Veronique Van Speybroeck

List of Publications by Year
in descending order

379	23,124	7561 77	12933 131
papers	citations	h-index	g-index

393	393	393	21122
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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

#	Article	IF	Citations
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
158	Mechanistic studies of aldol condensations in UiO-66 and UiO-66-NH 2 metal organic frameworks. Journal of Catalysis, 2015, 331, 1-12.	3.1	88
159	Shape-Selective Diffusion of Olefins in 8-Ring Solid Acid Microporous Zeolites. Journal of Physical Chemistry C, 2015, 119, 23721-23734.	1.5	65
160	Understanding Intrinsic Light Absorption Properties of UiO-66 Frameworks: A Combined Theoretical and Experimental Study. Inorganic Chemistry, 2015, 54, 10701-10710.	1.9	155
161	Binary and ternary Po-containing molecules relevant for LBE cooled reactors at operating temperature. Journal of Nuclear Materials, 2015, 458, 288-295.	1.3	9
162	Active site engineering in UiO-66 type metalâ€“organic frameworks by intentional creation of defects: a theoretical rationalization. CrystEngComm, 2015, 17, 395-406.	1.3	190

#	Article	IF	Citations
163	Accelerated living cationic ring-opening polymerization of a methyl ester functionalized 2-oxazoline monomer. Polymer Chemistry, 2015, 6, 514-518.	1.9	58
164	Quasi-1D physics in metal-organic frameworks: MIL-47(V) from first principles. Beilstein Journal of Nanotechnology, 2014, 5, 1738-1748.	1.5	23
165	Communication: DMRG-SCF study of the singlet, triplet, and quintet states of oxo-Mn(Salen). Journal of Chemical Physics, 2014, 140, 241103.	1.2	82
166	Solution enthalpy of Po and Te in solid leadâ€“bismuth eutectic. Journal of Nuclear Materials, 2014, 450, 287-291.	1.3	9
167	Exploring the vibrational fingerprint of the electronic excitation energy via molecular dynamics. Journal of Chemical Physics, 2014, 140, 134105.	1.2	5
168	Ab initiobased thermal property predictions at a low cost: An error analysis. Physical Review B, 2014, 89, .	1.1	23
169	Substituent effects on absorption spectra of pH indicators: An experimental and computational study of sulfonphthaleine dyes. Dyes and Pigments, 2014, 102, 241-250.	2.0	80
170	Critical Analysis of the Accuracy of Models Predicting or Extracting Liquid Structure Information. Journal of Physical Chemistry B, 2014, 118, 2451-2470.	1.2	5
171	Error Estimates for Solid-State Density-Functional Theory Predictions: An Overview by Means of the Ground-State Elemental Crystals. Critical Reviews in Solid State and Materials Sciences, 2014, 39, 1-24.	6.8	404
172	Tetravalent Doping of <scp><scp>CeO</scp></scp>₂: The Impact of Valence Electron Character on Group IV Dopant Influence. Journal of the American Ceramic Society, 2014, 97, 258-266.	1.9	36
173	Vanadium metalâ€“organic frameworks: structures and applications. New Journal of Chemistry, 2014, 38, 1853-1867.	1.4	57
174	Automated generation of radical species in crystalline carbohydrate using ab initio MD simulations. Physical Chemistry Chemical Physics, 2014, 16, 17196-17205.	1.3	4
175	Determining the storage, availability and reactivity of NH₃within Cu-Chabazite-based Ammonia Selective Catalytic Reduction systems. Physical Chemistry Chemical Physics, 2014, 16, 1639-1650.	1.3	181
176	Aliovalent doping of CeO₂: DFT study of oxidation state and vacancy effects. Journal of Materials Chemistry A, 2014, 2, 13723-13737.	5.2	93
177	Flexibility versus rigidity: what determines the stability of zeolite frameworks? A case study. Materials Horizons, 2014, 1, 582-587.	6.4	13
178	Catalytic Performance of Vanadium MILâ€47 and Linkerâ€Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. ChemPlusChem, 2014, 79, 1183-1197.	1.3	20
179	First principle chemical kinetics in zeolites: the methanol-to-olefin process as a case study. Chemical Society Reviews, 2014, 43, 7326-7357.	18.7	188
180	Triazolinediones enable ultrafast and reversible click chemistry for the design of dynamic polymer systems. Nature Chemistry, 2014, 6, 815-821.	6.6	285

