Vidar Remi Jensen

List of Publications by Year
in descending order

94 papers	3,435 citations	172207 29 h-index	155451 55 g-index
98 all docs	98 docs citations	98 times ranked	3291 citing authors

#	Article	IF	Citations
1	The accuracy of DFT-optimized geometries of functional transition metal compounds: a validation study of catalysts for olefin metathesis and other reactions in the homogeneous phase. Dalton Transactions, 2012, 41, 5526.	1.6	429
2	Quantitative Structureâˆ'Activity Relationships of Ruthenium Catalysts for Olefin Metathesis. Journal of the American Chemical Society, 2006, 128, 6952-6964.	6.6	202
3	Toward Quantitative Prediction of Stereospecificity of Metallocene-Based Catalysts for Î±-Olefin Polymerization. Chemical Reviews, 2000, 100, 1457-1470.	23.0	164
4	Simple and Highly <i>Z</i>-Selective Ruthenium-Based Olefin Metathesis Catalyst. Journal of the American Chemical Society, 2013, 135, 3331-3334.	6.6	145
5	Metalâˆ'Phosphine Bond Strengths of the Transition Metals: A Challenge for DFT. Journal of Physical Chemistry A, 2009, 113, 11833-11844.	1.1	127
6	Automated in Silico Design of Homogeneous Catalysts. ACS Catalysis, 2020, 10, 2354-2377.	5.5	119
7	Donor-Ligand-Substituted Cyclopentadienylchromium(III) Complexes:Â A New Class of Alkene Polymerization Catalyst. 2. Phosphinoalkyl-Substituted Systems. Organometallics, 2001, 20, 2234-2245.	1.1	96
8	Activity of Rhodium-Catalyzed Hydroformylation:Â Added Insight and Predictions from Theory. Journal of the American Chemical Society, 2007, 129, 8487-8499.	6.6	94
9	Synthesis and Stability of Homoleptic Metal(III) Tetramethylaluminates. Journal of the American Chemical Society, 2011, 133, 6323-6337.	6.6	90
10	Bimolecular Coupling as a Vector for Decomposition of Fast-Initiating Olefin Metathesis Catalysts. Journal of the American Chemical Society, 2018, 140, 6931-6944.	6.6	88
11	An Evolutionary Algorithm for <i>de Novo</i> Optimization of Functional Transition Metal Compounds. Journal of the American Chemical Society, 2012, 134, 8885-8895.	6.6	79
12	Loss and Reformation of Ruthenium Alkylidene: Connecting Olefin Metathesis, Catalyst Deactivation, Regeneration, and Isomerization. Journal of the American Chemical Society, 2017, 139, 16609-16619.	6.6	75
13	Complete Reaction Pathway of Ruthenium-Catalyzed Olefin Metathesis of Ethyl Vinyl Ether: Kinetics and Mechanistic Insight from DFT. Organometallics, 2013, 32, 2099-2111.	1.1	71
14	Activity of Homogeneous Chromium(III)-Based Alkene Polymerization Catalysts:Â Lack of Importance of the Barrier to Ethylene Insertion. Organometallics, 2000, 19, 403-410.	1.1	66
15	An investigation of the quantum chemical description of the ethylenic double bond in reactions: II. Insertion of ethylene into a titanium-carbon bond. Journal of Computational Chemistry, 1998, 19, 947-960.	1.5	56
16	Decomposition of Olefin Metathesis Catalysts by BrÃ¸nsted Base: Metallacyclobutane Deprotonation as a Primary Deactivating Event. Journal of the American Chemical Society, 2017, 139, 16446-16449.	6.6	53
17	Theory-assisted development of a robust and Z-selective olefin metathesis catalyst. Dalton Transactions, 2014, 43, 11106-11117.	1.6	50
18	Ziegler-Natta Ethylene Insertion Reaction for a Five-Coordinate Titanium Chloride Complex Bridged to an Aluminum Hydride Cocatalyst. Journal of the American Chemical Society, 1995, 117, 4109-4117.	6.6	47

