

# Christian Ehm

## List of Publications by Year in descending order

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52  
papers

1,036  
citations

361413

20  
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477307

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docs citations

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times ranked

548  
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#	ARTICLE	IF	CITATIONS
1	Role of Solvent Coordination on the Structure and Dynamics of <i>ansa</i> -Zirconocenium Ion Pairs in Aromatic Hydrocarbons. <i>Organometallics</i> , 2022, 41, 547-560.	2.3	11
2	Stabilizing Effect of Pre-equilibria: A Trifluoromethyl Complex as a CF <sub>2</sub> Reservoir in Catalytic Olefin Difluorocarbonation. <i>ACS Catalysis</i> , 2022, 12, 3719-3730.	11.2	6
3	A High-Throughput Approach to Repurposing Olefin Polymerization Catalysts for Polymer Upcycling. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	5
4	Isolation of an Elusive Phosphametallacyclobutadiene and Its Role in Reversible Carbon-Carbon Bond Cleavage. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	4
5	Isolation of an Elusive Phosphametallacyclobutadiene and Its Role in Reversible Carbon-Carbon Bond Cleavage. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	2
6	Selection of Low-Dimensional 3-D Geometric Descriptors for Accurate Enantioselectivity Prediction. <i>ACS Catalysis</i> , 2022, 12, 6934-6945.	11.2	9
7	SPAAC iClick: progress towards a bioorthogonal reaction in-corporating metal ions. <i>Dalton Transactions</i> , 2021, 50, 12681-12691.	3.3	11
8	Probing $\beta$ -alkyl elimination and selectivity in polyolefin hydrogenolysis through DFT. <i>Catalysis Science and Technology</i> , 2021, 11, 6155-6162.	4.1	8
9	Between T and Y: Asymmetry in the Interaction of LAu(I) with Bipy and $\beta$ -iminato-like Ligands. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 314-320.	2.0	2
10	Chain Transfer to Solvent and Monomer in Early Transition Metal Catalyzed Olefin Polymerization: Mechanisms and Implications for Catalysis. <i>Catalysts</i> , 2021, 11, 215.	3.5	8
11	Methylaluminoxane's Molecular Cousin: A Well-defined and Complete Al-Activator for Molecular Olefin Polymerization Catalysts. <i>ACS Catalysis</i> , 2021, 11, 4464-4475.	11.2	26
12	Polyolefin chain shuttling at <i>ansa</i> -metallocene catalysts: legend and reality. <i>European Polymer Journal</i> , 2021, 150, 110396.	5.4	5
13	<i>ansa</i> -Zirconocene Catalysts for Isotactic-Selective Propene Polymerization at High Temperature: A Long Story Finds a Happy Ending. <i>Journal of the American Chemical Society</i> , 2021, 143, 7641-7647.	13.7	28
14	Cyclic polyacetylene. <i>Nature Chemistry</i> , 2021, 13, 792-799.	13.6	51
15	Hafnium vs. Zirconium, the Perpetual Battle for Supremacy in Catalytic Olefin Polymerization: A Simple Matter of Electrophilicity?. <i>Polymers</i> , 2021, 13, 2621.	4.5	9
16	On the Nature of the Lewis Acidic Sites in TMA-Free Phenol-Modified Methylaluminoxane. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1088-1095.	2.0	25
17	High-Throughput Experimentation in Olefin Polymerization Catalysis: Facing the Challenges of Miniaturization. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 13940-13947.	3.7	26
18	On the limits of tuning comonomer affinity of Spaleck-type <i>ansa</i> -zirconocenes in ethene/1-hexene copolymerization: a high-throughput experimentation/QSAR approach. <i>Dalton Transactions</i> , 2020, 49, 10162-10172.	3.3	19

