

Curriculum Vitae **Klavs F. Jensen**

Warren K Lewis Professor of Chemical Engineering
Professor Materials Science and Engineering
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Education:

1980 Ph.D. (Chemical Engineering), University of Wisconsin - Madison
1976 M.Sc. (Chemical Engineering), Technical University of Denmark

Employment:

2015- Warren K. Lewis Professor, Chemical Engineering, Massachusetts Institute of Technology
2007-2015 Warren K. Lewis Professor and Department Head, Chemical Engineering, Massachusetts Institute of Technology
1996 - 07 Lamot du Pont Professor of Chemical Engineering
1989 - 94 Joseph R. Mares Career Development Chair in Chemical Engineering
1989 - Professor of Materials Science and Engineering, Massachusetts Institute of Technology
1988-89 Professor, Department of Chemical Engineering and Materials Science, University of Minnesota
1986-89 Fellow, Minnesota Supercomputer Institute
1984-88 Associate Professor, Department of Chemical Engineering and Materials Science, University of Minnesota
1980-84 Assistant Professor, Department of Chemical Engineering and Materials Science, University of Minnesota
1976-80 Research and Teaching Assistant, Department of Chemical Engineering, University of Wisconsin - Madison

Honors:

2022 Elected to the National Academy of Inventors
2022 Honorary Doctorate (*Doctor Honoris Causa*) the Technical University of Eindhoven, The Netherlands
2019 P.V. Danckwerts Memorial Lecture - European Federation of Chemical Engineering
2018 John Prausnitz American Institute of Chemical Engineers Institute Lecturer
2018 Inaugural Corning International Prize for Outstanding Work in Continuous-Flow Reactors and Chemistry for a Greener and Safer World
2017 Member of National Academy of Sciences
2017 Fellow Industrial and Engineering Chemistry Division of American Chemical Society
2016 Founders Award, American Institute of Chemical Engineers

- 2012 Inaugural recipient of the International Union of Pure and Applied Chemistry (IUPAC)-ThalesNano Prize in Flow Chemistry
- 2011 William H. Walker Award, American Institute of Chemical Engineers
- 2011 Knight of the order of "Dannebrogordenen"
- 2009 Fellow American Institute of Chemical Engineers
- 2008 Named one of the "One Hundred Chemical Engineers of the Modern Era" as part of the American Institute of Chemical Engineers Centennial
- 2008 Member of American Academy of Arts and Sciences
- 2007 Fellow American Association for the Advancement of Science
- 2006 Honorary Doctorate (*Doctor Technices Honoris Causa*) Technical University of Denmark
- 2004 Fellow of the Royal Society of Chemistry, London
- 2002 Member of National Academy of Engineering
- 2000 R. H. Wilhem Award, American Institute of Chemical Engineers
- 1995 Charles M.A. Stine Award of the Materials Engineering and Sciences Division, American Institute of Chemical Engineers
- 1987 Allan P. Colburn Award, American Institute of Chemical Engineers
- 1987 John Simon Guggenheim Fellowship
- 1985-90 Camille and Henry Dreyfus Teacher - Scholar
- 1984-89 Presidential Young Investigator Award, National Science Foundation
- 1984 Young Chemical Engineer of the Year, AIChE Twin City Section
- 1983 Young Authors' Award, Electrochemical Society
- 1982 Shell Faculty Career Initiation Award
- 1981 Outstanding Junior Faculty Award, ARCO Oil and Gas Company

Lectureships

- 2019 Kelly Lecturers, School of Chemical Engineering, Purdue University
- 2019 Henry A. McGee Lecture, Virginia Commonwealth University, April 4, 2019
- 2015 Bruce A. Finlayson Lecture, University of Washington, Seattle
- 2014 Jacobus van 't Hoff Lecture, Technical University Delft, The Netherlands
- 2014 ExxonMobil Lecture, University of Massachusetts, Amherst
- 2013 Schlumberger Lecture, University of Alberta, Canada
- 2012 Richard H. Wilhelm Lectures, Princeton University
- 2012 Distinguished McFerrin Lecturer, Texas A&M University
- 2011 Robert Pigford Lecture, University of Delaware
- 2010 Ashton Cary Lectures, Georgia Institute of Technology
- 2010 Basore Distinguished Lecturer, Auburn University
- 2007 Inaugural Jeanne and Martin Sussman Lecture in Chemical and Biological Engineering, Tufts University
- 2007 Ashland Distinguish Lecturer, University of Kentucky
- 2007 Bergveld Lecture, Twente University, The Netherlands
- 2005 Adams Distinguished Lecture, Purdue University
- 2005 Distinguish Lindsay Lecturer, Texas A&M University
- 2003 Julian C. Smith Lectureship, Cornell, Ithaca, NY
- 2003 William N. Lacey Lectureship, California Institute of Technology, Pasadena