#	Article	IF	Citations
181	Base catalytic activity of alkaline earth MOFs: a (micro)spectroscopic study of active site formation by the controlled transformation of structural anions. Chemical Science, 2014, 5, 4517-4524.	3.7	58
182	Metal-dioxidoterephthalate MOFs of the MOF-74 type: Microporous basic catalysts with well-defined active sites. Journal of Catalysis, 2014, 317, 1-10.	3.1	138
183	Metalâ€“organic frameworks as potential shock absorbers: the case of the highly flexible MIL-53(Al). Chemical Communications, 2014, 50, 9462-9464.	2.2	122
184	Insight into the Formation and Reactivity of Frameworkâ€Bound Methoxide Species in Hâ€ZSMâ€5 from Static and Dynamic Molecular Simulations. ChemCatChem, 2014, 6, 1906-1918.	1.8	69
185	Reactivity of CO on Carbon-Covered Cobalt Surfaces in Fischerâ€“Tropsch Synthesis. Journal of Physical Chemistry C, 2014, 118, 5317-5327.	1.5	42
186	Cationic Ring-Opening Polymerization of 2-Propyl-2-oxazolines: Understanding Structural Effects on Polymerization Behavior Based on Molecular Modeling. ACS Macro Letters, 2013, 2, 651-654.	2.3	26
187	Covalent immobilization of the Jacobsen catalyst on mesoporous phenolic polymer: A highly enantioselective and stable asymmetric epoxidation catalyst. Materials Chemistry and Physics, 2013, 141, 967-972.	2.0	19
188	Synthesis Modulation as a Tool To Increase the Catalytic Activity of Metalâ€“Organic Frameworks: The Unique Case of UiO-66(Zr). Journal of the American Chemical Society, 2013, 135, 11465-11468.	6.6	871
189	Ranking the Stars: A Refined Pareto Approach to Computational Materials Design. Physical Review Letters, 2013, 111, 075501.	2.9	23
190	trans effect and trans influence: importance of metal mediated ligandâ€“ligand repulsion. Physical Chemistry Chemical Physics, 2013, 15, 17354.	1.3	57
191	Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. ACS Catalysis, 2013, 3, 2556-2567.	5.5	91
192	Insight in the activity and diastereoselectivity of various Lewis acid catalysts for the citronellal cyclization. Journal of Catalysis, 2013, 305, 118-129.	3.1	51
193	Crystal structure prediction for supersaturated AZO: the case of Zn3Al2O6. CrystEngComm, 2013, 15, 10440.	1.3	3
194	New Functionalized Metalâ€“Organic Frameworks MIL-47-X (X = â^'Cl, â^'Br, â^'CH₃,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Adsorption Properties. Journal of Physical Chemistry C, 2013, 117, 22784-22796.	1.5	79
195	Mn-salen@MIL101(Al): a heterogeneous, enantioselective catalyst synthesized using a â€˜bottle around the shipâ€™ approach. Chemical Communications, 2013, 49, 8021.	2.2	70
196	New V^{IV}-Based Metalâ€“Organic Framework Having Framework Flexibility and High CO₂ Adsorption Capacity. Inorganic Chemistry, 2013, 52, 113-120.	1.9	68
197	Mechanistic Studies on Chabaziteâ€Type Methanolâ€toâ€Olefin Catalysts: Insights from Timeâ€Resolved UV/Vis Microspectroscopy Combined with Theoretical Simulations. ChemCatChem, 2013, 5, 173-184.	1.8	70
198	Enthalpy and Entropy Barriers Explain the Effects of Topology on the Kinetics of Zeoliteâ€Catalyzed Reactions. Chemistry - A European Journal, 2013, 19, 11568-11576.	1.7	63

#	Article	IF	Citations
199	Origins of the solvent effect on the propagation kinetics of acrylic acid and methacrylic acid. Journal of Polymer Science Part A, 2013, 51, 2024-2034.	2.5	23
200	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order. Journal of Chemical Physics, 2013, 138, 074108.	1.2	84
201	Polycaprolactone and polycaprolactone/chitosan nanofibres functionalised with the pH-sensitive dye Nitrazine Yellow. Carbohydrate Polymers, 2013, 91, 284-293.	5.1	95
202	Synthesis of 2â€Hydroxyâ€1,4â€oxazinâ€3â€ones through Ring Transformation of 3â€Hydroxyâ€4â€(1,2â€dihydroxyethyl)â€²â€lactams and a Study of Their Reactivity. Chemistry - A European Journal, 2013, 19, 3383-3396.	5.7	20
203	Diphosphonylation of Aromatic Diazaheterocycles and Theoretical Rationalization of Product Yields. European Journal of Organic Chemistry, 2013, 2013, 1058-1067.	1.2	21
204	Ti-functionalized NH2-MIL-47: An effective and stable epoxidation catalyst. Catalysis Today, 2013, 208, 97-105.	2.2	31
205	Hirshfeld-E Partitioning: AIM Charges with an Improved Trade-off between Robustness and Accurate Electrostatics. Journal of Chemical Theory and Computation, 2013, 9, 2221-2225.	2.3	77
206	Bipyridine-Based Nanosized Metalâ€“Organic Framework with Tunable Luminescence by a Postmodification with Eu(III): An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 11302-11310.	1.5	85
207	On the Thermodynamics of Framework Breathing: A Free Energy Model for Gas Adsorption in MIL-53. Journal of Physical Chemistry C, 2013, 117, 11540-11554.	1.5	61
208	Quantification of silanol sites for the most common mesoporous ordered silicas and organosilicas: total versus accessible silanols. Physical Chemistry Chemical Physics, 2013, 15, 642-650.	1.3	110
209	Unraveling the Reaction Mechanisms Governing Methanolâ€toâ€Olefins Catalysis by Theory and Experiment. ChemPhysChem, 2013, 14, 1526-1545.	1.0	232
210	Complete low-barrier side-chain route for olefin formation during methanol conversion in H-SAPO-34. Journal of Catalysis, 2013, 305, 76-80.	3.1	102
211	Accurate prediction of 1H chemical shifts in interstrand cross-linked DNA. RSC Advances, 2013, 3, 3925.	1.7	12
212	Identification of Intermediates in Zeoliteâ€Catalyzed Reactions by In Situ UV/Vis Microspectroscopy and a Complementary Set of Molecular Simulations. Chemistry - A European Journal, 2013, 19, 16595-16606.	1.7	68
213	Bimetallicâ€“Organic Framework as a Zeroâ€Leaching Catalyst in the Aerobic Oxidation of Cyclohexene. ChemCatChem, 2013, 5, 3657-3664.	1.8	38
214	Analysis of the basis set superposition error in molecular dynamics of hydrogen-bonded liquids: Application to methanol. Journal of Chemical Physics, 2012, 137, 104506.	1.2	4
215	Computation of Charge Distribution and Electrostatic Potential in Silicates with the Use of Chemical Potential Equalization Models. Journal of Physical Chemistry C, 2012, 116, 490-504.	1.5	47
216	Synthesis, characterization and sorption properties of NH2-MIL-47. Physical Chemistry Chemical Physics, 2012, 14, 15562.	1.3	27

