

Vidar Remi Jensen

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91
papers

2,831
citations

27
h-index

50
g-index

98
ext. papers

3,157
ext. citations

6.4
avg, IF

5.44
L-index

#	Paper	IF	Citations
91	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. <i>Dalton Transactions</i> , 2012 , 41, 5526-41	4.3	346
90	Quantitative structure-activity relationships of ruthenium catalysts for olefin metathesis. <i>Journal of the American Chemical Society</i> , 2006 , 128, 6952-64	16.4	183
89	Toward Quantitative Prediction of Stereospecificity of Metallocene-Based Catalysts for alpha-Olefin Polymerization. <i>Chemical Reviews</i> , 2000 , 100, 1457-70	68.1	147
88	Simple and highly Z-selective ruthenium-based olefin metathesis catalyst. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3331-4	16.4	124
87	Metal-phosphine bond strengths of the transition metals: a challenge for DFT. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 11833-44	2.8	119
86	Donor-Ligand-Substituted Cyclopentadienylchromium(III) Complexes: A New Class of Alkene Polymerization Catalyst. 2. Phosphinoalkyl-Substituted Systems. <i>Organometallics</i> , 2001 , 20, 2234-2245	3.8	89
85	Synthesis and stability of homoleptic metal(III) tetramethylaluminates. <i>Journal of the American Chemical Society</i> , 2011 , 133, 6323-37	16.4	80
84	Activity of rhodium-catalyzed hydroformylation: added insight and predictions from theory. <i>Journal of the American Chemical Society</i> , 2007 , 129, 8487-99	16.4	80
83	Bimolecular Coupling as a Vector for Decomposition of Fast-Initiating Olefin Metathesis Catalysts. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6931-6944	16.4	69
82	Automated in Silico Design of Homogeneous Catalysts. <i>ACS Catalysis</i> , 2020 , 10, 2354-2377	13.1	66
81	An evolutionary algorithm for de novo optimization of functional transition metal compounds. <i>Journal of the American Chemical Society</i> , 2012 , 134, 8885-95	16.4	61
80	Activity of Homogeneous Chromium(III)-Based Alkene Polymerization Catalysts: Lack of Importance of the Barrier to Ethylene Insertion. <i>Organometallics</i> , 2000 , 19, 403-410	3.8	58
79	Loss and Reformation of Ruthenium Alkylidene: Connecting Olefin Metathesis, Catalyst Deactivation, Regeneration, and Isomerization. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16609-16619	16.4	56
78	Complete Reaction Pathway of Ruthenium-Catalyzed Olefin Metathesis of Ethyl Vinyl Ether: Kinetics and Mechanistic Insight from DFT. <i>Organometallics</i> , 2013 , 32, 2099-2111	3.8	55
77	An investigation of the quantum chemical description of the ethylenic double bond in reactions: II. Insertion of ethylene into a titanium-carbon bond. <i>Journal of Computational Chemistry</i> , 1998 , 19, 947-960	3.5	53
76	Decomposition of Olefin Metathesis Catalysts by Brønsted Base: Metallacyclobutane Deprotonation as a Primary Deactivating Event. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16446-16449	16.4	46
75	Theory-assisted development of a robust and Z-selective olefin metathesis catalyst. <i>Dalton Transactions</i> , 2014 , 43, 11106-17	4.3	43