- 2002 Ralph Peck Memorial Lecture, Illinois Institute of Technology, Chicago
- 2002 Bird, Stewart and Lightfoot Lecture, University of Wisconsin
- 2002 Donald L. Katz Lecture, University of Michigan
- 2002 L.K. Doraiswamy Lecture, National Chemical Laboratory, India and Iowa State University
- 2000 Berkeley Lecturer, Department of Chemical Engineering, UC Berkeley

Recent Professional Activities:

- 2021- Member editorial board Proceedings of the National Academy of Science
- 2019 - Scientific Advisory Board Automated Chemical Synthesis Enabled by Digital Molecular Technologies, Cambridge University
- 2019 - Scientific Advisory Board Molecule Maker Lab Institute University of Illinois (UIUC)
- 2018- Co-director (with Prof. R. Barzilay) of the MIT consortium, Machine Learning for Pharmaceutical Discovery and Synthesis
- 2016 Visiting Professor, Institute for Chemical and Bioengineering (ICB), ETH Zurich, Switzerland
- 2015- Inaugural Editor-in-Chief Editorial for the Royal Society of Chemistry Journal Reaction Chemistry and Engineering
- 2015 Member External Review Committee, Departments of Chemical Engineering, TU Delft, TU Eindhoven, and Twente University
- 2015 Member External Review Committee, Department of Chemical Engineering, Northwestern University
- 2014 - Member of the Scientific Advisory Board for Multiscale Catalytic Energy Conversion (MCEC) The Netherlands
- 2014 -15 Chair Chemical Engineering Section of the National Academy of Engineering
- 2014 -18 Member of the scientific advisory board for Snapdragon Chemistry
- 2013 Member External Review Committee, Department of Chemical Engineering, University of California, Berkeley
- 2013 - Founder and member of the board SQZ Biotech
- 2011 Member of the Graduate Program Review Committee, North Carolina State University
- 2010 Member External Review Committee, Department of Chemical Engineering, Stanford University
- 2010 Member External Advisory Council, Department of Chemical and Biomolecular Engineering, Korean Advanced Institute of Science and Technology
- 2009 -16 Member Advisory Council for the Department of Chemical Engineering, Princeton University
- 2009 -16 Member of the Board of Governors of the Technical University of Denmark
- 2007 Chair of the international evaluation committee Chemical Engineering, Technical University of Denmark
- 2007 - 13 Visiting Committee, Chemical Engineering, University of Wisconsin
- 2013 Evaluation committee, Chemical Engineering, University of California, Berkeley
- 2006 - 09 Advisory panel– Danish Ministry of Science, Technology and Innovation

- 2005 - Founding member of Chemical and Biological Microsystems Society (sponsors the International conferences on Miniaturized Systems for Chemistry and Life Sciences, μ TAS)
- 2005 Conference Chair for the Ninth International conference on Miniaturized Systems for Chemistry and Life Sciences
- 2005 International Evaluation Committee for the Danish National Laboratory Risø
- 2004 Member of evaluation committee of research profile of Technical University Eindhoven
- 2004 - Scientific Advisory Board for the A*STAR Institute for Bioengineering and Nanotechnology, Singapore

Recent MIT Service:

- 2022- Joint MIT-Harvard Landmark Bio Advisory Committee
- 2020- Steering Committee Takeda MIT program in artificial intelligence and health
- 2017-18 Advisory Committee for The Engine
- 2007-15 Department Head Chemical Engineering
- 2007-15 School of Engineering Council
- 2011- 15 Chair, School of Engineering Committee on Diversity
- 2009 -10 Co-chair MIT Institute-Wide Planning Task Force: Revenue Enhancement Working Group
- 2008-10 Committees on education, engineering - life science interface, and materials science infrastructure
- 2005-07 Faculty Policy Committee

Memberships in Professional Societies:

- American Association for the Advancement of Science (Fellow)
- American Institute of Chemical Engineers (Fellow)
- American Chemical Society
- Materials Research Society
- Royal Society of Chemistry (Fellow)

Teaching and Research Interests:

Research interests include on-demand multistep synthesis, methods for automated synthesis, and machine learning techniques for chemical synthesis and interpreting large chemical data sets. Catalysis, chemical kinetics, and transport phenomena are also topics of interest, along with the development of methods for predicting the performance of reactive chemical systems.

