Veronique Van Speybroeck

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8237254/publications.pdf

Version: 2024-02-01

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	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
2	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
3	Metalâ€“organic and covalent organic frameworks as single-site catalysts. Chemical Society Reviews, 2017, 46, 3134-3184.	18.7	861
4	Thermal unequilibrium of strained black CsPbI ₃ thin films. Science, 2019, 365, 679-684.	6.0	444
5	Advances in theory and their application within the field of zeolite chemistry. Chemical Society Reviews, 2015, 44, 7044-7111.	18.7	405
6	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
7	Regioselectivity in the ring opening of non-activated aziridines. Chemical Society Reviews, 2012, 41, 643-665.	18.7	401
8	Electrophilicity and Nucleophilicity Index for Radicals. Organic Letters, 2007, 9, 2721-2724.	2.4	396
9	Electronic Effects of Linker Substitution on Lewis Acid Catalysis with Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 4887-4890.	7.2	384
10	Triazolinediones enable ultrafast and reversible click chemistry for the design of dynamic polymer systems. Nature Chemistry, 2014, 6, 815-821.	6.6	285
11	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
12	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
13	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
14	Unraveling the Reaction Mechanisms Governing Methanolâ€toâ€Olefins Catalysis by Theory and Experiment. ChemPhysChem, 2013, 14, 1526-1545.	1.0	232
15	Structureâ€“performance descriptors and the role of Lewis acidity in the methanol-to-propylene process. Nature Chemistry, 2018, 10, 804-812.	6.6	221
16	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
17	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
18	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
19	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
20	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
21	Missing Linkers: An Alternative Pathway to UiO-66 Electronic Structure Engineering. Chemistry of Materials, 2017, 29, 3006-3019.	3.2	176
22	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
23	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
24	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. Matter, 2019, 1, 219-234.	5.0	170
25	Design of zeolite by inverse sigma transformation. Nature Materials, 2012, 11, 1059-1064.	13.3	161
26	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
27	TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics. Journal of Chemical Information and Modeling, 2010, 50, 1736-1750.	2.5	155
28	Understanding Intrinsic Light Absorption Properties of UiO-66 Frameworks: A Combined Theoretical and Experimental Study. Inorganic Chemistry, 2015, 54, 10701-10710.	1.9	155
29	Zeolite Shape-Selectivity in thegem-Methylation of Aromatic Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 1311-1314.	7.2	154
30	First Principle Kinetic Studies of Zeolite-Catalyzed Methylation Reactions. Journal of the American Chemical Society, 2011, 133, 888-899.	6.6	153
31	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
32	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
33	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
34	Theoretical Study of the Thermodynamics and Kinetics of Hydrogen Abstractions from Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 11771-11786.	1.1	134
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. Journal of Chemical Theory and Computation, 2016, 12, 3894-3912.	2.3	119
41	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
42	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
43	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
44	Levofloxacin ozonation in water: Rate determining process parameters and reaction pathway elucidation. Chemosphere, 2009, 76, 683-689.	4.2	109
45	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
46	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
47	Electronic structure and band gap of zinc spinel oxides beyond LDA: ZnAl₂O₄, ZnGa₂O₄and Znln₂O₄. New Journal of Physics, 2011, 13, 063002.	1.2	105
48	Thermodynamic insight into stimuli-responsive behaviour of soft porous crystals. Nature Communications, 2018, 9, 204.	5.8	104
49	A Flexible Photoactive Titanium Metalâ€“Organic Framework Based on a [Ti^{IV}₃(Ì¼₃â€O)(O)₂(COO)₆] Cluster. Angewandte Chemie - International Edition, 2015, 54, 13912-13917.	7.2	103
50	Mechanical energy storage performance of an aluminum fumarate metalâ€“organic framework. Chemical Science, 2016, 7, 446-450.	3.7	103
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	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
56	The calculation of thermodynamic properties of molecules. Chemical Society Reviews, 2010, 39, 1764.	18.7	96
57	Vibrational modes in partially optimized molecular systems. Journal of Chemical Physics, 2007, 126, 224102.	1.2	95
58	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
59	Polycaprolactone and polycaprolactone/chitosan nanofibres functionalised with the pH-sensitive dye Nitrazine Yellow. Carbohydrate Polymers, 2013, 91, 284-293.	5.1	95
60	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
61	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
62	Aliovalent doping of CeO₂: DFT study of oxidation state and vacancy effects. Journal of Materials Chemistry A, 2014, 2, 13723-13737.	5.2	93
63	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
64	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
65	Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. ACS Catalysis, 2013, 3, 2556-2567.	5.5	91
66	Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. Nature Communications, 2018, 9, 4899.	5.8	90
67	Ab initio group contribution method for activation energies for radical additions. AIChE Journal, 2004, 50, 426-444.	1.8	88
68	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
69	Reliably Modeling the Mechanical Stability of Rigid and Flexible Metalâ€“Organic Frameworks. Accounts of Chemical Research, 2018, 51, 138-148.	7.6	88
70	Carbonâ€centered Radical Addition and Î²â€scission Reactions: Modeling of Activation Energies and Preâ€exponential Factors. ChemPhysChem, 2008, 9, 124-140.	1.0	87
71	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
72	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

