Christian Ehm

List of Publications by Year
in descending order

52 papers	1,036 citations	361413 20 h-index	477307 29 g-index
57 all docs	57 docs citations	57 times ranked	548 citing authors

#	Article	IF	Citations
1	Role(s) of TMA in polymerization. Dalton Transactions, 2016, 45, 6847-6855.	3.3	68
2	Catalyst activation and the dimerization energy of alkylaluminium compounds. Journal of Organometallic Chemistry, 2014, 772-773, 161-171.	1.8	59
3	Calculating accurate barriers for olefin insertion and related reactions. Journal of Organometallic Chemistry, 2015, 775, 39-49.	1.8	56
4	Accurate Prediction of Copolymerization Statistics in Molecular Olefin Polymerization Catalysis: The Role of Entropic, Electronic, and Steric Effects in Catalyst Comonomer Affinity. ACS Catalysis, 2017, 7, 1512-1519.	11.2	54
5	Cyclic polyacetylene. Nature Chemistry, 2021, 13, 792-799.	13.6	51
6	Selective Copper Complex-Catalyzed Hydrodefluorination of Fluoroalkenes and Allyl Fluorides: A Tale of Two Mechanisms. Journal of the American Chemical Society, 2019, 141, 11506-11521.	13.7	42
7	Connection of Stereoselectivity, Regioselectivity, and Molecular Weight Capability in <i>rac</i>-Râ€²₂Si(2-Me-4-R-indenyl)₂ZrCl₂ Type Catalysts. Macromolecules, 2018, 51, 8073-8083.	4.8	40
8	Backbone rearrangement during olefin capture as the rate limiting step in molecular olefin polymerization catalysis and its effect on comonomer affinity. Journal of Polymer Science Part A, 2017, 55, 2807-2814.	2.3	39
9	Chain Transfer to Solvent in Propene Polymerization with Ti Cp-phosphinimide Catalysts: Evidence for Chain Termination via Tiâ€“C Bond Homolysis. ACS Catalysis, 2016, 6, 7989-7993.	11.2	31
10	MgCl₂-Supported Zieglerâ€“Natta Catalysts: a DFT-D â€œFlexible-Clusterâ€•Approach to Internal Donor Adducts. Journal of Physical Chemistry C, 2018, 122, 9046-9053.	3.1	30
11	An Integrated High Throughput Experimentation/Predictive QSAR Modeling Approach to ansa-Zirconocene Catalysts for Isotactic Polypropylene. Polymers, 2020, 12, 1005.	4.5	29
12	Reactivity Trends of Lewis Acidic Sites in Methylaluminoxane and Some of Its Modifications. Inorganic Chemistry, 2020, 59, 5751-5759.	4.0	28
13	<i>ansa</i>-Zirconocene Catalysts for Isotactic-Selective Propene Polymerization at High Temperature: A Long Story Finds a Happy Ending. Journal of the American Chemical Society, 2021, 143, 7641-7647.	13.7	28
14	BHT-Modified MAO: Cage Size Estimation, Chemical Counting of Strongly Acidic Al Sites, and Activation of a Ti-Phosphinimide Precatalyst. ACS Catalysis, 2019, 9, 2996-3010.	11.2	26
15	High-Throughput Experimentation in Olefin Polymerization Catalysis: Facing the Challenges of Miniaturization. Industrial & Engineering Chemistry Research, 2020, 59, 13940-13947.	3.7	26
16	A Systematic Study of the Temperature-Induced Performance Decline of <i>ansa</i>-Metallocenes for iPP. Macromolecules, 2020, 53, 9325-9336.	4.8	26
17	Methylaluminoxaneâ€™s Molecular Cousin: A Well-defined and â€œCompleteâ€•Al-Activator for Molecular Olefin Polymerization Catalysts. ACS Catalysis, 2021, 11, 4464-4475.	11.2	26
18	On the Nature of the Lewis Acidic Sites in â€œTMAâ€Freeâ€•Phenolâ€Modified Methylaluminoxane. European Journal of Inorganic Chemistry, 2020, 2020, 1088-1095.	2.0	25