Teaching interests include kinetics and chemical reaction engineering, transport phenomena, fundamentals of microfluidics

Current Students, Postdocs, Visitors, and Staff

PhD Students: Richard B. Canty,

Postdocs: Jakob Dahl, Seung Kyun Ha, Federico Florit, Brent Koscher, Joshua Lansford, Shinje Lee, Matthew McDonald, Karthik Sankar, Dylan Walsh, Andrew Zahrt

Visiting students: Nicola Hagger (ETH-Z), Leo Maeser (ETH-Z)

Staff: Alina Haverty, Brooke Jin, Mark Murnin

Past Students, Postdocs, Research Associates, Visitors, and Staff

PhD Students: Natalie S. Eyck, Anirudh M.K. Nambiar, Lagnajit Pattanaik, Jessica Xu, Yiming Mo, Dale A. Thomas, Connor Coley, Kosi Aroh, Marcella Lusardi, Lu Yang, Lisi Xie, Tatyana Shatova, Nopphon Weeranoppanant, Brandon Reizman, Wen-Hsuan (Jen) Lee, María José Nieves, Everett O'Neal, Patrick Heider, Armon Sharei, Jason Moore, Jinyoung Baek, EthelMae Victoria Dydek, Kevin Nagy, Jaroslav Keybl, Chris Marton, Jonathan McMullen, Mahmooda Sultana, Nikolay Zaborenko, Ling Chao, Hemantkumar Sahoo, Linlin Ye, Jane Rempel, Jacob Albrecht, Brandon Blackwell, Saif Khan, Jason Kralj, Ole M. Nielsen, Edward R. Murphy, Brian K. Yen, Zhiyu "Ben" Zhang, Thomas Gervais, Andrea Zanzotto, Nuria de Mas, Leonel Arana, Hang Lu, Sameer K. Ajmera, Gwang-Soo Kim, Jinwook Lee, Maria A. Nemirovskaya, Samara L. Firebaugh, Chris Vineis, Tamara M. Floyd, Jason R. Heine, Matthew W. Losey, Seth Thomas Rodgers, Rajesh Venkataramani, Theodoros Mihopoulos, Kathleen M. Vaeth, Brian G. Willis, Suman K. Banerjee, I-Ming Hsing, Harsano S. Simka, Ravi Srinivasan, Jeffrey P. Hebb, Brian H. Cumpston, Shih-Tung Ngiam, Michal Danek, Jeung-Soo Huh, Sateria Salim, Tushar P. Merchant, Daniel G. Coronell, Jaesung Han, Kwok-Lun Ho, (Univ. Minnesota) Erik Oddmund Einset, Jihperng Leu, Rajesh R. Melkote, Sadavisan Shankar, Donald R. McKenna, James B. Planeaux, Harry K. Moffat, Peter E. Price Jr., Mark F. Ellis, Dimitrios I. Fotiadis, Manoj Dalvie, Konstantinos P. Giapis, Thomas R. Omstead, David C. Skouby, Peter Wai-Man Lee, Victor Gonzalez, Karl F. Roenigk, Mark D. Foster, David B. Graves, Sebastian Reyes

M.Sc. Students: Ylva Olsson, Jacqueline T. Underberg, Samuel B. Schaevitz, Douglas S. Fong, Michael Z. Gu, Kim-Marie Levis, , Lawrence J. Foley, Brad Houston, (Univ. Minnesota) , Dimitious Vlachos, Simon Brandon, Anthony M. Kremer, Carl Allen Houtman, Thomas P. Kempf, Devesh Kapur, Harald C. Lyche, Charles W. Plumb,