74	Palladium Precatalysts for Decarbonylative Dehydration of Fatty Acids to Linear Alpha Olefins. <i>ACS Catalysis</i> , 2016 , 6, 7784-7789	13.1	41
73	Ziegler-Natta Ethylene Insertion Reaction for a Five-Coordinate Titanium Chloride Complex Bridged to an Aluminum Hydride Cocatalyst. <i>Journal of the American Chemical Society</i> , 1995 , 117, 4109-4117	16.4	40
72	Ruthenium Alkylidene Complexes of Chelating Amine Ligands. <i>Organometallics</i> , 2007 , 26, 5803-5814	3.8	39
71	A Heterogeneous Catalyst for the Transformation of Fatty Acids to α -Olefins. <i>ACS Catalysis</i> , 2017 , 7, 2543-2547	13.1	38
70	Nature of the Transition Metal-Carbene Bond in Grubbs Olefin Metathesis Catalysts. <i>Organometallics</i> , 2011 , 30, 3522-3529	3.8	37
69	The Nature of the Barrier to Phosphane Dissociation from Grubbs Olefin Metathesis Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2012 , 2012, 1507-1516	2.3	34
68	Synthesis of a new bidentate NHC-Ag(I) complex and its unanticipated reaction with the Hoveyda-Grubbs first generation catalyst. <i>Tetrahedron</i> , 2009 , 65, 7186-7194	2.4	34
67	Evolutionary de novo design of phenothiazine derivatives for dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 9851-9860	13	32
66	The First Imidazolium-Substituted Metal Alkylidene. <i>Organometallics</i> , 2007 , 26, 4383-4385	3.8	32
65	Ethene Copolymerization with Trialkylsilyl Protected Polar Norbornene Derivates. <i>Macromolecular Chemistry and Physics</i> , 2004 , 205, 308-318	2.6	32
64	Selective production of linear α -olefins via catalytic deoxygenation of fatty acids and derivatives. <i>Catalysis Science and Technology</i> , 2018 , 8, 1487-1499	5.5	26
63	Automated design of realistic organometallic molecules from fragments. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 767-80	6.1	26
62	DFT Investigation of the Single-Center, Two-State Model for the Broken Rate Order of Transition Metal Catalyzed Olefin Polymerization. <i>Macromolecules</i> , 2005 , 38, 10266-10278	5.5	25
61	Sterically (un)encumbered mer-tridentate N-heterocyclic carbene complexes of titanium(IV) for the copolymerization of cyclohexene oxide with CO ₂ . <i>Dalton Transactions</i> , 2016 , 45, 14734-44	4.3	23
60	Automated building of organometallic complexes from 3D fragments. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 1919-31	6.1	23
59	Quantum Chemical Investigation of Ethylene Insertion into the Cr-CH ₃ Bond in CrCl(H ₂ O)CH ₃ ⁺ as a Model of Homogeneous Ethylene Polymerization. <i>Organometallics</i> , 1997 , 16, 2514-2522	3.8	23
58	Evaluation of PM3(tm) as a Geometry Generator in Theoretical Studies of Transition-Metal-Based Catalysts for Polymerizing Olefins. <i>Journal of Molecular Modeling</i> , 1997 , 3, 193-202	2	23
57	A novel efficient deoxygenation process for N-heteroarene N-oxides. <i>Journal of Organic Chemistry</i> , 2005 , 70, 3218-24	4.2	23

56	Computational Investigation of Ethylene Insertion into the Metal-Methyl Bond of First-Row Transition Metal(III) Species. <i>Organometallics</i> , 2001 , 20, 4852-4862	3.8	22
55	Phosphine-Based Z-Selective Ruthenium Olefin Metathesis Catalysts. <i>Organometallics</i> , 2016 , 35, 1825-1837	3.8	21
54	Computer-aided molecular design of imidazole-based absorbents for CO ₂ capture. <i>International Journal of Greenhouse Gas Control</i> , 2016 , 49, 55-63	4.2	20
53	Neutral nickel ethylene oligo- and polymerization catalysts: towards computational catalyst prediction and design. <i>Chemistry - A European Journal</i> , 2014 , 20, 7962-78	4.8	19
52	Pyridine-Stabilized Fast-Initiating Ruthenium Monothiolate Catalysts for Z-Selective Olefin Metathesis. <i>Organometallics</i> , 2017 , 36, 3284-3292	3.8	19
51	Green and efficient synthesis of bidentate Schiff base Ru catalysts for olefin metathesis. <i>Journal of Organic Chemistry</i> , 2007 , 72, 3561-4	4.2	19
50	Catalytic dehydrogenation of ethane over mononuclear Cr(III) silica surface sites. Part 2: C-H activation by oxidative addition. <i>Journal of Physical Organic Chemistry</i> , 2006 , 19, 25-33	2.1	19
49	Theoretical Investigation of Bis(imido)chromium(VI) Cations as Polymerization Catalysts. <i>Organometallics</i> , 2001 , 20, 616-626	3.8	19
48	Structure and Thermodynamics of Gaseous Oxides, Hydroxides, and Mixed Oxohydroxides of Chromium: CrO _m (OH) _n (m, n = 0-3) and CrO ₃ . A Computational Study. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 10414-10423	2.8	18
47	Raman Spectroscopic and ab initio Quantum Chemical Investigations of Molecules and Complex Ions in the Molten System CsCl-NbCl ₅ -NbOCl ₃ . <i>Inorganic Chemistry</i> , 1995 , 34, 4360-4369	5.1	18
46	The role of intermediate chain migration in propene polymerization using substituted {iPr(CpFlu)}ZrCl ₂ /MAO catalysts. <i>Macromolecular Rapid Communications</i> , 2000 , 21, 91-97	4.8	17
45	Synthesis of methoxy-substituted phenols by peracid oxidation of the aromatic ring. <i>Journal of Organic Chemistry</i> , 2005 , 70, 7290-6	4.2	16
44	Neutral nickel oligo- and polymerization catalysts: the importance of alkyl phosphine intermediates in chain termination. <i>Chemistry - A European Journal</i> , 2011 , 17, 14628-42	4.8	15
43	Influence of multidentate N-donor ligands on highly electrophilic zinc initiator for the ring-opening polymerization of epoxides. <i>Journal of Organometallic Chemistry</i> , 2011 , 696, 1691-1697	2.3	15
42	Site epimerization in ansa-zirconocene polymerization catalysts. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 4367-4378	2.3	15
41	Theoretical Investigation of the Low-Energy States of CpMoCl(PMe ₃) ₂ and Their Role in the Spin-Forbidden Addition of N ₂ and CO. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1424-1432	2.8	15
40	DENOPTIM: Software for Computational Design of Organic and Inorganic Molecules. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4077-4082	6.1	13
39	Striking a Compromise: Polar Functional Group Tolerance versus Insertion Barrier Height for Olefin Polymerization Catalysts. <i>Organometallics</i> , 2012 , 31, 6022-6031	3.8	13