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19	Palladium Precatalysts for Decarbonylative Dehydration of Fatty Acids to Linear Alpha Olefins. ACS Catalysis, 2016, 6, 7784-7789.	5.5	47
20	Nature of the Transition Metalâ€"Carbene Bond in Grubbs Olefin Metathesis Catalysts. Organometallics, 2011, 30, 3522-3529.	1.1	43
21	A Heterogeneous Catalyst for the Transformation of Fatty Acids to Î±-Olefins. ACS Catalysis, 2017, 7, 2543-2547.	5.5	43
22	Ruthenium Alkylidene Complexes of Chelating Amine Ligands. Organometallics, 2007, 26, 5803-5814.	1.1	40
23	Synthesis of a new bidentate NHCâ€"Ag(I) complex and its unanticipated reaction with the Hoveydaâ€"Grubbs first generation catalyst. Tetrahedron, 2009, 65, 7186-7194.	1.0	39
24	The First Imidazolium-Substituted Metal Alkylidene. Organometallics, 2007, 26, 4383-4385.	1.1	38
25	The Nature of the Barrier to Phosphane Dissociation from Grubbs Olefin Metathesis Catalysts. European Journal of Inorganic Chemistry, 2012, 2012, 1507-1516.	1.0	38
26	Automated Design of Realistic Organometallic Molecules from Fragments. Journal of Chemical Information and Modeling, 2014, 54, 767-780.	2.5	37
27	Evolutionary de novo design of phenothiazine derivatives for dye-sensitized solar cells. Journal of Materials Chemistry A, 2015, 3, 9851-9860.	5.2	36
28	Ethene Copolymerization with Trialkylsilyl Protected Polar Norbornene Derivates. Macromolecular Chemistry and Physics, 2004, 205, 308-318.	1.1	33
29	Selective production of linear Î±-olefins <i>via</i> catalytic deoxygenation of fatty acids and derivatives. Catalysis Science and Technology, 2018, 8, 1487-1499.	2.1	32
30	Automated Building of Organometallic Complexes from 3D Fragments. Journal of Chemical Information and Modeling, 2014, 54, 1919-1931.	2.5	31
31	Sterically (un)encumbered mer-tridentate N-heterocyclic carbene complexes of titanium(<scp>iv</scp>) for the copolymerization of cyclohexene oxide with CO₂. Dalton Transactions, 2016, 45, 14734-14744.	1.6	31
32	Phosphine-Based <i>Z</i>-Selective Ruthenium Olefin Metathesis Catalysts. Organometallics, 2016, 35, 1825-1837.	1.1	30
33	DENOPTIM: Software for Computational <i>de Novo</i> Design of Organic and Inorganic Molecules. Journal of Chemical Information and Modeling, 2019, 59, 4077-4082.	2.5	29
34	Computational Investigation of Ethylene Insertion into the Metalâ^'Methyl Bond of First-Row Transition Metal(III) Species. Organometallics, 2001, 20, 4852-4862.	1.1	26
35	A Novel Efficient Deoxygenation Process forN-HeteroareneN-Oxides. Journal of Organic Chemistry, 2005, 70, 3218-3224.	1.7	26
36	DFT Investigation of the Single-Center, Two-State Model for the Broken Rate Order of Transition Metal Catalyzed Olefin Polymerization. Macromolecules, 2005, 38, 10266-10278.	2.2	26