Postdocs: Camille Bilodeau, Pritha Verma, Jiannan Liu, Max Lübbsmeyer, Kakasaheb Y. Nandiwale, Romaric Gérardy, Christian Haas, Hanyu Gao, Ioannis Lignos, Yanfei Guan, Yiming Mo, Mike Fortunato, Thomas Struble, Victor Schultz, Xiaoxue Wang, Agnieska Ladosz, Luke Rogers, Haomiao Zhang, Yi Shen, Joseph Imbrogno, Stefano Lazzari, Hongkun Lin, Kyoungmi Lee, Maryam Peer, Ye-Jin Wang, Andrew Teixeira, Xioyun Ding, Nopphon Weeranoppanant, Milad Albolhasani, Norman Horn, Saurabh Shahane, Gaurav Giri, Yanxiang Shi, Yanjie Zhang, Cuixian Yang, Fumihio Sassa, Baris Unal, Stephen Born, Steve Newman, Armon Sharei, Mohsen Behnam, Jean Christophe Monbaliu, Ulrich Neuenschwander, Seung Kon Lee, Sidy Ndao, Simon Kuhn, Patrick Bazinet, Anand Kumar, Xiaoying Liu, Damien Webb, Lei Gu, Victor Sebastian Cabeza, Woo Young Sim, Chris Smith, Soubir Basak ,Ketan Pimparkar, Ryan Hartman, Jian Wen, Bernard Yen, Samuel Marre, Kishori Deshpande, Jamil El-Ali, Axel Günther, Hyun Goo Choi, Nuria De Mas,

Yongbae Joen, Benjamin Wilhite, Nicolas Szita, Chelsey Baertsch, Carlo Cavalotti, Cyril Delattre, Rebecca Jackman, Constance Bauer, Ratna Shekhar, Istvan Lengyl, Javier Rodriguez-Viejo, Ajit Balakrishna, Charles Musgrave, XiaYong, Peter Futerko, Vernon Cole, Narasimha Acharya, Ming Xi, Karson Knutson, Chris Kleijn, Jiong-Ping Lu, Maurizio Masi, Kun-Ho Lie, Sanjay Patnaik, Ananth Annapragada, Lakis Mountziaris

Research Associates: Aleksander Franz, Guohua Liang, Andrea Adamo

Staff: Mengjie (Max) Liu, Travis Hart, Tim Kulesza, Joshua Byington, Joan Chisholm

Visitors:

Students: Timo Nicola Schneider (ETHZ), Federico Florit (Milano Polytechnico), Aaron Löwenstein (ETH), Leif-Thore Deck (ETH), Anna Pawlowska (Adam Mickiewicz University, Poland), Cyril Schroeder (ETH), Vignesh Somnath (ETH), Aniket Udepurkar (KU Leuven), Christina Kuhnle (KIT), Alexander Pomberger (Vienna), Tingliang Xie (Tsinghua), Clemens Isert (ETH), Oliver Schilter (ETH), Wenhao Gao (Johns Hopkins), Robbert van Putten (Delft) Lorenz Baumgartner (TU Munich), Thomas Kopfmüller (TU Munich), Esther Chen (ETH), Pius Theiler (ETH), Ramona Achermann (ETH), Kim Duembgen (ETH), Kristina Pedersen (DTU), Lukas Weimann (ETH), Quirin Grossman (ETH), Kevin Gao (Caltech), Baptiste Hardy (UCL, Belgium), Ronan O’Connell (U. Glasgow) Francisco J. Navarro-Brull (Alicante, Spain), Shusaku Asano (Kyoto), Thilo Kögl (TU Munich), Maud Fevre (Bordeaux), Gerrit Schatte (Munich), Alexander Woitalka (Munich), Filipa Castro (Minho, Portugal), Alessandro Arione (EPFL), Flurin Hänseler (ETH), Norbert Heublein (Munich), Francesco Venturini (Milan), Lars Johansen (DTU), Ruud Brand (Delft), Nora Langhorst (Hannover), Maurizio Rondanini (Milan), Gian Caviezel (ETH), Veronique Gondoin (ETH), Ruben Kolfschoten (ETH), Nicolas Imlinger (Austria), Gerardo Perozziello (DTU), Franz Trachsel (ETH), Martina Thalmann (ETH), Tobias Kraus (Munich), Jamil El-Ali (DTU), Uwe Hansen (Munich), Joost Driessen (Eindhoven), Ester Hurtos (Barcelona), Søren Eriksen (DTU), Tim Lund (Berlin)

