, 11286-11293.	1.7	5
97	Metalâ€“organic and covalent organic frameworks as single-site catalysts. Chemical Society Reviews, 2017, 46, 3134-3184.	18.7	861
98	Benzene co-reaction with methanol and dimethyl ether over zeolite and zeotype catalysts: Evidence of parallel reaction paths to toluene and diphenylmethane. Journal of Catalysis, 2017, 349, 136-148.	3.1	70
99	Missing Linkers: An Alternative Pathway to UiO-66 Electronic Structure Engineering. Chemistry of Materials, 2017, 29, 3006-3019.	3.2	176
100	Tandem Addition of Phosphite Nucleophiles Across Unsaturated Nitrogen-Containing Systems: Mechanistic Insights on Regioselectivity. Journal of Organic Chemistry, 2017, 82, 188-201.	1.7	6
101	Effect of temperature and branching on the nature and stability of alkene cracking intermediates in H-ZSM-5. Journal of Catalysis, 2017, 345, 53-69.	3.1	92
102	High-Throughput Screening of Extrinsic Point Defect Properties in Si and Ge: Database and Applications. Chemistry of Materials, 2017, 29, 975-984.	3.2	10
103	Reactivity of 3â€Oxoâ€²â€lactams with Respect to Primary Aminesâ€”An Experimental and Computational Approach. Chemistry - A European Journal, 2017, 23, 18002-18009.	1.7	8
104	A series of sulfonic acid functionalized mixed-linker DUT-4 analogues: synthesis, gas sorption properties and catalytic performance. Dalton Transactions, 2017, 46, 14356-14364.	1.6	15
105	Asymmetric Synthesis of 3,4-Disubstituted 2-(Trifluoromethyl)pyrrolidines through Rearrangement of Chiral 2-(2,2,2-Trifluoro-1-hydroxyethyl)azetidines. Journal of Organic Chemistry, 2017, 82, 10092-10109.	1.7	13
106	Hydrogen Transfer versus Methylation: On the Genesis of Aromatics Formation in the Methanol-To-Hydrocarbons Reaction over H-ZSM-5. ACS Catalysis, 2017, 7, 5773-5780.	5.5	102
107	Efficient Construction of Free Energy Profiles of Breathing Metalâ€“Organic Frameworks Using Advanced Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5861-5873.	2.3	45
108	Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. Journal of Physical Chemistry C, 2017, 121, 25309-25322.	1.5	34

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109	Nature of active sites on UiO-66 and beneficial influence of water in the catalysis of Fischer esterification. Journal of Catalysis, 2017, 352, 401-414.	3.1	172
110	The Monomer Electron Density Force Field (MEDFF): A Physically Inspired Model for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 161-179.	2.3	53
111	A Breathing Zirconium Metalâ€“Organic Framework with Reversible Loss of Crystallinity by Correlated Nanodomain Formation. Chemistry - A European Journal, 2016, 22, 3264-3267.	1.7	41
112	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. Journal of Chemical Theory and Computation, 2016, 12, 3894-3912.	2.3	119
113	Vibrational fingerprint of the absorption properties of UiO-type MOF materials. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
114	Towards metalâ€“organic framework based field effect chemical sensors: UiO-66-NH₂ for nerve agent detection. Chemical Science, 2016, 7, 5827-5832.	3.7	108
115	Cutting the cost of carbon capture: a case for carbon capture and utilization. Faraday Discussions, 2016, 192, 391-414.	1.6	33
116	Is the error on first-principles volume predictions absolute or relative?. Computational Materials Science, 2016, 117, 390-396.	1.4	15
117	Effect of Lewis acids on the stereoregularity of N,N-dimethyl acrylamide: A computational approach. European Polymer Journal, 2016, 83, 67-76.	2.6	3
118	Suppression of the Aromatic Cycle in Methanol-to-Olefins Reaction over ZSM-5 by Post-Synthetic Modification Using Calcium. ChemCatChem, 2016, 8, 3005-3005.	1.8	5
119	Water coordination and dehydration processes in defective UiO-66 type metal organic frameworks. CrystEngComm, 2016, 18, 7056-7069.	1.3	58
120	Suppression of the Aromatic Cycle in Methanolâ€toâ€Olefins Reaction over ZSMâ€5 by Postâ€Synthetic Modification Using Calcium. ChemCatChem, 2016, 8, 3057-3063.	1.8	71
121	Acidity Constant (pK_a) Calculation of Large Solvated Dye Molecules: Evaluation of Two Advanced Molecular Dynamics Methods. ChemPhysChem, 2016, 17, 3447-3459.	1.0	20
122	Heterogeneous Ru(<scp>iii</scp>) oxidation catalysts via â€˜clickâ€™ bidentate ligands on a periodic mesoporous organosilica support. Green Chemistry, 2016, 18, 6035-6045.	4.6	14
123	Thermodynamic Insight in the High-Pressure Behavior of UiO-66: Effect of Linker Defects and Linker Expansion. Chemistry of Materials, 2016, 28, 5721-5732.	3.2	97
124	Exploring the Flexibility of MIL-47(V)-Type Materials Using Force Field Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 14934-14947.	1.5	48
125	DMRG-CASPT2 study of the longitudinal static second hyperpolarizability of all-trans polyenes. Journal of Chemical Physics, 2016, 145, 054120.	1.2	58
126	Facile Synthesis of Cooperative Acidâ€“Base Catalysts by Clicking Cysteine and Cysteamine on an Ethyleneâ€Bridged Periodic Mesoporous Organosilica. European Journal of Inorganic Chemistry, 2016, 2016, 2144-2151.	1.0	20