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37	Computer-aided molecular design of imidazole-based absorbents for CO 2 capture. International Journal of Greenhouse Gas Control, 2016, 49, 55-63.	2.3	26
38	Pyridine-Stabilized Fast-Initiating Ruthenium Monothiolate Catalysts for <i>Z</i>-Selective Olefin Metathesis. Organometallics, 2017, 36, 3284-3292.	1.1	26
39	Bimolecular Coupling in Olefin Metathesis: Correlating Structure and Decomposition for Leading and Emerging Rutheniumâˆ’Carbene Catalysts. Journal of the American Chemical Society, 2021, 143, 11072-11079.	6.6	26
40	Quantum Chemical Investigation of Ethylene Insertion into the Crâˆ’CH3Bond in CrCl(H2O)CH3+as a Model of Homogeneous Ethylene Polymerization. Organometallics, 1997, 16, 2514-2522.	1.1	25
41	Evaluation of PM3(tm) as a Geometry Generator in Theoretical Studies of Transition-Metal-Based Catalysts for Polymerizing Olefins. Journal of Molecular Modeling, 1997, 3, 193-202.	0.8	25
42	Theoretical Investigation of Bis(imido)chromium(VI) Cations as Polymerization Catalysts. Organometallics, 2001, 20, 616-626.	1.1	24
43	Green and Efficient Synthesis of Bidentate Schiff Base Ru Catalysts for Olefin Metathesis. Journal of Organic Chemistry, 2007, 72, 3561-3564.	1.7	23
44	Raman Spectroscopic and ab initio Quantum Chemical Investigations of Molecules and Complex Ions in the Molten System CsCl-NbCl5-NbOCl3. Inorganic Chemistry, 1995, 34, 4360-4369.	1.9	22
45	Structure and Thermodynamics of Gaseous Oxides, Hydroxides, and Mixed Oxohydroxides of Chromium:Â CrOm(OH)n(m,n= 0âˆ'2) and CrO3. A Computational Study. Journal of Physical Chemistry A, 1998, 102, 10414-10423.	1.1	21
46	Challenging Metathesis Catalysts with Nucleophiles and BrÃ¸nsted Base: Examining the Stability of State-of-the-Art Ruthenium Carbene Catalysts to Attack by Amines. ACS Catalysis, 2020, 10, 11623-11633.	5.5	21
47	The role of intermediate chain migration in propene polymerization using substituted {iPr(CpFlu)}ZrCl2/MAO catalysts. Macromolecular Rapid Communications, 2000, 21, 91-97.	2.0	20
48	Catalytic dehydrogenation of ethane over mononuclear Cr(III)-silica surface sites. Part 2: Cï£¿H activation by oxidative addition. Journal of Physical Organic Chemistry, 2006, 19, 25-33.	0.9	20
49	Neutral Nickel Ethylene Oligoâ€•and Polymerization Catalysts: Towards Computational Catalyst Prediction and Design. Chemistry - A European Journal, 2014, 20, 7962-7978.	1.7	20
50	<i>Z</i>-Selective Monothiolate Ruthenium Indenylidene Olefin Metathesis Catalysts. Organometallics, 2020, 39, 397-407.	1.1	20
51	Synthesis of Methoxy-Substituted Phenols by Peracid Oxidation of the Aromatic Ring. Journal of Organic Chemistry, 2005, 70, 7290-7296.	1.7	18
52	Influence of multidentate N-donor ligands on highly electrophilic zinc initiator for the ring-opening polymerization of epoxides. Journal of Organometallic Chemistry, 2011, 696, 1691-1697.	0.8	18
53	Ring Closure To Form Metal Chelates in 3D Fragment-Based de Novo Design. Journal of Chemical Information and Modeling, 2015, 55, 1844-1856.	2.5	18
54	Reduction of chromium in ethylene polymerisation using bis(imido)chromium(vi) catalyst precursorsElectronic supplementary information available: Cartesian coordinate files of the computed stationary points. See http://www.rsc.org/suppdata/cc/b1/b110296f/. Chemical Communications, 2002, , 542-543.	2.2	16

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55	Neutral Nickel Oligoâ€•and Polymerization Catalysts: The Importance of Alkyl Phosphine Intermediates in Chain Termination. Chemistry - A European Journal, 2011, 17, 14628-14642.	1.7	16
56	Theoretical Investigation of the Low-Energy States of CpMoCl(PMe3)2and Their Role in the Spin-Forbidden Addition of N2and CO. Journal of Physical Chemistry A, 2003, 107, 1424-1432.	1.1	15
57	Site epimerization in ansa-zirconocene polymerization catalysts. Journal of Organometallic Chemistry, 2006, 691, 4367-4378.	0.8	15
58	Vibrational spectra and ab initio quantum mechanical calculation of energy, geometry and vibrational frequencies of the oxothiophosphate ions PO3S3â^', PO2S3â^'2 and POS3â^'3. Journal of Molecular Structure, 1994, 319, 85-100.	1.8	14
59	Multiple Additions of Palladium to C60. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 365-371.	1.0	14
60	Striking a Compromise: Polar Functional Group Tolerance versus Insertion Barrier Height for Olefin Polymerization Catalysts. Organometallics, 2012, 31, 6022-6031.	1.1	14
61	Vibrational frequencies of AlF3. Chemical Physics Letters, 1994, 230, 196-202.	1.2	13
62	Integration of Ligand Field Molecular Mechanics in Tinker. Journal of Chemical Information and Modeling, 2015, 55, 1282-1290.	2.5	13
63	Titanium-Ethylene Complexes Proposed To Be Intermediates in Ziegler-Natta Catalysis. Can They Be Detected through Vibrational Spectroscopy?. Organometallics, 1995, 14, 4349-4358.	1.1	12
64	2001, 173, 117-122.	0.4	12
65	Structure and Stability of Substitutional Metallofullerenes of the Firstâ€Row Transition Metals. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 269-278.	1.0	12
66	Formation of the Ironâ€"Oxo Hydroxylating Species in the Catalytic Cycle of Aromatic Amino Acid Hydroxylases. Chemistry - A European Journal, 2011, 17, 3746-3758.	1.7	12
67	Chromium dichloride: the unusually flat bending potential of the5Îg-derived5B2ground state. Molecular Physics, 1997, 91, 131-138.	0.8	11
68	Structure and Stability of Networked Metallofullerenes of the Transition Metals. Journal of Physical Chemistry A, 2006, 110, 11711-11716.	1.1	11
69	The Aromatic Amino Acid Hydroxylase Mechanism: A Perspective From Computational Chemistry. Advances in Inorganic Chemistry, 2010, , 437-500.	0.4	11
70	Spin Crossover in a Hexaamineiron(II) Complex: Experimental Confirmation of a Computational Prediction. Chemistry - A European Journal, 2018, 24, 5082-5085.	1.7	11
71	Rapid Decomposition of Olefin Metathesis Catalysts by a Truncated N-Heterocyclic Carbene: Efficient Catalyst Quenching and N-Heterocyclic Carbene Vinylation. ACS Catalysis, 2018, 8, 11822-11826.	5.5	11
72	Ethylene-Triggered Formation of Ruthenium Alkylidene from Decomposed Catalyst. ACS Catalysis, 2020, 10, 6788-6797.	5.5	11