Scientists: Fang Zhao (East China University of Science and Technology), Toku Fujioka (Kao, Japan), Kai Wang (Tsinghua), Mathiew Odijk (Twente), Thomas Gendrineau (Bordeaux), Amol Kulkarni (Indian Chemical Laboratory), Masay Hamano (Ono Pharmaceuticals), Kenichiro Hashimoto (Tokyo), Michiel Kreutzer (Delft), Elizabeth Podlaha-Murphy (Louisiana), Kunio Watanabe (Asahi Glass), Tomoya Inoue (Asahi Chemicals), Yasuhiro Wada (Misubishi), Shinji Isogai (Misubishi), Masanobu Ichida (Misubishi), Shige Kieda (Hitachi)

Bibliography

Google Scholar (h-index 134, citations ~ 67,300)

<https://scholar.google.com/citations?user=aiPql48AAAAJ&hl=en>

Refereed Journal Publications

- 490 C. P. Haas, M. Lübbesmeyer, E. Jin, M.A McDonald, B. Koscher, N. Guimond, L. Di Rocco, H. Kayser, S. Leweke, S. Niefenführ, R. Nicholls, E. Greeves, D. Barber, J. Hillenbrand, G. Volpin, and K.F. Jensen, Open-Source Chromatographic Data Analysis for Reaction Optimization and Screening, accepted *ACS Cent. Sci.* DOI: 10.1021/acscentsci.2c01042.
- 489 A.F. Zahrt, Y. Mo, K.Y. Nandiwale, R. Shprints, E. Heid, K.F. Jensen, Machine Learning Guided Discovery of Electrochemical Reactions, *J. Am. Chem. Soc.* **144**, 49, 22599–22610 (2022). Highlighted in <https://www.science.org/content/blog-post/searching-wilderness-new-chemistry>
488. M.E. Deagen, D.J. Walsh, D.J. Audus, K. Kroenlein, J.J. de Pablo, K. Aou, Kyle Chard, K.F. Jensen, and B.D. Olsen, Networks and interfaces as catalysts for polymer materials innovation, *Cell Reports Physical Science* **2022** DOI: 10.1016/j.xcrp.2022.101126
487. D.J. Walsh, T.N. Schneider, B.D. Olsen, and K.F. Jensen, Design and simulation of a uniform irradiance photochemical platform, *React. Chem. Eng.* **8**, 416–423 (2023) DOI: 10.1039/d2re00329e
486. J.L. Lansford, B.C. Barnes, B.M. Rice, and K.F. Jensen, Building Chemical Property Models for Energetic Materials from Small Datasets Using a Transfer Learning Approach, *J. Chem. Inf. Model.* **62**, 22, 5397–5410 (2022).
- 485 A.M.K. Nambiar, C.P. Breen, T. Hart, T. Kulesza, T. F. Jamison, and K.F. Jensen, Bayesian optimization of computer-proposed multistep synthetic routes on an automated robotic flow platform, *ACS Cent. Sci.*, **8**, 6, 825–836 (2022)
- 484 R. Gérardy, A.M.K. Nambiar, T. Hart, P.T. Mahesh, and K.F. Jensen, Photochemical synthesis of the bioactive fragment of salbutamol and derivatives in a self-optimizing flow chemistry platform, *Chem. Eur. J.* **15**, e202201385 (2022)
- 483 K.Y. Nandiwale, T. Hart, A.F. Zahrt, A.M. K. Nambiar, P.T. Mahesh, Y. Mo, M.J. Nieves-Remacha, M.D. Johnson, P. García-Losada, C. Mateos, J.A. Rincón and K.F. Jensen, Continuous stirred-tank reactor cascade platform for self-optimization of reactions involving solids, *React. Chem. Eng.* **7**, 1315-1327 (2022).
- 482 K. Sankaranarayanan, E. Heid, C.W. Coley, D. Verma, W.H. Green, and K.F. Jensen, Similarity based enzymatic retrosynthesis, *Chem. Sci.*, **13**, 6039–6053 (2022)
- 481 R. van Putten, N.S. Eyke, L.M. Baumgartner, V.L. Schultz, Georgy A. Filonenko, K.F. Jensen, and E. A. Pidko, Automation and microfluidics for the efficient, fast, and focused reaction development of asymmetric hydrogenation catalysis, *ChemSusChem* **2022**, e202200333
- 480 C. Bilodeau, W. Jin, T. Jaakkola, R. Barzilay, and K.F. Jensen, Generative models for molecular discovery: Recent advances and challenges, *WIREs Comput Mol Sci.*;e1608 (2022).
- 479 M.G. Booty, K.A. Hlavaty, A. Stockmann, E.I. Ozay, Carolyne Smith, L. Tian, E. How, D. Subramanya, A. Venkitaraman, C. Yee, O. Pryor, K. Volk, K. Blagovic, I. Vicente-Suarez, D. Yarar, M. Myint, A. Merino, J. Chow, T. Abdeljawad, H. An, S. Liu, S. Mao, M.