#	Article	IF	Citations
217	Solvent-Controlled Selective Transformation of 2-Bromomethyl-2-methylaziridines to Functionalized Aziridines and Azetidines. Journal of Organic Chemistry, 2012, 77, 3181-3190.	1.7	26
218	Diastereoselective Aldol Reaction of Zincated 3-Chloro-3-methyl-1-azaallylic Anions as Key Step in the Synthesis of 1,2,3,4-Tetrasubstituted 3-Chloroazetidines. Journal of Organic Chemistry, 2012, 77, 3415-3425.	1.7	14
219	Entropyâ€Driven Chemisorption of NO_x on Phosphotungstic Acid. Angewandte Chemie - International Edition, 2012, 51, 11010-11013.	7.2	4
220	Mechanistic insight into the cyclohexene epoxidation with VO(acac)2 and tert-butyl hydroperoxide. Journal of Catalysis, 2012, 294, 1-18.	3.1	40
221	Efficient Approach for the Computational Study of Alcohol and Nitrile Adsorption in H-ZSM-5. Journal of Physical Chemistry C, 2012, 116, 5499-5508.	1.5	77
222	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. Journal of Chemical Theory and Computation, 2012, 8, 661-676.	2.3	66
223	Free radical polymerization of ethyl methacrylate and ethyl Î±-hydroxy methacrylate: A computational approach to the propagation kinetics. Polymer, 2012, 53, 3211-3219.	1.8	18
224	Tuning of CeO2 buffer layers for coated superconductors through doping. Applied Surface Science, 2012, 260, 32-35.	3.1	29
225	Methylation of benzene by methanol: Single-site kinetics over H-ZSM-5 and H-beta zeolite catalysts. Journal of Catalysis, 2012, 292, 201-212.	3.1	126
226	Solventâ€Catalyzed Ringâ€“Chainâ€“Ring Tautomerization in Axially Chiral Compounds. Chemistry - A European Journal, 2012, 18, 12725-12732.	1.7	14
227	Design of zeolite by inverse sigma transformation. Nature Materials, 2012, 11, 1059-1064.	13.3	161
228	Ab Initio Parametrized Force Field for the Flexible Metalâ€“Organic Framework MIL-53(Al). Journal of Chemical Theory and Computation, 2012, 8, 3217-3231.	2.3	69
229	The conformational sensitivity of iterative stockholder partitioning schemes. Chemical Physics Letters, 2012, 545, 138-143.	1.2	35
230	Accurate spinâ€“orbit and spinâ€“other-orbit contributions to the g-tensor for transition metal containing systems. Physical Chemistry Chemical Physics, 2012, 14, 10690.	1.3	20
231	Synthesis, Structural Characterization, and Catalytic Performance of a Vanadium-Based Metal-Organic Framework (COMOC-3). European Journal of Inorganic Chemistry, 2012, 2012, 2819-2827.	1.0	47
232	Electronic Effects of Linker Substitution on Lewis Acid Catalysis with Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 4887-4890.	7.2	384
233	Investigating the Halochromic Properties of Azo Dyes in an Aqueous Environment by Using a Combined Experimental and Theoretical Approach. Chemistry - A European Journal, 2012, 18, 8120-8129.	1.7	41
234	Regioselectivity in the ring opening of non-activated aziridines. Chemical Society Reviews, 2012, 41, 643-665.	18.7	401