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73	The Zieglerâ€"Natta olefin insertion reaction for cationic metals. Chemical Physics Letters, 1993, 212, 353-361.	1.2	10
74	Strength of the metal-olefin bond in titanium complexes related to Ziegler-Natta catalysis. A theoretical model study of a square-pyramidal active center postulated to be found in titanium halide-based catalysts. Organometallics, 1994, 13, 282-288.	1.1	9
75	The Mechanism of Rh-Catalyzed Transformation of Fatty Acids to Linear Alpha olefins. Inorganics, 2017, 5, 87.	1.2	9
76	Green Solvent for the Synthesis of Linear Î±-Olefins from Fatty Acids. ACS Sustainable Chemistry and Engineering, 2019, 7, 4903-4911.	3.2	9
77	Silica-supported Z-selective Ru olefin metathesis catalysts. Molecular Catalysis, 2020, 483, 110743.	1.0	9
78	On the nature of the active site in ruthenium olefin coordinationâ€"insertion polymerization catalystsâ˜†. Journal of Molecular Catalysis A, 2010, 324, 64-74.	4.8	8
79	Accurate metalâ€"ligand bond energies in the Î·²-C₂H₄ and Î·²-C₆₀ complexes of Pt(PH₃)₂, with application to their Bis(triphenylphosphine) analogues. Molecular Physics, 2013, 111, 1599-1611.	0.8	8
80	Unsaturated and Benzannulated N-Heterocyclic Carbene Complexes of Titanium and Hafnium: Impact on Catalysts Structure and Performance in Copolymerization of Cyclohexene Oxide with CO2. Molecules, 2020, 25, 4364.	1.7	8
81	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	1.5	8
82	The Janus face of high trans-effect carbenes in olefin metathesis: gateway to both productivity and decomposition. Chemical Science, 2022, 13, 5107-5117.	3.7	8
83	An investigation of the quantum chemical description of the ethylenic double bond in reactions. I. The electrophilic addition of hydrochloric acid to ethylene. Journal of Chemical Physics, 1996, 105, 6910-6920.	1.2	7
84	Unusual Temperature Effects in Propene Polymerization Using Stereorigid Zirconocene Catalysts. ChemPhysChem, 2005, 6, 1929-1933.	1.0	7
85	Toward E-selective Olefin Metathesis: Computational Design and Experimental Realization of Ruthenium Thio-Indolate Catalysts. Topics in Catalysis, 0, , 1.	1.3	7
86	The Reaction Mechanism of Phenylalanine Hydroxylase. â€" A Question of Coordination. Pteridines, 2005, 16, 27-34.	0.5	6
87	Soft Bending Modes of Terminal Chlorides in Gaseous Two- and Three-Coordinate Cu(II)â^'Cl Species. Inorganic Chemistry, 1999, 38, 3985-3993.	1.9	5
88	Water Dissociation and Dioxygen Binding in Phenylalanine Hydroxylase. European Journal of Inorganic Chemistry, 2010, 2010, 351-356.	1.0	5
89	Substrate Hydroxylation by the Oxidoâ€"Iron Intermediate in Aromatic Amino Acid Hydroxylases: A DFT Mechanistic Study. European Journal of Inorganic Chemistry, 2011, 2011, 2720-2732.	1.0	5
90	Supported Ru olefin metathesis catalysts <i>via</i> a thiolate tether. Dalton Transactions, 2019, 48, 2886-2890.	1.6	5

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91	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	1.5	4
92	Benefit of a hemilabile ligand in deoxygenation of fatty acids to 1-alkenes. Faraday Discussions, 2019, 220, 231-248.	1.6	4
93	Evolution inspector: Interactive visual analysis for evolutionary molecular design. , 2015, , .		1
94	Synthesis of Methoxy-Substituted Phenols by Peracid Oxidation of the Aromatic Ring.. ChemInform, 2006, 37, no.	0.1	0