- Heimann, L. Talarico, M.K. Jacques, E. Chong, L. Pomerance, J.T. Gonzalez, U.H. von Andrian, K.F. Jensen, R.Langer, H. Knoetgen, C. Trumpfheller, P. Umaña, H. Bernstein, A. Sharei and S.M. Loughhead, Microfluidic squeezing enables MHC class I antigen presentation by diverse immune cells to elicit CD8⁺ T cell responses with antitumor activity, *J. Immunol*, ji2100656 (2022), DOI: 10.4049/jimmunol.2100656
- 478 C. Bilodeau, W. Jin, H. Xu, J.A. Emerson, S. Mukhopadhyay, T. H. Kalantar, T. Jaakkola, R. Barzilay, and K. F. Jensen, Generating molecules with optimized aqueous solubility using iterative graph translation, *React. Chem. Eng* **7**, 297 (2022)
- 477 S.M. Kearnes, M.R. Maser, M. Wleklinski, A. Kast, A.G. Doyle, S.D. Dreher, J.M. Hawkins, K.F. Jensen, and C.W. Coley, The Open Reaction Database, *J. Am. Chem. Soc.* **143**, 18820–18826 (2021)
- 476 R. Duvadie, A. Pomberger, Y. Mo, E.I. Altinoglu, H.-W. Hsieh, K.Y. Nandiwale, V.L. Schultz, K.F. Jensen, and R.I. Robinson, Photoredox iridium–nickel dual catalyzed cross-electrophile coupling: from a batch to a continuous stirred-tank reactor via an automated segmented flow reactor, *Org. Process Res. Dev.* **25**, 2323–2330 (2021)
- 475 H. Zhang, A. Ładosz, K.F. Jensen, Design and operation of an enhanced pervaporation device with static mixers, *AIChE J.*, 2021, e17455. DOI: 10.1002/aic.17455
- 474 F. Florit, A.M.K. Nambiar, C.P. Breen, T.F. Jamison and K. F. Jensen, Design of dynamic trajectories for efficient and data-rich exploration of flow reaction design spaces, *React. Chem. Eng.*, **6** 2306-231 (2021).
- 473 C. Armstrong, Y. Miyai, A. Formosa, D. Thomas, E. Chen, T. Hart, V. Schultz, B.K. Desai, A.Y. Cai, A. Almasy, K.F. Jensen, L. Rogers, and T Roper, On-Demand Continuous Manufacturing of Ciprofloxacin in Portable Plug-and-Play Factories: Development of a Highly Efficient Synthesis for Ciprofloxacin, *Org. Process Res. Dev.* **25**, 7, 1524–1533 (2021)
- 472 J. Guo, A.S. Ibanez-Lopez, H. Gao, V. Quach, C.W. Coley, K.F. Jensen, and R. Barzilay, Automated Chemical Reaction Extraction from Scientific Literature, *J. Chem. Inf. Model.* **61**, 4124 (2021) 10.1021/acs.jcim.1c00284
- 471 C. P. Breen, A.M.K. Nambiar, T. F. Jamison, and K.F. Jensen, Ready, Set, Flow! Automated Continuous Synthesis and Optimization, *Trends in Chemistry*, **3** 373-386 (2021)
- 470 I. Lignos, Y. Mo, L. Carayannopoulos, M. Ginterseder, M.G. Bawendi, and K.F. Jensen, A high-temperature continuous stirred-tank reactor cascade for the multistep synthesis of InP/ZnS quantum dots, *React. Chem. Eng.*, **6**, (2021). DOI: 10.1039/d0re00454e
- 469 F. Florit, R. Rota, K.F. Jensen, Dispersion in coiled tubular reactors: A CFD and experimental analysis on the effect of pitch, *Chem. Eng. Sci.*, **233** 116393 (2021)
- 468 Y. Guan, C.W. Coley, H. Wu, D. Ranasinghe, E. Heid, T.J. Struble, L. Pattanaik, W.H. Green, and K.F. Jensen Regio-selectivity prediction with a machine learned reaction representation and on-the-fly quantum mechanical descriptors, *Chem. Sci.*, **12**, 2198-208 (2021).
- 467 N.S. Eyke, B.A. Koscher, and K.F. Jensen, Toward machine learning-enhanced high-throughput experimentation, *Trends in Chemistry*, **3** 120-132 (2021)