#	Article	IF	Citations
73	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
74	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
75	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order. Journal of Chemical Physics, 2013, 138, 074108.	1.2	84
76	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
77	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
78	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
79	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
80	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
81	New Functionalized Metalâ€“Organic Frameworks MIL-47-X (X = â^'Cl, â^'Br, â^'CH₃,) Tj ETQq1 1 0.784314 rgBT /Overlock Adsorption Properties. Journal of Physical Chemistry C, 2013, 117, 22784-22796.	1.5	79
82	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
83	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
84	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
85	DFT Study on the Propagation Kinetics of Free-Radical Polymerization of Î±-Substituted Acrylates. Macromolecules, 2009, 42, 3033-3041.	2.2	72
86	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
87	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
88	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
89	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
90	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

#	Article	IF	Citations
91	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
92	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
93	How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. ACS Catalysis, 2018, 8, 9579-9595.	5.5	70
94	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
95	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
96	New V^{IV}-Based Metalâ€“Organic Framework Having Framework Flexibility and High CO₂ Adsorption Capacity. Inorganic Chemistry, 2013, 52, 113-120.	1.9	68
97	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
98	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
99	Ab Initio Group Contribution Method for Activation Energies of Hydrogen Abstraction Reactions. ChemPhysChem, 2006, 7, 188-199.	1.0	66
100	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
101	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. Journal of Chemical Theory and Computation, 2012, 8, 661-676.	2.3	66
102	Scope and Mechanism of the (4+3) Cycloaddition Reaction of Furfuryl Cations. Angewandte Chemie - International Edition, 2011, 50, 11990-11993.	7.2	65
103	Shape-Selective Diffusion of Olefins in 8-Ring Solid Acid Microporous Zeolites. Journal of Physical Chemistry C, 2015, 119, 23721-23734.	1.5	65
104	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
105	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
106	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
107	Ab Initio Study of Free-Radical Polymerization: Polyethylene Propagation Kinetics. ChemPhysChem, 2006, 7, 131-140.	1.0	60
108	MFI Fingerprint: How Pentasil-Induced IR Bands Shift during Zeolite Nanogrowth. Journal of Physical Chemistry C, 2008, 112, 9186-9191.	1.5	59

#	Article	IF	Citations
109	Theoretical evaluation of zeolite confinement effects on the reactivity of bulky intermediates. Physical Chemistry Chemical Physics, 2009, 11, 5222.	1.3	59
110	Au@UiO-66: a base free oxidation catalyst. RSC Advances, 2015, 5, 22334-22342.	1.7	59
111	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
112	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
113	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
114	Accelerated living cationic ring-opening polymerization of a methyl ester functionalized 2-oxazoline monomer. Polymer Chemistry, 2015, 6, 514-518.	1.9	58
115	Water coordination and dehydration processes in defective UiO-66 type metal organic frameworks. CrystEngComm, 2016, 18, 7056-7069.	1.3	58
116	DMRG-CASPT2 study of the longitudinal static second hyperpolarizability of all-trans polyenes. Journal of Chemical Physics, 2016, 145, 054120.	1.2	58
117	trans effect and trans influence: importance of metal mediated ligandâ€“ligand repulsion. Physical Chemistry Chemical Physics, 2013, 15, 17354.	1.3	57
118	Vanadium metalâ€“organic frameworks: structures and applications. New Journal of Chemistry, 2014, 38, 1853-1867.	1.4	57
119	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
120	Thermal Engineering of Metalâ€“Organic Frameworks for Adsorption Applications: A Molecular Simulation Perspective. ACS Applied Materials & Interfaces, 2019, 11, 38697-38707.	4.0	56
121	Regio- and stereospecific ring opening of 1,1-dialkyl-2-(aryloxymethyl)aziridinium salts by bromide. Chemical Communications, 2006, , 1554.	2.2	55
122	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
123	Ethene Dimerization on Zeolite-Hosted Ni Ions: Reversible Mobilization of the Active Site. ACS Catalysis, 2019, 9, 5645-5650.	5.5	54
124	Porous organic polymers as metal free heterogeneous organocatalysts. Green Chemistry, 2021, 23, 7361-7434.	4.6	54
125	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
126	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