38	Multiple Additions of Palladium to C60. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2006 , 14, 365-378	3.7	13
37	Vibrational frequencies of AlF ₃ . <i>Chemical Physics Letters</i> , 1994 , 230, 196-202	2.5	13
36	Formation of the iron-oxo hydroxylating species in the catalytic cycle of aromatic amino acid hydroxylases. <i>Chemistry - A European Journal</i> , 2011 , 17, 3746-58	4.8	12
35	Reduction of chromium in ethylene polymerisation using bis(imido)chromium(VI) catalyst precursors. <i>Chemical Communications</i> , 2002 , 542-3	5.8	12
34	Challenging Metathesis Catalysts with Nucleophiles and Brønsted Base: Examining the Stability of State-of-the-Art Ruthenium Carbene Catalysts to Attack by Amines. <i>ACS Catalysis</i> , 2020 , 10, 11623-11633	13.1	12
33	Ring Closure To Form Metal Chelates in 3D Fragment-Based de Novo Design. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1844-56	6.1	11
32	Integration of Ligand Field Molecular Mechanics in Tinker. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1282-90	6.1	11
31	Z-Selective Monothiolate Ruthenium Indenylidene Olefin Metathesis Catalysts. <i>Organometallics</i> , 2020 , 39, 397-407	3.8	10
30	Chromium dichloride: the unusually flat bending potential of the 5g-derived 5B2 ground state. <i>Molecular Physics</i> , 1997 , 91, 131-138	1.7	10
29	Structure and Stability of Substitutional Metallofullerenes of the First-Row Transition Metals. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2006 , 14, 269-278	1.8	10
28	Structure and stability of networked metallofullerenes of the transition metals. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 11711-6	2.8	10
27	Steric control of the chromium-catalyzed oligomerization of ethylene ¹). <i>Macromolecular Symposia</i> , 2001 , 173, 117-122	0.8	10
26	The Ziegler-Natta olefin insertion reaction for cationic metals. <i>Chemical Physics Letters</i> , 1993 , 212, 353-361	1.5	10
25	Titanium-Ethylene Complexes Proposed To Be Intermediates in Ziegler-Natta Catalysis. Can They Be Detected through Vibrational Spectroscopy?. <i>Organometallics</i> , 1995 , 14, 4349-4358	3.8	9
24	Vibrational spectra and ab initio quantum mechanical calculation of energy, geometry and vibrational frequencies of the oxothiophosphate ions PO ₃ S ₃ ²⁻ and PO ₃ S ₃ ³⁻ . <i>Journal of Molecular Structure</i> , 1994 , 319, 85-100	3.4	9
23	Ethylene-Triggered Formation of Ruthenium Alkylidene from Decomposed Catalyst. <i>ACS Catalysis</i> , 2020 , 10, 6788-6797	13.1	8
22	The Mechanism of Rh-Catalyzed Transformation of Fatty Acids to Linear Alpha olefins. <i>Inorganics</i> , 2017 , 5, 87	2.9	8
21	Spin Crossover in a Hexamineiron(II) Complex: Experimental Confirmation of a Computational Prediction. <i>Chemistry - A European Journal</i> , 2018 , 24, 5082-5085	4.8	8