#	Article	IF	Citations
235	Hostâ€“guest and guestâ€“guest interactions between xylene isomers confined in the MIL-47(V) pore system. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	23
236	The influence of a polyamide matrix on the halochromic behaviour of the pH-sensitive azo dye Nitrazine Yellow. Dyes and Pigments, 2012, 94, 443-451.	2.0	53
237	The coordinatively saturated vanadium MIL-47 as a low leaching heterogeneous catalyst in the oxidation of cyclohexene. Journal of Catalysis, 2012, 285, 196-207.	3.1	100
238	Atomic Velocity Projection Method: A New Analysis Method for Vibrational Spectra in Terms of Internal Coordinates for a Better Understanding of Zeolite Nanogrowth. Journal of Chemical Theory and Computation, 2011, 7, 1045-1061.	2.3	10
239	display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Ce<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math	1.1	43
240	²⁹Si NMR and UVâ^'Raman Investigation of Initial Oligomerization Reaction Pathways in Acid-Catalyzed Silica Solâ^'Gel Chemistry. Journal of Physical Chemistry C, 2011, 115, 3562-3571.	1.5	72
241	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	2.3	42
242	First Principle Kinetic Studies of Zeolite-Catalyzed Methylation Reactions. Journal of the American Chemical Society, 2011, 133, 888-899.	6.6	153
243	Synthesis of 3-Methoxyazetidines via an Aziridine to Azetidine Rearrangement and Theoretical Rationalization of the Reaction Mechanism. Journal of Organic Chemistry, 2011, 76, 2157-2167.	1.7	42
244	Electronic structure and band gap of zinc spinel oxides beyond LDA: ZnAl₂O₄, ZnGa₂O₄and ZnIn₂O₄. New Journal of Physics, 2011, 13, 063002.	1.2	105
245	Normal Mode Analysis in Zeolites: Toward an Efficient Calculation of Adsorption Entropies. Journal of Chemical Theory and Computation, 2011, 7, 1090-1101.	2.3	94
246	UV-Raman and ²⁹Si NMR Spectroscopy Investigation of the Nature of Silicate Oligomers Formed by Acid Catalyzed Hydrolysis and Polycondensation of Tetramethylorthosilicate. Journal of Physical Chemistry C, 2011, 115, 11077-11088.	1.5	33
247	Assessment of Periodic and Cluster-in-Vacuo Models for First Principles Calculation of EPR Parameters of Paramagnetic Defects in Crystals: Rh²⁺ Defects in NaCl as Case Study. Journal of Physical Chemistry A, 2011, 115, 1721-1733.	1.1	11
248	Crystal structure prediction for iron as inner core material in heavy terrestrial planets. Earth and Planetary Science Letters, 2011, 312, 237-242.	1.8	32
249	Stereoselective Synthesis of cis-3,4-Disubstituted Piperidines through Ring Transformation of 2-(2-Mesyloxyethyl)azetidines. Journal of Organic Chemistry, 2011, 76, 8364-8375.	1.7	33
250	Reactivity of Activated versus Nonactivated 2-(Bromomethyl)aziridines with respect to Sodium Methoxide: A Combined Computational and Experimental Study. Journal of Organic Chemistry, 2011, 76, 8698-8709.	1.7	17
251	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. Polymer, 2011, 52, 5503-5512.	1.8	20
252	Experimental and theoretical IR study of methanol and ethanol conversion over H-SAPO-34. Catalysis Today, 2011, 177, 12-24.	2.2	41

#	Article	IF	Citations
253	Full Theoretical Cycle for both Ethene and Propene Formation during Methanolâ€toâ€Olefin Conversion in Hâ€ZSMâ€5. ChemCatChem, 2011, 3, 208-212.	1.8	116
254	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	2.3	32
255	Validation of DFT-Based Methods for Predicting Qualitative Thermochemistry of Large Polyaromatics. ChemPhysChem, 2011, 12, 1100-1108.	1.0	8
256	Scope and Mechanism of the (4+3) Cycloaddition Reaction of Furfuryl Cations. Angewandte Chemie - International Edition, 2011, 50, 11990-11993.	7.2	65
257	Furanâ€Oxidationâ€Triggered Inducible DNA Crossâ€Linking: Acyclic Versus Cyclic Furanâ€Containing Building Blocksâ€"On the Benefit of Restoring the Cyclic Sugar Backbone. Chemistry - A European Journal, 2011, 17, 6940-6953.	1.7	25
258	Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. Chemistry - A European Journal, 2011, 17, 12027-12036.	1.7	23
259	Theoretical Simulations Elucidate the Role of Naphthalenic Species during Methanol Conversion within Hâ€SAPOâ€34. Chemistry - A European Journal, 2011, 17, 9083-9093.	1.7	36
260	Catalytic and molecular separation properties of Zeogrids and Zeotiles. Catalysis Today, 2011, 168, 17-27.	2.2	15
261	Assessment of a low-cost protocol for anab initiobased prediction of the mixing enthalpy at elevated temperatures: The Fe-Mo system. Physical Review B, 2011, 83, .	1.1	23
262	Comparative study of various normal mode analysis techniques based on partial Hessians. Journal of Computational Chemistry, 2010, 31, 994-1007.	1.5	43
263	TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics. Journal of Chemical Information and Modeling, 2010, 50, 1736-1750.	2.5	155
264	The remarkable catalytic activity of the saturated metal organic framework V-MIL-47 in the cyclohexene oxidation. Chemical Communications, 2010, 46, 5085.	2.2	109
265	Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate. Macromolecules, 2010, 43, 5602-5610.	2.2	38
266	Assembly of cyclic hydrocarbons from ethene and propene in acid zeolite catalysis to produce active catalytic sites for MTO conversion. Journal of Catalysis, 2010, 271, 67-78.	3.1	86
267	Systematic Study of Halideâ€Induced Ring Opening of 2â€Substituted Aziridinium Salts and Theoretical Rationalization of the Reaction Pathways. European Journal of Organic Chemistry, 2010, 2010, 4920-4931.	1.2	63
268	Opposite Regiospecific Ring Opening of 2-(Cyanomethyl)aziridines by Hydrogen Bromide and Benzyl Bromide: Experimental Study and Theoretical Rationalization. Journal of Organic Chemistry, 2010, 75, 4530-4541.	1.7	56
269	A coordinative saturated vanadium containing metal organic framework that shows a remarkable catalytic activity. Studies in Surface Science and Catalysis, 2010, 175, 329-332.	1.5	9
270	Influence of Protein Environment on the Electron Paramagnetic Resonance Properties of Flavoprotein Radicals: A QM/MM Study. Journal of Physical Chemistry B, 2010, 114, 16655-16665.	1.2	20