#	Article	IF	Citations
127	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
128	Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts. Nature Materials, 2020, 19, 1081-1087.	13.3	52
129	High-rate nanofluidic energy absorption in porous zeolitic frameworks. Nature Materials, 2021, 20, 1015-1023.	13.3	52
130	Reactivity and aromaticity of polyaromatics in radical cyclization reactions. International Journal of Quantum Chemistry, 2004, 96, 568-576.	1.0	51
131	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
132	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
133	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
134	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
135	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
136	Halochromic properties of sulfonphthaleine dyes in a textile environment: The influence of substituents. Dyes and Pigments, 2016, 124, 249-257.	2.0	49
137	Coordination and activation of nitrous oxide by iron zeolites. Nature Catalysis, 2021, 4, 332-340.	16.1	49
138	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
139	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
140	Ab Initio Study of Free-Radical Polymerization:Â Defect Structures in Poly(vinyl chloride). Macromolecules, 2007, 40, 1321-1331.	2.2	47
141	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
142	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
143	Unraveling the thermodynamic criteria for size-dependent spontaneous phase separation in soft porous crystals. Nature Communications, 2019, 10, 4842.	5.8	47
144	The Remarkable Amphoteric Nature of Defective UiOâ€66 in Catalytic Reactions. ChemCatChem, 2017, 9, 2203-2210.	1.8	46

#	Article	IF	Citations
145	Ab Initio Study of Free-Radical Polymerizations: Cost-Effective Methods to Determine the Reaction Rates. ChemPhysChem, 2005, 6, 180-189.	1.0	45
146	Hydrocarbon Bond Dissociation Enthalpies: From Substituted Aromatics to Large Polyaromatics. ChemPhysChem, 2006, 7, 2205-2214.	1.0	45
147	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
148	Design of a thermally controlled sequence of triazolinedione-based click and transclick reactions. Chemical Science, 2017, 8, 3098-3108.	3.7	45
149	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
150	Comparative study of various normal mode analysis techniques based on partial Hessians. Journal of Computational Chemistry, 2010, 31, 994-1007.	1.5	43
151	Quantum chemical study of [illegible] 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 xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	1.1	43
152	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
153	Collective action of water molecules in zeolite dealumination. Catalysis Science and Technology, 2019, 9, 3721-3725.	2.1	43
154	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
155	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
156	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	2.3	42
157	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
158	Reactivity of CO on Carbon-Covered Cobalt Surfaces in Fischerâ€“Tropsch Synthesis. Journal of Physical Chemistry C, 2014, 118, 5317-5327.	1.5	42
159	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
160	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
161	Experimental and theoretical IR study of methanol and ethanol conversion over H-SAPO-34. Catalysis Today, 2011, 177, 12-24.	2.2	41
162	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

