# CV – Vidar R. Jensen

Role in the project Centre director I Principal investigator I Personal information				
First name, Surname:	Jensen, Vidar Remi			
Date of birth:	15.07.1966	Sex:	Male	
Nationality:	Norwegian			
Researcher unique identifier(s)ORCID: 0000-0003-2444-3220, Research ID: F-8740-2012		2012		
URL for personal website:	http://jensen.uib.no/			

#### Education

Year	Faculty/department - University/institution - Country
1995	Ph.D. Dept. of Inorganic Chemistry - The Norwegian Institute of Technology (NTNU)

# **Positions - current and previous**

Year	Job title – Employer - Country
2007–	Full Professor - Department of Chemistry, University of Bergen (UiB) - Norway. Group leader: 2 permanent researchers, 1 postdoc, 4 PhD students, 4 master students.
2003–08	Associate Professor at Department of Chemistry, UiB.
2002	CNRS Research Associate, Université de Bourgogne

# **Project management experience – most important projects**

Year	Project owner - Project - Role - Funder
2019–2023	UiB. Water-tolerant catalysis. WP Leader. Research Council of Norway (RCN) (Total budget: 1000 k€). Via the prestigious FRIPRO-mechanism (success rate in molecular chemistry < 5%). Collaboration between the two Centre Directors (Fogg/Jensen), with equal sharing of the resources between expt and comput. activities.
2017–2021	UiB. Sustainable and Selective Metathesis. <b>Principal Investigator (PI)</b> . RCN (Total budget: 1000 k€). <b>FRIPRO</b> project, close Jensen/Fogg collaboration, and mix of expt./comput.
2016–2020	UiB. Renewable aromatic hydrocarbons for fuel blending from lignin by novel homogenous catalysis. PI. RCN (Total budget: 1000 k€). Role: Computational catalyst design.
2015–2021	UiB and Univ. of Oslo. <b>Two FRIPRO projects</b> . <b>WP leader</b> . RCN (Combined total: ca. 1800 k€, WP share: ca. 600 k€). Role: Mechanistic and predictive calculations in catalysis.
2014–2017	UiB. µAlgae for climate, food, and feed. PI. RCN (Total budget: 850 k€). IdeaLab (sandbox) project. 6 partners covering genetics, optics, visualization, chemistry, and RRI.
2014–2017	Charles University (Prague). <i>Phosphine Ligands for Environmentally Friendly C-C Bond</i> <i>Forming Reactions</i> . <b>Node Leader</b> . EEA/Norway Grants (Total: 600 k€, Node: 280 k€)
2012–2016	UiB. Catalyst and process optimization for petrochemical applications of stereoselective olefin metathesis. PI. RCN (Total budget: 1000 k€)

2012–2015	NTNU. A method for automated de novo optimisation of functional transition-metal complexes. WP Leader. RCN (Total budget: 830 k€, WP budget: 310 k€).
2010–2017	Bergen Technology Transfer Office. <b>Two</b> commercialization projects on stereoselective olefin metathesis (a CDCM topi). <b>PI</b> and <b>WP leader</b> , respectively. RCN (Total budget: 1100 k€ and 550 k€, respectively). I led the technology development and IPR protection.
1998-2011	UiB. <b>PI</b> of <b>four</b> RCN-funded research projects, totalling ca. 1050 k€.

# Supervision of students

Master's students	Ph.D. students	Postdocs	University/institution - Country
8/0	8/1	6/0	University of Bergen/Norwegian University of Science and Technology

### Other relevant professional experiences

Year	Description - Role	
	INSTITUTIONAL / LEADERSHIP RESPONSIBILITIES	
2009–2015	Board member, the Research Council of Norway e-science program eVITA	
2007–2017	Department Council member, Department of Chemistry, UiB.	
2006–2010	Head of Section, Inorganic Chemistry, Nanostructures and Modeling, Department of Chemistry, UiB, encompassing 8 professors and their groups.	
	REVIEWING ACTIVITY	
2020	<b>Reviewer</b> , ERC Synergy, ETH, Agency for Science, Technology and Research (A*STAR, Singapore), The Polish National Science Centre, and Austrian Science Fund.	
2010-	<b>Reviewer</b> , Science, J. Am. Chem. Soc., Acc. Chem. Res., Chem. Sci., ACS Cat., ChemEur. J., Organometallics, J. Catal., and many more.	
2007–	<b>Reviewer</b> (repeated), the Technology Foundation STW (the Netherlands), The National Research Foundation (South Africa), ACS Petroleum Research Fund (USA).	
	COMMISSIONS OF TRUST	
2013–2018	Management Committee member of COST Actions CM1205 and CM1305.	
2012–2017	Scientific Advisory Board member, CTCC (a Centre of Excellence).	
2011–	Full professorship evaluation committees: NTNU (Norway), KTH (Sweden), DTU (Denmark).	
2008–	<b>Board member</b> , Organometallic Division of The European Association for Chemical and Molecular Sciences (EuCheMS).	