20	The Aromatic Amino Acid Hydroxylase Mechanism: A Perspective From Computational Chemistry. <i>Advances in Inorganic Chemistry</i> , 2010 , 437-500	2.1	8
19	Rapid Decomposition of Olefin Metathesis Catalysts by a Truncated N-Heterocyclic Carbene: Efficient Catalyst Quenching and N-Heterocyclic Carbene Vinylation. <i>ACS Catalysis</i> , 2018 , 8, 11822-11826 ^{13.1}		8
18	Accurate metal-olefin bond energies in the η^2 -C ₂ H ₄ and η^2 -C ₆₀ complexes of Pt(PH ₃) ₂ , with application to their Bis(triphenylphosphine) analogues. <i>Molecular Physics</i> , 2013 , 111, 1599-1611	1.7	7
17	On the nature of the active site in ruthenium olefin coordination-insertion polymerization catalysts?. <i>Journal of Molecular Catalysis A</i> , 2010 , 324, 64-74		7
16	Bimolecular Coupling in Olefin Metathesis: Correlating Structure and Decomposition for Leading and Emerging Ruthenium-Carbene Catalysts. <i>Journal of the American Chemical Society</i> , 2021 , 143, 11072-11079 ^{16.1}		7
15	Use of multivariate methods in the analysis of calculated reaction pathways. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1197-1216	3.5	7
14	An investigation of the quantum chemical description of the ethylenic double bond in reactions. I. The electrophilic addition of hydrochloric acid to ethylene. <i>Journal of Chemical Physics</i> , 1996 , 105, 6910-6920 ^{3.9}		6
13	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. <i>Organometallics</i> , 1994 , 13, 282-288	3.8	6
12	Silica-supported Z-selective Ru olefin metathesis catalysts. <i>Molecular Catalysis</i> , 2020 , 483, 110743	3.3	5
11	Substrate Hydroxylation by the Oxidation Intermediate in Aromatic Amino Acid Hydroxylases: A DFT Mechanistic Study. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 2720-2732	2.3	5
10	Water Dissociation and Dioxygen Binding in Phenylalanine Hydroxylase. <i>European Journal of Inorganic Chemistry</i> , 2010 , 2010, 351-356	2.3	5
9	The Reaction Mechanism of Phenylalanine Hydroxylase. A Question of Coordination. <i>Pteridines</i> , 2005 , 16, 27-34	0.6	5
8	Green Solvent for the Synthesis of Linear α -Olefins from Fatty Acids. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 4903-4911	8.3	4
7	Supported Ru olefin metathesis catalysts via a thiolate tether. <i>Dalton Transactions</i> , 2019 , 48, 2886-2890 ^{4.3}		4
6	Unusual temperature effects in propene polymerization using stereorigid zirconocene catalysts. <i>ChemPhysChem</i> , 2005 , 6, 1929-33	3.2	4
5	Benefit of a hemilabile ligand in deoxygenation of fatty acids to 1-alkenes. <i>Faraday Discussions</i> , 2019 , 220, 231-248	3.6	3
4	Soft Bending Modes of Terminal Chlorides in Gaseous Two- and Three-Coordinate Cu(II)Cl Species. <i>Inorganic Chemistry</i> , 1999 , 38, 3985-3993	5.1	3
3	Use of multivariate methods in the analysis of calculated reaction pathways. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1197-1216	3.5	3

- 2 Unsaturated and Benzannulated -Heterocyclic Carbene Complexes of Titanium and Hafnium: Impact on Catalysts Structure and Performance in Copolymerization of Cyclohexene Oxide with CO. *Molecules*, **2020**, 25, 4.8 3
- 1 Toward E-selective Olefin Metathesis: Computational Design and Experimental Realization of Ruthenium Thio-Indolate Catalysts. *Topics in Catalysis*, 1 2.3 3