#	Article	IF	Citations
163	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
164	On the intrinsic dynamic nature of the rigid UiO-66 metalâ€“organic framework. Chemical Science, 2018, 9, 2723-2732.	3.7	41
165	Shape-selective Câ€“H activation of aromatics to biarylic compounds using molecular palladium in zeolites. Nature Catalysis, 2020, 3, 1002-1009.	16.1	41
166	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
167	A recent development in computational chemistry: chemical reactions from first principles molecular dynamics simulations. Chemical Society Reviews, 2003, 32, 151-157.	18.7	40
168	Reactivity Indices for Radical Reactions Involving Polyaromatics. Journal of Physical Chemistry A, 2004, 108, 7281-7290.	1.1	40
169	Density Functional Theory Study of Free-Radical Polymerization of Acrylates and Methacrylates:Â Structureâ”Reactivity Relationship. Macromolecules, 2007, 40, 9590-9602.	2.2	40
170	Mechanistic insight into the cyclohexene epoxidation with VO(acac)2 and tert-butyl hydroperoxide. Journal of Catalysis, 2012, 294, 1-18.	3.1	40
171	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
172	Non-food applications of natural dyes extracted from agro-food residues: A critical review. Journal of Cleaner Production, 2021, 301, 126920.	4.6	40
173	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
174	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
175	Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate. Macromolecules, 2010, 43, 5602-5610.	2.2	38
176	Bimetallicâ€“Organic Framework as a Zeroâ€Leaching Catalyst in the Aerobic Oxidation of Cyclohexene. ChemCatChem, 2013, 5, 3657-3664.	1.8	38
177	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
178	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
179	Nucleophile-dependent regioselective ring opening of 2-substituted N,N-dibenzylaziridinium ions: bromide versus hydride. Chemical Communications, 2009, , 2508.	2.2	37
180	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

#	Article	IF	Citations
181	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
182	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
183	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
184	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
185	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
186	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
187	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
188	Bond Dissociation Enthalpies of Large Aromatic Carbon-Centered Radicals. Journal of Physical Chemistry A, 2008, 112, 13566-13573.	1.1	35
189	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
190	The conformational sensitivity of iterative stockholder partitioning schemes. Chemical Physics Letters, 2012, 545, 138-143.	1.2	35
191	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
192	Pillared-layered metalâ€“organic frameworks for mechanical energy storage applications. Journal of Materials Chemistry A, 2019, 7, 22663-22674.	5.2	34
193	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
194	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
195	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
196	Cutting the cost of carbon capture: a case for carbon capture and utilization. Faraday Discussions, 2016, 192, 391-414.	1.6	33
197	Ligand Addition Energies and the Stoichiometry of Colloidal Nanocrystals. ACS Nano, 2016, 10, 1462-1474.	7.3	33
198	The Kinetics of Cyclization Reactions on Polyaromatics from First Principles. ChemPhysChem, 2002, 3, 863-870.	1.0	32

#	Article	IF	Citations
199	Modeling elementary reactions in coke formation from first principles. Molecular Simulation, 2007, 33, 879-887.	0.9	32
200	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
201	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	2.3	32
202	A general synthesis of azetidines by copper-catalysed photoinduced anti-Baldwin radical cyclization of ynamides. Nature Communications, 2022, 13, 560.	5.8	32
203	Multi-level Modeling of Silicaâ€“Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
204	Ti-functionalized NH2-MIL-47: An effective and stable epoxidation catalyst. Catalysis Today, 2013, 208, 97-105.	2.2	31
205	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
206	Towards modeling spatiotemporal processes in metalâ€“organic frameworks. Trends in Chemistry, 2021, 3, 605-619.	4.4	31
207	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
208	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
209	Tuning of CeO2 buffer layers for coated superconductors through doping. Applied Surface Science, 2012, 260, 32-35.	3.1	29
210	A DFTâ€Based Investigation of Hydrogen Abstraction Reactions from Methylated Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2008, 9, 2349-2358.	1.0	27
211	Synthesis, characterization and sorption properties of NH2-MIL-47. Physical Chemistry Chemical Physics, 2012, 14, 15562.	1.3	27
212	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
213	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
214	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
215	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
216	DFT Investigation of Alkoxide vs Alkylammonium Formation in Amine-Substituted Zeolites. Journal of Physical Chemistry B, 2005, 109, 7952-7960.	1.2	26

#	Article	IF	Citations
217	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
218	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
219	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
220	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
221	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
222	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
223	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
224	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
225	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
226	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
227	Ab initio enhanced sampling kinetic study on MTO ethene methylation reaction. Journal of Catalysis, 2020, 388, 38-51.	3.1	24
228	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
229	Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. Chemistry - A European Journal, 2011, 17, 12027-12036.	1.7	23
230	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
231	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
232	Ranking the Stars: A Refined Pareto Approach to Computational Materials Design. Physical Review Letters, 2013, 111, 075501.	2.9	23
233	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
234	Quasi-1D physics in metal-organic frameworks: MIL-47(V) from first principles. Beilstein Journal of Nanotechnology, 2014, 5, 1738-1748.	1.5	23