#### **Publication statistics**

91 articles published in peer-reviewed journals (61 as corresponding author); in total 2165 citations without self-citations; >200 per year and increasing. *h*-index: 25, i10 index: 62 (ISI WoS, 15.11.2020). Examples: *J. Am. Chem. Soc.* (9), *ACS Catalysis* (6), *Organometallics* (15), *J. Chem. Inf. Model.* (5).

# 10-year track record

Prof. Jensen envisions a future in which molecular and materials discovery is realized via "Big Computing / Big Data", not serendipity. Over the last 10 years, he has pursued this vision by developing fundamental and truly general-purpose methods for automated, *de novo* design of any kind of molecule, including catalysts and other metal-containing functional molecules. A related priority has been to verify predicted functional molecules by synthesis and testing. A second related track has been to uncover mechanistic insight to be used in subsequent computationally guided design.

### Representative publications last 10 years (Corresponding author of all)

- 10. Foscato, M.; Jensen, V. R. Automated in Silico Design of Homogeneous Catalysts. *ACS Catal.* **2020**, *10*, 2354–2377. (Perspective on **topic of proposal**: automation in catalyst design, **already cited 11 times**.)
- 9. Bernhardt, P. V. (10); **Jensen**, V. R. (author #7) Spin Crossover in a Hexaamineiron(II) Complex: Experimental Confirmation of a Computational Prediction. *Chem. Eur. J.* **2018**, 24, 5082–5085. (Firstever experimentally confirmed inorganic molecule designed using an automated de novo approach.)
- 8. Engel, J. (6); **Jensen**, V. R. (author #6) *Loss and Reformation of Ruthenium Alkylidene: Connecting Olefin Metathesis, Catalyst Deactivation, Regeneration, and Isomerization. J. Am. Chem. Soc.* **2017**, 139, 16609–16619. (High-impact study on metathesis catalyst stability (relevant for MD1), **36 citations**.)
- 7. Foscato, M.; Houghton, B. J.; Occhipinti, G.; Deeth, R. J.; **Jensen**, V. R. Ring Closure to Form Metal Chelates in 3D Fragment-Based de Novo Design. *J. Chem. Inf. Model.* **2015**, *55*, 1844–1856. (Method development for de novo design and conformational selection (relevant for EM1), 10 citations.)
- 6. Occhipinti, G.; Koudriavtsev, V; Törnroos, K. W.; **Jensen**, V. R. Theory-Assisted Development of a Robust and Z-Selective Olefin Metathesis Catalyst. *Dalton Trans*. **2014**, 43, 11106–11117. (Expt. verified design of a robust and stereoselective metathesis catalyst (relevant for MD1), **34 citations**.)
- Foscato, M.; Venkatraman, V.; Occhipinti, G.; Alsberg, B.; Jensen, V. R. Automated Building of Organometallic Complexes from 3D Fragments. *J. Chem. Inf. Model.* 2014, *54*, 1919–1931. (Fundamental method development for de novo design (relevant for EM1), 18 citations.)
- 4. Foscato, M.; Occhipinti, G.; Venkatraman, V.; Alsberg, B.; **Jensen**, V. R. Automated design of realistic organometallic molecules from fragments. *J. Chem. Inf. Model.* **2014**, *54*, 767–780. (Fundamental method development for de novo design (relevant for EM1), 24 citations.)
- 3. Occhipinti, G.; Hansen, F. R.; Törnroos, K. W.; **Jensen**, V. R. Simple and Highly Z-Selective Ruthenium-Based Olefin Metathesis Catalyst. *J. Am. Chem. Soc.* **2013**, 135, 3331–3334. (High-impact breakthrough in metathesis (relevant for MD1) and demonstration of design, **99 citations**.)
- Chu, Y.; Heyndrickx, W.; Occhipinti, G.; Jensen, V. R.; Alsberg, B. K. An Evolutionary Algorithm for de Novo Optimization of Functional Transition Metal Compounds. *J. Am. Chem. Soc.* 2012, 134, 8885– 8895. (High-impact, first report on general-purpose de novo method, 50 citations.)
- Minenkov, Y.; Singstad, Å; Occhipinti, G.; Jensen, V. R. 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 Trans.* 2012, *41*, 5526–5541. (Benchmark study to gauge and improve the accuracy of molecular-level computational methods in mechanism and design studies, 276 citations, ISI Highly Cited Paper, among top 1% in chemistry)

# **Granted patents**

Catalysts developed using the *in silico* molecular design strategy championed by Prof. Jensen have so far been protected by three granted patents: United States Patent US 8,716,488 B2, May 6, 2014; United States Patent US 9,303,100 B2, Apr 5, 2016; United States Patent US 10,265,691 B2, Apr 23, 2019.