#	Article	IF	Citations
271	Conformational Sampling of Macrocyclic Alkenes Using a Kennardâ˜Stone-Based Algorithm. Journal of Physical Chemistry A, 2010, 114, 6879-6887.	1.1	17
272	Intramolecular Ï€âˆ’Ï€ Stacking Interactions in 2-Substituted N,N-Dibenzylaziridinium Ions and Their Regioselectivity in Nucleophilic Ring-Opening Reactions. Journal of Organic Chemistry, 2010, 75, 885-896.	1.7	66
273	Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures. Journal of Physical Chemistry A, 2010, 114, 2864-2873.	1.1	35
274	Kinetic and Mechanistic Study onp-Quinodimethane Formation in the Sulfinyl Precursor Route for the Polymerization of Poly(p-phenylenevinylene) (PPV). Macromolecules, 2010, 43, 7424-7433.	2.2	26
275	Solvent Effects on Free Radical Polymerization Reactions: The Influence of Water on the Propagation Rate of Acrylamide and Methacrylamide. Macromolecules, 2010, 43, 827-836.	2.2	50
276	The calculation of thermodynamic properties of molecules. Chemical Society Reviews, 2010, 39, 1764.	18.7	96
277	Experimental and computational study of the ring opening of tricyclic oxanorbornenes to polyhydro isoindole phosphonates. Organic and Biomolecular Chemistry, 2010, 8, 3644.	1.5	14
278	Normal modes for large molecules with arbitrary link constraints in the mobile block Hessian approach. Journal of Chemical Physics, 2009, 130, 084107.	1.2	22
279	Insight into the Solvation and Isomerization of 3â€Haloâ€1â€azaallylic Anions from Ab Initio Metadynamics Calculations and NMR Experiments. Chemistry - A European Journal, 2009, 15, 580-584.	1.7	10
280	Theoretical Insights on Methylbenzene Sideâ€Chain Growth in ZSMâ€5 Zeolites for Methanolâ€toâ€Olefin Conversion. Chemistry - A European Journal, 2009, 15, 10803-10808.	1.7	131
281	Multi-level Modeling of Silicaâ€“Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
282	The Effect of Confined Space on the Growth of Naphthalenic Species in a Chabaziteâ€Type Catalyst: A Molecular Modeling Study. ChemCatChem, 2009, 1, 373-378.	1.8	45
283	Theoretical Study on the Structural Properties of Various Solvated Metalated 3-Halo-1-azaallylic Anions. Journal of Physical Chemistry A, 2009, 113, 6375-6380.	1.1	9
284	Reversibility from DFT-Based Reactivity Indices: Intramolecular Side Reactions in the Polymerization of Poly(vinyl chloride). Journal of Physical Chemistry A, 2009, 113, 7899-7908.	1.1	11
285	DFT Study on the Propagation Kinetics of Free-Radical Polymerization of Î±-Substituted Acrylates. Macromolecules, 2009, 42, 3033-3041.	2.2	72
286	Mobile Block Hessian Approach with Adjoined Blocks: An Efficient Approach for the Calculation of Frequencies in Macromolecules. Journal of Chemical Theory and Computation, 2009, 5, 1203-1215.	2.3	30
287	Levofloxacin ozonation in water: Rate determining process parameters and reaction pathway elucidation. Chemosphere, 2009, 76, 683-689.	4.2	109
288	The electronegativity equalization method and the split charge equilibration applied to organic systems: Parametrization, validation, and comparison. Journal of Chemical Physics, 2009, 131, 044127.	1.2	82