#	Article	IF	Citations
235	Ab initiobased thermal property predictions at a low cost: An error analysis. Physical Review B, 2014, 89, .	1.1	23
236	DFT-EPR study of radiation-induced radicals in ?-D-glucose. International Journal of Quantum Chemistry, 2004, 99, 102-108.	1.0	22
237	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
238	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
239	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
240	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
241	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
242	Access to Biorenewable and CO₂-Based Polycarbonates from Exovinylene Cyclic Carbonates. ACS Sustainable Chemistry and Engineering, 2021, 9, 1714-1728.	3.2	22
243	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
244	Theoretical study on the alteration of fundamental zeolite properties by methylene functionalization. Microporous and Mesoporous Materials, 2006, 96, 350-356.	2.2	21
245	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
246	Diphosphonylation of Aromatic Diazaheterocycles and Theoretical Rationalization of Product Yields. European Journal of Organic Chemistry, 2013, 2013, 1058-1067.	1.2	21
247	Semi-analytical mean-field model for predicting breathing in metalâ€“organic frameworks. Molecular Simulation, 2015, 41, 1311-1328.	0.9	21
248	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
249	Charting the Metal-Dependent High-Pressure Stability of Bimetallic UiO-66 Materials. , 2020, 2, 438-445.		21
250	Crystals springing into action: metalâ€“organic framework CUK-1 as a pressure-driven molecular spring. Chemical Science, 2021, 12, 5682-5687.	3.7	21
251	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
252	Ab initio study on elementary radical reactions in coke formation. International Journal of Quantum Chemistry, 2003, 91, 384-388.	1.0	20

#	Article	IF	Citations
253	The Rhâ€“ligand bond: RhX (X=C, N, O, F, P and Cl) molecules. Chemical Physics Letters, 2006, 421, 281-286.	1.2	20
254	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
255	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. Polymer, 2011, 52, 5503-5512.	1.8	20
256	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
257	Synthesis of 2â€Hydroxyâ€1,4â€oxazinâ€3â€ones through Ring Transformation of 3â€Hydroxyâ€4â€(1,2â€dihydroxyethyl)â€Î²â€lactams and a Study of Their Reactivity. Chemistry - A European Journal, 2013, 19, 3383-3396.	1.7	20
258	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
259	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
260	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
261	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
262	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
263	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
264	Carbon capture turned upside down: high-temperature adsorption & low-temperature desorption (HALD). Energy and Environmental Science, 2015, 8, 2480-2491.	15.6	19
265	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
266	Overview of Nâ€Rich Antennae Investigated in Lanthanideâ€Based Temperature Sensing. Chemistry - A European Journal, 2021, 27, 7214-7230.	1.7	19
267	First-principles calculation of the EPRgtensor in extended periodic systems. Physical Review B, 2006, 73, .	1.1	18
268	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
269	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
270	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

#	Article	IF	Citations
271	Texture Formation in Polycrystalline Thin Films of Allâ€Inorganic Lead Halide Perovskite. Advanced Materials, 2021, 33, e2007224.	11.1	18
272	Bifunctional acidâ€“base catalyzed reactions in zeolites from the HSAB viewpoint. Chemical Physics Letters, 2006, 419, 10-15.	1.2	17
273	Conformational Sampling of Macrocyclic Alkenes Using a Kennardâ^'Stone-Based Algorithm. Journal of Physical Chemistry A, 2010, 114, 6879-6887.	1.1	17
274	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
275	Convergence of Atomic Charges with the Size of the Enzymatic Environment. Journal of Chemical Information and Modeling, 2015, 55, 564-571.	2.5	17
276	Influence of a Confined Methanol Solvent on the Reactivity of Active Sites in UiOâ€66. ChemPhysChem, 2018, 19, 420-429.	1.0	17
277	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
278	Elucidating the promotional effect of a covalent triazine framework in aerobic oxidation. Applied Catalysis B: Environmental, 2020, 269, 118769.	10.8	17
279	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
280	Mechanistic Characterization of Zeolite-Catalyzed Aromatic Electrophilic Substitution at Realistic Operating Conditions. Jacs Au, 2022, 2, 502-514.	3.6	17
281	Comparative study of kinetics and reactivity indices of free radical polymerization reactions. International Journal of Quantum Chemistry, 2005, 102, 454-460.	1.0	16
282	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
283	Theoretical insight into the regioselective ring-expansions of bicyclic aziridinium ions. Organic and Biomolecular Chemistry, 2018, 16, 796-806.	1.5	16
284	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
285	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
286	Catalytic and molecular separation properties of Zeogrids and Zeotiles. Catalysis Today, 2011, 168, 17-27.	2.2	15
287	Is the error on first-principles volume predictions absolute or relative?. Computational Materials Science, 2016, 117, 390-396.	1.4	15
288	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