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127	On the stability and nature of adsorbed pentene in BrÃ¸nsted acid zeolite H-ZSM-5 at 323 K. Journal of Catalysis, 2016, 340, 227-235.	3.1	55
128	Halochromic properties of sulfonphthaleine dyes in a textile environment: The influence of substituents. Dyes and Pigments, 2016, 124, 249-257.	2.0	49
129	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
130	Insight into the Effect of Water on the Methanol-to-Olefins Conversion in H-SAPO-34 from Molecular Simulations and in Situ Microspectroscopy. ACS Catalysis, 2016, 6, 1991-2002.	5.5	110
131	Towards molecular control of elementary reactions in zeolite catalysis by advanced molecular simulations mimicking operating conditions. Catalysis Science and Technology, 2016, 6, 2686-2705.	2.1	38
132	Ab initio study of the trapping of polonium on noble metals. Journal of Nuclear Materials, 2016, 472, 35-42.	1.3	6
133	Influence of Solvation and Dynamics on the Mechanism and Kinetics of Nucleophilic Aromatic Substitution Reactions in Liquid Ammonia. Journal of Organic Chemistry, 2016, 81, 1635-1644.	1.7	18
134	Systematic study of the chemical and hydrothermal stability of selected â€œstableâ€•Metal Organic Frameworks. Microporous and Mesoporous Materials, 2016, 226, 110-116.	2.2	277
135	Ligand Addition Energies and the Stoichiometry of Colloidal Nanocrystals. ACS Nano, 2016, 10, 1462-1474.	7.3	33
136	Mechanical energy storage performance of an aluminum fumarate metalâ€“organic framework. Chemical Science, 2016, 7, 446-450.	3.7	103
137	Normal mode analysis of macromolecular systems with the mobile block Hessian method. , 2015, , .		0
138	Synthesis of poly(2â€oxazoline)s with side chain methyl ester functionalities: Detailed understanding of living copolymerization behavior of methyl ester containing monomers with 2â€alkylâ€2â€oxazolines. Journal of Polymer Science Part A, 2015, 53, 2649-2661.	2.5	43
139	Mechanistic Investigation on Oxygen Transfer with the Manganeseâ€Salen Complex. ChemCatChem, 2015, 7, 2711-2719.	1.8	10
140	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. Chemistry - A European Journal, 2015, 21, 19176-19185.	1.7	9
141	A Flexible Photoactive Titanium Metalâ€“Organic Framework Based on a [Ti^{IV}₃(Î¼₃â€O)(O)₂(COO)₆] Cluster. Angewandte Chemie - International Edition, 2015, 54, 13912-13917.	7.2	103
142	How zeolitic acid strength and composition alter the reactivity of alkenes and aromatics towards methanol. Journal of Catalysis, 2015, 328, 186-196.	3.1	49
143	QuickFF: A program for a quick and easy derivation of force fields for metalâ€organic frameworks from ab initio input. Journal of Computational Chemistry, 2015, 36, 1015-1027.	1.5	132
144	Possibility of [1,5] Sigmatropic Shifts in Bicyclo[4.2.0]octa-2,4-dienes. Journal of Organic Chemistry, 2015, 80, 2609-2620.	1.7	13

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145	Convergence of Atomic Charges with the Size of the Enzymatic Environment. Journal of Chemical Information and Modeling, 2015, 55, 564-571.	2.5	17
146	Elucidating the Structural Isomerism of Fluorescent Strigolactone Analogue CISAâ€1. European Journal of Organic Chemistry, 2015, 2015, 1211-1217.	1.2	3
147	Au@UiO-66: a base free oxidation catalyst. RSC Advances, 2015, 5, 22334-22342.	1.7	59
148	Beyond the Diketopiperazine Family with Alternatively Bridged Brevianamide F Analogues. Journal of Organic Chemistry, 2015, 80, 8046-8054.	1.7	5
149	The enantioselectivity of the manganese-salen complex in the epoxidation of unfunctionalized olefins and the influence of grafting. Journal of Molecular Catalysis A, 2015, 406, 106-113.	4.8	7
150	Carbon capture turned upside down: high-temperature adsorption & low-temperature desorption (HALD). Energy and Environmental Science, 2015, 8, 2480-2491.	15.6	19
151	Advances in theory and their application within the field of zeolite chemistry. Chemical Society Reviews, 2015, 44, 7044-7111.	18.7	405
152	Complex Reaction Environments and Competing Reaction Mechanisms in Zeolite Catalysis: Insights from Advanced Molecular Dynamics. Chemistry - A European Journal, 2015, 21, 9385-9396.	1.7	53
153	A Comparison of Barostats for the Mechanical Characterization of Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2015, 11, 5583-5597.	2.3	83
154	Mechanical Properties from Periodic Plane Wave Quantum Mechanical Codes: The Challenge of the Flexible Nanoporous MIL-47(V) Framework. Journal of Physical Chemistry C, 2015, 119, 23752-23766.	1.5	37
155	Determination of the Nature of the Cu Coordination Complexes Formed in the Presence of NO and NH₃ within SSZ-13. Journal of Physical Chemistry C, 2015, 119, 24393-24403.	1.5	36
156	Semi-analytical mean-field model for predicting breathing in metalâ€“organic frameworks. Molecular Simulation, 2015, 41, 1311-1328.	0.9	21
157	Fine-tuning the theoretically predicted structure of MIL-47(V) with the aid of powder X-ray diffraction. CrystEngComm, 2015, 17, 8612-8622.	1.3	7
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