#	Article	IF	Citations
289	Theoretical evaluation of zeolite confinement effects on the reactivity of bulky intermediates. Physical Chemistry Chemical Physics, 2009, 11, 5222.	1.3	59
290	Nucleophile-dependent regioselective ring opening of 2-substituted N,N-dibenzylaziridinium ions: bromide versus hydride. Chemical Communications, 2009, , 2508.	2.2	37
291	Carbonâ€Centered Radical Addition and Î²â€Scission Reactions: Modeling of Activation Energies and Preâ€exponential Factors. ChemPhysChem, 2008, 9, 124-140.	1.0	87
292	A DFTâ€Based Investigation of Hydrogen Abstraction Reactions from Methylated Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2008, 9, 2349-2358.	1.0	27
293	A Complete Catalytic Cycle for Supramolecular Methanolâ€toâ€Olefins Conversion by Linking Theory with Experiment. Angewandte Chemie - International Edition, 2008, 47, 5179-5182.	7.2	240
294	Synthesis of Tricyclic Phosphonopyrrolidines via IMDAF: Experimental and Theoretical Investigation of the Observed Stereoselectivity. Journal of Organic Chemistry, 2008, 73, 7921-7927.	1.7	12
295	Recent theoretical insights into the role of the zeolite framework on methanol-to-olefin conversion. Studies in Surface Science and Catalysis, 2008, , 741-744.	1.5	1
296	MD-TRACKS: A Productive Solution for the Advanced Analysis of Molecular Dynamics and Monte Carlo simulations. Journal of Chemical Information and Modeling, 2008, 48, 2414-2424.	2.5	21
297	Experimental and Computational Study of the Conrotatory Ring Opening of Various 3-Chloro-2-azetines. Journal of Organic Chemistry, 2008, 73, 5481-5488.	1.7	38
298	An Intrinsic Radical Stability Scale from the Perspective of Bond Dissociation Enthalpies: A Companion to Radical Electrophilicities. Journal of Organic Chemistry, 2008, 73, 9109-9120.	1.7	50
299	MFI Fingerprint: How Pentasil-Induced IR Bands Shift during Zeolite Nanogrowth. Journal of Physical Chemistry C, 2008, 112, 9186-9191.	1.5	59
300	Using elementary reactions to model growth processes of polyaromatic hydrocarbons under pyrolysis conditions of light feedstocks. Molecular Simulation, 2008, 34, 193-199.	0.9	11
301	Temperature Study of a Glycine Radical in the Solid State Adopting a DFT Periodic Approach: Vibrational Analysis and Comparison with EPR Experiments. Journal of Physical Chemistry B, 2008, 112, 7618-7630.	1.2	15
302	ZEOBUILDER: A GUI Toolkit for the Construction of Complex Molecular Structures on the Nanoscale with Building Blocks. Journal of Chemical Information and Modeling, 2008, 48, 1530-1541.	2.5	48
303	Calculating Reaction Rates with Partial Hessians: Validation of the Mobile Block Hessian Approach. Journal of Chemical Theory and Computation, 2008, 4, 614-625.	2.3	35
304	Molecular Environment and Temperature Dependence of Hyperfine Interactions in Sugar Crystal Radicals from First Principles. Journal of Physical Chemistry B, 2008, 112, 1508-1514.	1.2	9
305	Bond Dissociation Enthalpies of Large Aromatic Carbon-Centered Radicals. Journal of Physical Chemistry A, 2008, 112, 13566-13573.	1.1	35
306	Evidence for a Grotthuss-Like Mechanism in the Formation of the Rhamnose Alkoxy Radical Based on Periodic DFT Calculations. Radiation Research, 2008, 169, 8-18.	0.7	18

#	Article	IF	Citations
307	Vibrational modes in partially optimized molecular systems. Journal of Chemical Physics, 2007, 126, 224102.	1.2	95
308	Refinement of the supramolecular concept in methanol-to-olefin catalysis. Studies in Surface Science and Catalysis, 2007, 170, 1668-1676.	1.5	5
309	Density Functional Theory Study of Free-Radical Polymerization of Acrylates and Methacrylates:Â Structureâ^'Reactivity Relationship. Macromolecules, 2007, 40, 9590-9602.	2.2	40
310	The Rise and Fall of Direct Mechanisms in Methanol-to-Olefin Catalysis:Â An Overview of Theoretical Contributions. Industrial & Engineering Chemistry Research, 2007, 46, 8832-8838.	1.8	95
311	Spin-Polarized Conceptual Density Functional Theory Study of the Regioselectivity in Ring Closures of Radicals. Journal of Organic Chemistry, 2007, 72, 348-356.	1.7	36
312	Modeling elementary reactions in coke formation from first principles. Molecular Simulation, 2007, 33, 879-887.	0.9	32
313	Theoretical Study of the Thermodynamics and Kinetics of Hydrogen Abstractions from Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 11771-11786.	1.1	134
314	Ab Initio Study of Free-Radical Polymerization:Â Defect Structures in Poly(vinyl chloride). Macromolecules, 2007, 40, 1321-1331.	2.2	47
315	Four-Membered Heterocycles with a Carbonâ^'Heteroatom Exocyclic Double Bond at the 3-Position:â€‰ Puckering Potential and Thermodynamic Properties. Journal of Physical Chemistry A, 2007, 111, 2797-2803.	1.1	22
316	Ab Initio Thermochemistry and Kinetics for Carbon-Centered Radical Addition and Î²-Scission Reactions. Journal of Physical Chemistry A, 2007, 111, 8416-8428.	1.1	67
317	Novel Synthesis of 3,4-Diaminobutanenitriles and 4-Amino-2-butenenitriles from 2-(Cyanomethyl)aziridines through Intermediate Aziridinium Salts:Â An Experimental and Theoretical Approach. Journal of Organic Chemistry, 2007, 72, 4733-4740.	1.7	30
318	Global DFT-Based Reactivity Indicators:â€‰ An Assessment of Theoretical Procedures in Zeolite Catalysis. Journal of Physical Chemistry C, 2007, 111, 3028-3037.	1.5	14
319	The Gradient Curves Method:â€‰ An Improved Strategy for the Derivation of Molecular Mechanics Valence Force Fields from ab Initio Data. Journal of Chemical Theory and Computation, 2007, 3, 1420-1434.	2.3	19
320	Zeolite Shape-Selectivity in thegem-Methylation of Aromatic Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 1311-1314.	7.2	154
321	Ab Initio Study of Poly(vinyl chloride) Propagation Kinetics: Head-to-Head versus Head-to-Tail Additions. ChemPhysChem, 2007, 8, 541-552.	1.0	26
322	How useful are reactivity indicators for the description of hydrogen abstraction reactions on polycyclic aromatic hydrocarbons?. Chemical Physics Letters, 2007, 444, 17-22.	1.2	12
323	Electrophilicity and Nucleophilicity Index for Radicals. Organic Letters, 2007, 9, 2721-2724.	2.4	396
324	An extended hindered-rotor model with incorporation of Coriolis and vibrational-rotational coupling for calculating partition functions and derived quantities. Journal of Chemical Physics, 2006, 124, 044314.	1.2	86