#	Article	IF	Citations
289	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
290	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
291	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
292	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
293	Solventâ€Catalyzed Ringâ€“Chainâ€“Ring Tautomerization in Axially Chiral Compounds. Chemistry - A European Journal, 2012, 18, 12725-12732.	1.7	14
294	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
295	Flexibility versus rigidity: what determines the stability of zeolite frameworks? A case study. Materials Horizons, 2014, 1, 582-587.	6.4	13
296	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
297	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
298	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
299	Dynamic Interplay between Defective UiOâ€66 and Protic Solvents in Activated Processes. Chemistry - A European Journal, 2019, 25, 15315-15325.	1.7	13
300	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
301	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
302	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
303	Accurate prediction of 1H chemical shifts in interstrand cross-linked DNA. RSC Advances, 2013, 3, 3925.	1.7	12
304	Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. Journal of Chemical Theory and Computation, 2018, 14, 6359-6369.	2.3	12
305	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
306	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

#	Article	IF	Citations
307	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
308	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
309	BrÃ¸nsted Acid Catalyzed Tandem Defunctionalization of Biorenewable Ferulic acid and Derivates into Bioâ€Catechol. Angewandte Chemie, 2020, 132, 3087-3092.	1.6	11
310	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
311	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
312	Elucidation of the pre-nucleation phase directing metal-organic framework formation. Cell Reports Physical Science, 2021, 2, 100680.	2.8	11
313	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
314	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
315	Mechanistic Investigation on Oxygen Transfer with the Manganeseâ€Salen Complex. ChemCatChem, 2015, 7, 2711-2719.	1.8	10
316	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
317	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
318	Acidity effect on benzene methylation kinetics over substituted H-MeAlPO-5 catalysts. Journal of Catalysis, 2021, 404, 594-606.	3.1	10
319	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
320	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
321	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
322	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
323	Solution enthalpy of Po and Te in solid leadâ€“bismuth eutectic. Journal of Nuclear Materials, 2014, 450, 287-291.	1.3	9
324	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. Chemistry - A European Journal, 2015, 21, 19176-19185.	1.7	9

#	Article	IF	Citations
325	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
326	Unraveling the thermodynamic conditions for negative gas adsorption in soft porous crystals. Communications Physics, 2019, 2, .	2.0	9
327	A Comparative Study on the Photophysical Properties of Anthocyanins and Pyranoanthocyanins. Chemistry - A European Journal, 2021, 27, 5956-5971.	1.7	9
328	Validation of DFT-Based Methods for Predicting Qualitative Thermochemistry of Large Polyaromatics. ChemPhysChem, 2011, 12, 1100-1108.	1.0	8
329	Reactivity of 3â€Oxoâ€Î²â€lactams with Respect to Primary Aminesâ€”An Experimental and Computational Approach. Chemistry - A European Journal, 2017, 23, 18002-18009.	1.7	8
330	Interfacial study of clathrates confined in reversed silica pores. Journal of Materials Chemistry A, 2021, 9, 21835-21844.	5.2	8
331	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
332	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
333	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
334	Vibrational fingerprint of the absorption properties of UiO-type MOF materials. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
335	Optical Properties of Isolated and Covalent Organic Framework-Embedded Ruthenium Complexes. Journal of Physical Chemistry A, 2019, 123, 6854-6867.	1.1	7
336	v-representability of one-body density matrices. Physical Review A, 2001, 64, .	1.0	6
337	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
338	Ab initio study of the trapping of polonium on noble metals. Journal of Nuclear Materials, 2016, 472, 35-42.	1.3	6
339	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
340	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
341	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
342	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