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19	Internal Donors in Zieglerâ€“Natta Systems: is Reduction by AlR₃ a Requirement for Donor Cleanâ€Up?. ChemCatChem, 2018, 10, 984-988.	3.7	21
20	How a Thermally Unstable Metal Hydrido Complex Can Yield High Catalytic Activity Even at Elevated Temperatures. Chemistry - A European Journal, 2016, 22, 9305-9310.	3.3	20
21	Tuning the Relative Energies of Propagation and Chain Termination Barriers in Polyolefin Catalysis through Electronic and Steric Effects. European Journal of Inorganic Chemistry, 2017, 2017, 3343-3349.	2.0	20
22	On the limits of tuning comonomer affinity of â€˜Spaleck-typeâ€™ <i>ansa</i>-zirconocenes in ethene/1-hexene copolymerization: a high-throughput experimentation/QSAR approach. Dalton Transactions, 2020, 49, 10162-10172.	3.3	19
23	Metalâ€“carbon bond strengths under polymerization conditions: 2,1-insertion as a catalyst stress test. Journal of Catalysis, 2017, 351, 146-152.	6.2	18
24	Fluorinated butatrienes. Journal of Fluorine Chemistry, 2010, 131, 1173-1181.	1.7	17
25	Organocatalytic Câ^'F Bond Activation with Alanes. Chemistry - A European Journal, 2018, 24, 6769-6777.	3.3	17
26	<i>C</i>₁-Symmetric Si-bridged (2-indenyl)(1-indenyl) <i>ansa</i>-metallocenes as efficient ethene/1-hexene copolymerization catalysts. Dalton Transactions, 2020, 49, 3015-3025.	3.3	17
27	Competition of Nucleophilic Aromatic Substitution, Ïƒâ€Bond Metathesis, and <i>syn</i> Hydrometalation in Titanium(III)â€Catalyzed Hydrodefluorination of Arenes. Chemistry - an Asian Journal, 2016, 11, 3062-3071.	3.3	15
28	Catalyst Mileage in Olefin Polymerization: The Peculiar Role of Toluene. Organometallics, 2018, 37, 2872-2879.	2.3	15
29	MgCl₂â€supported Zieglerâ€Natta catalysts: A DFTâ€D â€˜flexibleâ€clusterâ€™ approach. TiCl₄ and probe donor adducts. International Journal of Quantum Chemistry, 2018, 118, e25721.	2.0	14
30	Improving selectivity in catalytic hydrodefluorination by limiting S_NV reactivity. Dalton Transactions, 2016, 45, 16789-16798.	3.3	13
31	Toluene and Î±-Olefins as Radical Scavengers: Direct NMR Evidence for Homolytic Chain Transfer Mechanism Leading to Benzyl and â€œDormantâ€• Titanium Allyl Complexes. Organometallics, 2018, 37, 4189-4194.	2.3	13
32	Dielsâ€“Alder reactions of 1,1,4,4-tetrafluorobutatriene. Chemical Communications, 2010, 46, 2399.	4.1	12
33	Structure and Chemistry of SeF_{<i>x</i>}(CN)_{4-x} Compounds. Inorganic Chemistry, 2015, 54, 5220-5231.	4.0	12
34	SPAAC iClick: progress towards a bioorthogonal reaction in-corporating metal ions. Dalton Transactions, 2021, 50, 12681-12691.	3.3	11
35	Role of Solvent Coordination on the Structure and Dynamics of <i>ansa</i>-Zirconocenium Ion Pairs in Aromatic Hydrocarbons. Organometallics, 2022, 41, 547-560.	2.3	11
36	Separating Electronic from Steric Effects in Ethene/Î±-Olefin Copolymerization: A Case Study on Octahedral [ONNO] Zr-Catalysts. Processes, 2019, 7, 384.	2.8	9

#	Article	IF	Citations
37	Hafnium vs. Zirconium, the Perpetual Battle for Supremacy in Catalytic Olefin Polymerization: A Simple Matter of Electrophilicity?. Polymers, 2021, 13, 2621.	4.5	9
38	Selection of Low-Dimensional 3-D Geometric Descriptors for Accurate Enantioselectivity Prediction. ACS Catalysis, 2022, 12, 6934-6945.	11.2	9
39	Probing Î²-alkyl elimination and selectivity in polyolefin hydrogenolysis through DFT. Catalysis Science and Technology, 2021, 11, 6155-6162.	4.1	8
40	Chain Transfer to Solvent and Monomer in Early Transition Metal Catalyzed Olefin Polymerization: Mechanisms and Implications for Catalysis. Catalysts, 2021, 11, 215.	3.5	8
41	Gallium Hydrides and O/Nâ€Donors as Tunable Systems in Câˆ’F Bond Activation. Chemistry - an Asian Journal, 2018, 13, 2908-2915.	3.3	7
42	Stabilizing Effect of Pre-equilibria: A Trifluoromethyl Complex as a CF₂ Reservoir in Catalytic Olefin Difluorocarbenation. ACS Catalysis, 2022, 12, 3719-3730.	11.2	6
43	Polyolefin chain shuttling at ansa-metallocene catalysts: legend and reality. European Polymer Journal, 2021, 150, 110396.	5.4	5
44	A Highâ€Throughput Approach to Repurposing Olefin Polymerization Catalysts for Polymer Upcycling. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
45	Partially Fluorinated Butatrienes: A Coupled Cluster Study. Journal of Physical Chemistry A, 2010, 114, 3609-3614.	2.5	4
46	Cyclic dimers of tetrafluorobutatriene. Theoretical Chemistry Accounts, 2011, 129, 507-515.	1.4	4
47	From Mechanistic Investigation to Quantitative Prediction. , 2019, , 287-326.		4
48	Isolation of an Elusive Phosphametallacyclobutadiene and Its Role in Reversible Carbonâˆ’Carbon Bond Cleavage. Angewandte Chemie - International Edition, 2022, 61, .	13.8	4
49	Between T and Y: Asymmetry in the Interaction of LAu(I) with Bipy and Î²â€Diiminateâ€like Ligands. European Journal of Inorganic Chemistry, 2021, 2021, 314-320.	2.0	2
50	Isolation of an Elusive Phosphametallacyclobutadiene and Its Role in Reversible Carbonâˆ’Carbon Bond Cleavage. Angewandte Chemie, 2022, 134, .	2.0	2
51	Internal Donors in Ziegler-Natta Systems: is Reduction by AlR3 a Requirement for Donor Clean-Up?. ChemCatChem, 2018, 10, 863-863.	3.7	1
52	A Highâ€Throughput Approach to Repurposing Olefin Polymerization Catalysts for Polymer Upcycling. Angewandte Chemie, 0, , .	2.0	0