#	Article	IF	Citations
325	Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2006, 110, 13624-13631.	1.1	41
326	Regio- and stereospecific ring opening of 1,1-dialkyl-2-(aryloxymethyl)aziridinium salts by bromide. Chemical Communications, 2006, , 1554.	2.2	55
327	X-(X = O, S, Se) Ions in Alkali Halide Lattices through Density Functional Calculations. 2. Interstitial Defect Models. Journal of Physical Chemistry B, 2006, 110, 8213-8218.	1.2	4
328	Study of Rhamnose Radicals in the Solid State Adopting a Density Functional Theory Cluster Approach. Journal of Physical Chemistry A, 2006, 110, 6504-6513.	1.1	19
329	Unexpected Four-Membered over Six-Membered Ring Formation during the Synthesis of Azaheterocyclic Phosphonates: Experimental and Theoretical Evaluation. Journal of the American Chemical Society, 2006, 128, 8468-8478.	6.6	37
330	Applicability of the Hindered Rotor Scheme to the Puckering Mode in Four-Membered Rings. Journal of Physical Chemistry A, 2006, 110, 3838-3844.	1.1	25
331	X-(X = O, S) Ions in Alkali Halide Lattices through Density Functional Calculations. 1. Substitutional Defect Models. Journal of Physical Chemistry B, 2006, 110, 8204-8212.	1.2	5
332	First-principles calculations of hyperfine parameters with the Gaussian and augmented-plane-wave method: Application to radicals embedded in a crystalline environment. Physical Review B, 2006, 74, .	1.1	42
333	What role do oxonium ions and oxonium ylides play in the ZSM-5 catalysed methanol-to-olefin process?. Chemical Physics Letters, 2006, 417, 309-315.	1.2	94
334	Bifunctional acidâ€“base catalyzed reactions in zeolites from the HSAB viewpoint. Chemical Physics Letters, 2006, 419, 10-15.	1.2	17
335	The Rhâ€“ligand bond: RhX (X=C, N, O, F, P and Cl) molecules. Chemical Physics Letters, 2006, 421, 281-286.	1.2	20
336	Ab initio calculation of entropy and heat capacity of gas-phase n-alkanes with hetero-elements O and S: Ethers/alcohols and sulfides/thiols. Chemical Physics, 2006, 328, 251-258.	0.9	25
337	Radiation-induced radicals in Î±-d-glucose: Comparing DFT cluster calculations with magnetic resonance experiments. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 795-801.	2.0	21
338	Theoretical study on the alteration of fundamental zeolite properties by methylene functionalization. Microporous and Mesoporous Materials, 2006, 96, 350-356.	2.2	21
339	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. Journal of Physical Chemistry A, 2006, 110, 8942-8951.	1.1	70
340	Understanding the Failure of Direct Cï£¿C Coupling in the Zeolite-Catalyzed Methanol-to-Olefin Process. Angewandte Chemie - International Edition, 2006, 45, 1714-1719.	7.2	220
341	Ab Initio Group Contribution Method for Activation Energies of Hydrogen Abstraction Reactions. ChemPhysChem, 2006, 7, 188-199.	1.0	66
342	Ab Initio Study of Free-Radical Polymerization: Polyethylene Propagation Kinetics. ChemPhysChem, 2006, 7, 131-140.	1.0	60