#	Article	IF	Citations
343	Refinement of the supramolecular concept in methanol-to-olefin catalysis. Studies in Surface Science and Catalysis, 2007, 170, 1668-1676.	1.5	5
344	Exploring the vibrational fingerprint of the electronic excitation energy via molecular dynamics. Journal of Chemical Physics, 2014, 140, 134105.	1.2	5
345	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
346	Beyond the Diketopiperazine Family with Alternatively Bridged Brevianamide F Analogues. Journal of Organic Chemistry, 2015, 80, 8046-8054.	1.7	5
347	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
348	Alternating Copolymer of Double Four Ring Silicate and Dimethyl Silicone Monomerâ€“PSSâ€1. Chemistry - A European Journal, 2017, 23, 11286-11293.	1.7	5
349	Entropy Contributions to Transition State Modeling. , 2018, , 189-228.		5
350	Structural and Photophysical Properties of Various Polypyridyl Ligands: A Combined Experimental and Computational Study. ChemPhysChem, 2020, 21, 2489-2505.	1.0	5
351	A comparative theoretical study on the solvent dependency of anthocyanin extraction profiles. Journal of Molecular Liquids, 2022, 351, 118606.	2.3	5
352	Micropatterning of polyurethanes with lasers. Polymer International, 2002, 51, 1172-1177.	1.6	4
353	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
354	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
355	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
356	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
357	Entropyâ€Driven Chemisorption of NO_x on Phosphotungstic Acid. Angewandte Chemie - International Edition, 2012, 51, 11010-11013.	7.2	4
358	Automated generation of radical species in crystalline carbohydrate using ab initio MD simulations. Physical Chemistry Chemical Physics, 2014, 16, 17196-17205.	1.3	4
359	Formation of Fluorinated Amido Esters through Unexpected C3â^'C4 Bond Fission in 4â€Trifluoromethylâ€3â€oxoâ€Î²â€lactams. Chemistry - an Asian Journal, 2018, 13, 421-431.	1.7	4
360	Cationâ^'Ï€ Interactions Accelerate the Living Cationic Ring-Opening Polymerization of Unsaturated 2-Alkyl-2-oxazolines. Macromolecules, 2020, 53, 3832-3846.	2.2	4

#	Article	IF	Citations
361	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
362	Crystal structure prediction for supersaturated AZO: the case of Zn3Al2O6. CrystEngComm, 2013, 15, 10440.	1.3	3
363	Elucidating the Structural Isomerism of Fluorescent Strigolactone Analogue CISAâ€‹1. European Journal of Organic Chemistry, 2015, 2015, 1211-1217.	1.2	3
364	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
365	Frontiers in Modeling Metalâ€“Organic Frameworks. Advanced Theory and Simulations, 2019, 2, 1900196.	1.3	3
366	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
367	Reaction of Electrophilic Allyl Halides with Amines: A Reinvestigation. Synthesis, 2006, 2006, 2260-2264.	1.2	1
368	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
369	Identification of vanadium dopant sites in the metalâ€“organic framework DUT-5(Al). Physical Chemistry Chemical Physics, 2021, 23, 7088-7100.	1.3	1
370	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
371	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
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	Normal mode analysis of macromolecular systems with the mobile block Hessian method. , 2015, , .		0
374	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
375	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
376	Structural and Photophysical Properties of Various Polypyridyl Ligands: A Combined Experimental and Computational Study. ChemPhysChem, 2020, 21, 2488-2488.	1.0	0
377	Quantifying the Likelihood of Structural Models through a Dynamically Enhanced Powder Xâ€‹Ray Diffraction Protocol. Angewandte Chemie, 2021, 133, 8995-9004.	1.6	0
378	Frontispiece: Overview of Nâ€‹Rich Antennae Investigated in Lanthanideâ€‹Based Temperature Sensing. Chemistry - A European Journal, 2021, 27, .	1.7	0

#	Article	IF	Citations
379	Dynamic evolution of catalytic active sites within zeolite catalysis. , 2021, , .		0