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19	A Systematic Study of the Temperature-Induced Performance Decline of <i>ansa</i> -Metalloenes for iPP. <i>Macromolecules</i> , 2020, 53, 9325-9336.	4.8	26
20	An Integrated High Throughput Experimentation/Predictive QSAR Modeling Approach to <i>ansa</i> -Zirconocene Catalysts for Isotactic Polypropylene. <i>Polymers</i> , 2020, 12, 1005.	4.5	29
21	<i>C</i> <sub>1</sub> -Symmetric Si-bridged (2-indenyl)(1-indenyl) <i>ansa</i> -metalloenes as efficient ethene/1-hexene copolymerization catalysts. <i>Dalton Transactions</i> , 2020, 49, 3015-3025.	3.3	17
22	Reactivity Trends of Lewis Acidic Sites in Methylaluminoxane and Some of Its Modifications. <i>Inorganic Chemistry</i> , 2020, 59, 5751-5759.	4.0	28
23	Selective Copper Complex-Catalyzed Hydrodefluorination of Fluoroalkenes and Allyl Fluorides: A Tale of Two Mechanisms. <i>Journal of the American Chemical Society</i> , 2019, 141, 11506-11521.	13.7	42
24	Separating Electronic from Steric Effects in Ethene/ $\pm$ -Olefin Copolymerization: A Case Study on Octahedral [ONNO] Zr-Catalysts. <i>Processes</i> , 2019, 7, 384.	2.8	9
25	BHT-Modified MAO: Cage Size Estimation, Chemical Counting of Strongly Acidic Al Sites, and Activation of a Ti-Phosphinimide Precatalyst. <i>ACS Catalysis</i> , 2019, 9, 2996-3010.	11.2	26
26	From Mechanistic Investigation to Quantitative Prediction. , 2019, , 287-326.		4
27	MgCl <sub>2</sub> -Supported Ziegler-Natta Catalysts: a DFT-D $\infty$ -Flexible-Cluster Approach to Internal Donor Adducts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9046-9053.	3.1	30
28	Internal Donors in Ziegler-Natta Systems: is Reduction by AlR <sub>3</sub> a Requirement for Donor Clean-Up?. <i>ChemCatChem</i> , 2018, 10, 863-863.	3.7	1
29	Organocatalytic C-F Bond Activation with Alanes. <i>Chemistry - A European Journal</i> , 2018, 24, 6769-6777.	3.3	17
30	Internal Donors in Ziegler-Natta Systems: is Reduction by AlR <sub>3</sub> a Requirement for Donor Clean-Up?. <i>ChemCatChem</i> , 2018, 10, 984-988.	3.7	21
31	Toluene and $\pm$ -Olefins as Radical Scavengers: Direct NMR Evidence for Homolytic Chain Transfer Mechanism Leading to Benzyl and $\infty$ -Dormant-Titanium Allyl Complexes. <i>Organometallics</i> , 2018, 37, 4189-4194.	2.3	13
32	Connection of Stereoselectivity, Regioselectivity, and Molecular Weight Capability in <i>rac</i> - $\text{Si}(2\text{-Me-4-R-indenyl})_2\text{ZrCl}_2$ Type Catalysts. <i>Macromolecules</i> , 2018, 51, 8073-8083.	4.8	40
33	MgCl <sub>2</sub> -supported Ziegler-Natta catalysts: A DFT $\infty$ -flexible-cluster approach. TiCl <sub>4</sub> and probe donor adducts. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25721.	2.0	14
34	Catalyst Mileage in Olefin Polymerization: The Peculiar Role of Toluene. <i>Organometallics</i> , 2018, 37, 2872-2879.	2.3	15
35	Gallium Hydrides and O/N-Donors as Tunable Systems in C-F Bond Activation. <i>Chemistry - an Asian Journal</i> , 2018, 13, 2908-2915.	3.3	7
36	Accurate Prediction of Copolymerization Statistics in Molecular Olefin Polymerization Catalysis: The Role of Entropic, Electronic, and Steric Effects in Catalyst Comonomer Affinity. <i>ACS Catalysis</i> , 2017, 7, 1512-1519.	11.2	54

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37	Metal–carbon bond strengths under polymerization conditions: 2,1-insertion as a catalyst stress test. <i>Journal of Catalysis</i> , 2017, 351, 146-152.	6.2	18
38	Backbone rearrangement during olefin capture as the rate limiting step in molecular olefin polymerization catalysis and its effect on comonomer affinity. <i>Journal of Polymer Science Part A</i> , 2017, 55, 2807-2814.	2.3	39
39	Tuning the Relative Energies of Propagation and Chain Termination Barriers in Polyolefin Catalysis through Electronic and Steric Effects. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3343-3349.	2.0	20
40	How a Thermally Unstable Metal Hydrido Complex Can Yield High Catalytic Activity Even at Elevated Temperatures. <i>Chemistry - A European Journal</i> , 2016, 22, 9305-9310.	3.3	20
41	Improving selectivity in catalytic hydrodefluorination by limiting $S_{N2}$ reactivity. <i>Dalton Transactions</i> , 2016, 45, 16789-16798.	3.3	13
42	Competition of Nucleophilic Aromatic Substitution, $\sigma$ -Bond Metathesis, and <i>syn</i> Hydrometalation in Titanium(III)-Catalyzed Hydrodefluorination of Arenes. <i>Chemistry - an Asian Journal</i> , 2016, 11, 3062-3071.	3.3	15
43	Chain Transfer to Solvent in Propene Polymerization with Ti Cp-phosphinimide Catalysts: Evidence for Chain Termination via Ti–C Bond Homolysis. <i>ACS Catalysis</i> , 2016, 6, 7989-7993.	11.2	31
44	Role(s) of TMA in polymerization. <i>Dalton Transactions</i> , 2016, 45, 6847-6855.	3.3	68
45	Structure and Chemistry of $SeF_x(CN)_4-x$ Compounds. <i>Inorganic Chemistry</i> , 2015, 54, 5220-5231.	4.0	12
46	Calculating accurate barriers for olefin insertion and related reactions. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 39-49.	1.8	56
47	Catalyst activation and the dimerization energy of alkylaluminium compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 161-171.	1.8	59
48	Cyclic dimers of tetrafluorobutatriene. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 507-515.	1.4	4
49	Fluorinated butatrienes. <i>Journal of Fluorine Chemistry</i> , 2010, 131, 1173-1181.	1.7	17
50	Partially Fluorinated Butatrienes: A Coupled Cluster Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3609-3614.	2.5	4
51	Diels–Alder reactions of 1,1,4,4-tetrafluorobutatriene. <i>Chemical Communications</i> , 2010, 46, 2399.	4.1	12
52	A High-Throughput Approach to Repurposing Olefin Polymerization Catalysts for Polymer Upcycling. <i>Angewandte Chemie</i> , 0, , .	2.0	0