#	Article	IF	Citations
343	Hydrocarbon Bond Dissociation Enthalpies: From Substituted Aromatics to Large Polyaromatics. ChemPhysChem, 2006, 7, 2205-2214.	1.0	45
344	Reaction of Electrophilic Allyl Halides with Amines: A Reinvestigation. Synthesis, 2006, 2006, 2260-2264.	1.2	1
345	First-principles calculation of the EPRgtensor in extended periodic systems. Physical Review B, 2006, 73, .	1.1	18
346	How should we calculate multi-dimensional potential energy surfaces for an accurate reproduction of partition functions?. Chemical Physics, 2005, 314, 109-117.	0.9	22
347	Why does the uncoupled hindered rotor model work well for the thermodynamics of n-alkanes?. Chemical Physics Letters, 2005, 402, 479-484.	1.2	84
348	Group Additive Values for the Gas Phase Standard Enthalpy of Formation of Hydrocarbons and Hydrocarbon Radicals. Journal of Physical Chemistry A, 2005, 109, 7466-7480.	1.1	127
349	Ab Initio Study of Free-Radical Polymerizations: Cost-Effective Methods to Determine the Reaction Rates. ChemPhysChem, 2005, 6, 180-189.	1.0	45
350	Study of radical defects in crystalline lattices from first-principles molecular dynamics simulations. International Journal of Quantum Chemistry, 2005, 101, 761-769.	1.0	4
351	Comparative study of kinetics and reactivity indices of free radical polymerization reactions. International Journal of Quantum Chemistry, 2005, 102, 454-460.	1.0	16
352	Ab initio EPR study of S?3 and Se?3 defects in alkali halides. International Journal of Quantum Chemistry, 2005, 102, 409-414.	1.0	4
353	Level of theory study of magnetic resonance parameters of chalcogen XYâ^'(X, Y = O, S and Se) defects in alkali halides. Physical Chemistry Chemical Physics, 2005, 7, 240-249.	1.3	7
354	Rules for Generating Conformers and Their Relative Energies inn-Alkanes with a Heteroelement O or S:Â Ethers and Alcohols, or Sulfides and Thiols. Journal of Physical Chemistry A, 2005, 109, 9617-9626.	1.1	12
355	DFT Investigation of Alkoxide vs Alkylammonium Formation in Amine-Substituted Zeolites. Journal of Physical Chemistry B, 2005, 109, 7952-7960.	1.2	26
356	N-Alkenyl-2-aziridinylmethyl Radicals andN-Alkenylaminyl Radicals in Cascade Cyclizations to Pyrrolizidines and Indolizidines. Journal of Organic Chemistry, 2005, 70, 3674-3681.	1.7	16
357	Reactivity and aromaticity of polyaromatics in radical cyclization reactions. International Journal of Quantum Chemistry, 2004, 96, 568-576.	1.0	51
358	DFT-EPR study of radiation-induced radicals in ?-D-glucose. International Journal of Quantum Chemistry, 2004, 99, 102-108.	1.0	22
359	Ab initio group contribution method for activation energies for radical additions. AICHE Journal, 2004, 50, 426-444.	1.8	88
360	Density functional theory as a tool for the structure determination of radiation-induced bioradicals. Magnetic Resonance in Chemistry, 2004, 42, S3-S19.	1.1	6

#	Article	IF	Citations
361	Reactivity Indices for Radical Reactions Involving Polyaromatics. Journal of Physical Chemistry A, 2004, 108, 7281-7290.	1.1	40
362	Evaluation of Different Model Space Approaches Based on DFT to Examine the EPR Parameters of a Radiation-Induced Radical in Solid-State Î±-Glycine. Journal of Physical Chemistry A, 2004, 108, 11321-11332.	1.1	33
363	Efficient Use of Bifunctional Acidâ^'Base Properties for Alkylammonium Formation in Amine-Substituted Zeolites. Journal of the American Chemical Society, 2004, 126, 9162-9163.	6.6	25
364	Ab Initio Calculations for Hydrocarbons:Â Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. Journal of Physical Chemistry A, 2003, 107, 9147-9159.	1.1	170
365	Ab initio and experimental study on thermally degradable polycarbonates: Effect of structure on reactivity. International Journal of Quantum Chemistry, 2003, 91, 363-368.	1.0	1
366	Application of molecular cluster models to study the amino acidL-?-alanine and its derived radicals in the crystalline state. International Journal of Quantum Chemistry, 2003, 91, 511-516.	1.0	9
367	Ab initio study on elementary radical reactions in coke formation. International Journal of Quantum Chemistry, 2003, 91, 384-388.	1.0	20
368	Ab Initio Calculation of Entropy and Heat Capacity of Gas-Phase n-Alkanes Using Internal Rotations. Journal of Physical Chemistry A, 2003, 107, 3139-3145.	1.1	101
369	A recent development in computational chemistry: chemical reactions from first principles molecular dynamics simulations. Chemical Society Reviews, 2003, 32, 151-157.	18.7	40
370	Ab Initio Studies of Thermal Syn-Elimination Reactions in Carbonates:Â Effect of Structure on Reactivity. Journal of Physical Chemistry A, 2002, 106, 12370-12375.	1.1	5
371	Ab Initio Study of Radical Reactions: Role of Coupled Internal Rotations on the Reaction Kinetics (III). Journal of Physical Chemistry A, 2002, 106, 8945-8950.	1.1	58
372	Reactivity and kinetics of polyaromatic hydrocarbons in elementary radical reactions. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 315-318.	0.1	0
373	The Kinetics of Cyclization Reactions on Polyaromatics from First Principles. ChemPhysChem, 2002, 3, 863-870.	1.0	32
374	Micropatterning of polyurethanes with lasers. Polymer International, 2002, 51, 1172-1177.	1.6	4
375	Density Functional Calculations on Alanine-Derived Radicals:â€‰ Influence of Molecular Environment on EPR Hyperfine Coupling Constants. Journal of Physical Chemistry A, 2001, 105, 8794-8804.	1.1	40
376	Ab Initio and Experimental Study on Thermally Degradable Polycarbonates:â€‰ The Effect of Substituents on the Reaction Rates. Journal of the American Chemical Society, 2001, 123, 10650-10657.	6.6	26
377	Ab Initio Study of Radical Reactions: Cyclization Pathways for the Butylbenzene Radical (II). Journal of Physical Chemistry A, 2001, 105, 7713-7723.	1.1	23
378	v-representability of one-body density matrices. Physical Review A, 2001, 64, .	1.0	6

#	Article	IF	Citations
379	Ab Initio Study of Radical Addition Reactions: Addition of a Primary Ethylbenzene Radical to Ethene (I). Journal of Physical Chemistry A, 2000, 104, 10939-10950.	1.1	139