# Most important invited presentations to established conferences last 10 years

 Wenner-Gren Foundations International Symposium "Mechanistic Homogeneous Catalysis – A Meeting between Theory and Experiment", Stockholm, 4-7.09.2019. Invited lecture: *The Life, Death,* and Resurrection of Ruthenium Olefin Metathesis Catalysts.

- 9. International Symposium on Olefin Metathesis and Related Chemistry, Barcelona, Spain, 30.06-03.07.2019, **Invited Plenary lecture**: *Synergy Between Theory and Experiment: Overcoming Challenges in Ru-Catalyzed Olefin Metathesis.*
- 8. 102nd Canadian Chemistry Conference and Exhibition; 3-7.06.2019, Québec City, Canada. Invited lecture: *De Novo Design of Functional Transition-Metal Compounds*.
- 7. International Symposium on Olefin Metathesis and Related Chemistry, Zurich, Switzerland, 9-12.07.2017, Invited lecture: *Loss and Reformation of Ruthenium Alkylidene: Connecting Olefin Metathesis, Catalyst Deactivation, Regeneration, and Isomerization.*
- 6. XXII EuCheMS Conference on Organometallic Chemistry, 9-13.07.2017, Amsterdam, The Netherlands, **Invited keynote lecture**: *Computational Design of Organometallic Compounds.*
- 5. 3rd meeting on Challenges in Computational Homogeneous Catalysis, 3-4.09.2015, Stockholm, Sweden. Invited lecture: *Artificial Evolution of Homogeneous Catalysts*.
- 4. Indaba 8 Serendipity vs Prediction, 16-21.08.2015, Skukuza, South-Africa. Invited lecture: In *Silico Design of Homogeneous Catalysts*.
- 3. International Symposium on Olefin Metathesis and Related Chemistry, Nara, Japan, 14-19.07.2013, Nara, Japan. Invited lecture: *Z-selective ruthenium-based olefin metathesis catalysts*.
- 2. 95th Canadian Chemistry Conference and Exhibition; 26-30.05.2012, Calgary, Canada. Invited lecture: *Theory-assisted design of homogeneous catalysts: New strategies.*
- 1. Challenges in Computational Homogeneous Catalysis, 3-4.09.2011, Stockholm, Sweden. Invited lecture: *Darwinian Optimization of Homogeneous Catalysts*.

# **Organisation of international conferences**

- 2022 Organizer (with D. E. Fogg), 24th International Symposium on **Olefin Metathesis** (ISOM24), Bergen.
- 2019 Organizer, International workshop: Artificial Intelligence in Molecular Design, Bergen.
- 2019 Track-organizer, 10th Congress, Int. Soc. for Theoretical Chemical Physics (ISTCP), Tromsø, Norway.

# Major contributions to the early careers of excellent researchers

10 previous students or postdocs hold permanent positions (researcher positions / professorships) at universities or public research institutions, among them Nicolas Merle, Assist. Prof. at University of Lille and Yury Minenkov, Senior Research Scientist at Moscow Institute of Physics and Technology. Even though the group does not work within medicinal chemistry, its focus on molecular design and discovery has made its students and postdocs popular with pharmaceutical companies. Six previous students and postdocs have taken researcher positions in companies such as AstraZeneca, Novartis, and Janssen Pharmaceutica (part of Johnson & Johnson). In addition to undergraduate course development, Prof. Jensen has developed a PhDlevel course (KJEM324) on computational transition-metal chemistry, given ca. every second year.

# Example of leadership in industrial innovation or design

Prof. Jensen has used this strategy in breakthrough, theory-guided development and realization (synthesis, testing, IPR protection, and commercialization) of stereoselective olefin metathesis catalysts. One of these catalysts is on track to enter the catalogue of a major provider of chemicals. His computationally derived catalyst technology has received, together with the technology transfer office in Bergen, two innovation grants from the Research Council of Norway (listed under "Project management experience" in the CV). The first and largest of these grants was awarded in 2010: "Selective Ruthenium Olefin Metathesis Catalysts" (ca. 1100 k $\in$ ), with Prof. Jensen as **Principal Investigator**.