- 466 H. Gao, J. Pauphilet, T.J. Struble, C.W. Coley, and K.F. Jensen, Direct optimization across computer-generated reaction networks balances materials use and feasibility of synthesis plans for molecule libraries, *J. Chem. Inf. Model.* **61**, 493-504 (2021).
- 465 Y. Mo, Y. Guan, P. Verma, J. Guo, M. E. Fortunato, Z. Lu, C. W. Coley and K. F. Jensen, Evaluating and clustering retrosynthesis pathways with learned strategy, *Chem. Sci.*, **12** 1461-1478 (2021).
- 464 A. Ładosz, C. Kuhnle, and K.F. Jensen, Characterization of reaction enthalpy and kinetics in a microscale flow platform, *React. Chem. Eng.*, **5**, 2115-2122 (2020).
- 463 X. Wang, Y. Qian, H. Gao, C.W. Coley, Y. Mo, R. Barzilay, and K.F. Jensen, Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning, *Chem. Sci.* **11**, 10959-10972 (2020).
- 462 X. Duan, J. Tu, A.R. Teixeira, L. Sang, K.F. Jensen and J. Zhang, An automated flow platform for accurate determination of gas–liquid–solid reaction kinetics, *React. Chem. Eng.*, **5**, 1751-1758 (2020).
- 461 Y. Mo, G. Rughoobur, A.M K. Nambiar, K. Zhang, and K.F. Jensen, A multifunctional microfluidic platform for high-throughput experimentation of electroorganic chemistry, *Angew. Chemie Int. Ed.*, **59** (47) 20890-20894 (2020).
- 460 N.S. Eyke, W.H. Green, K.F. Jensen, Iterative experimental design based on active machine learning reduces the experimental burden associated with reaction screening, *React. Chem. Eng.* **5**, 1963–1972 (2020).
- 459 L. Rogers, N. Briggs, R. Achermann, A. Adamo, M. Azad, D. Brancazio, G. Capellades, G. Hammersmith, T. Hart, J. Imbrogno, L.P. Kelly, G. Liang, C. Neurohr, K. Rapp, M.G. Russell, C. Salz, D.A. Thomas, L. Weimann, T.F. Jamison, A.S. Myerson, and K.F. Jensen, Continuous production of five active pharmaceutical ingredients in flexible plug-and-play modules: A demonstration campaign, *Org. Process Res. Dev.* **24**, 10, 2183–2196 (2020).
- 458 T. Hart, V.L. Schultz, D.A. Thomas, T. Kulesza, and K.F. Jensen, Development of a versatile modular flow chemistry benchtop system, *Org. Process Res. Dev.* **24**, 10, 2105–2112 (2020).
- 457 M.E. Fortunato, C.W. Coley, B.C. Barnes, and K. F. Jensen, Data augmentation and pretraining for template-based retrosynthetic prediction in computer-aided synthesis planning, *J. Chem. Inf. Model.* **60**, 7, 3398–3407 (2020).
- 456 Y. Mo, Z. Lu, G. Rughoobur, P. Patil, N. Gershenfeld, A. I. Akinwande, S.L. Buchwald, and K.F. Jensen Microfluidic electrochemistry for single-electron transfer redox-neutral reactions, *Science* **368**, 1352–1357 (2020).
- 455 A.B. Wood, K.Y. Nandiwale, Y. Mo, B. Jin, A. Pomberger, V.L. Schultz, F. Gallou, and K.F. Jensen, and B.H. Lipshutz, Continuous flow Suzuki–Miyaura couplings in water under micellar conditions in a CSTR cascade catalyzed by Fe/ppm Pd nanoparticles, *Green Chemistry*, **22**, 3441-3444 (2020)

- 454 I. Lignos, H. Utzat, M.G. Bawendi, and K.F. Jensen, Nanocrystal synthesis, μ fluidic sample dilution and direct extraction of single emission linewidths in continuous flow, *Lab Chip* **20**, 1975-1980 (2020).
- 453 T.J. Struble, J.C. Alvarez, S.P. Brown, M. Chytil, J. Cisar, R.L. DesJarlais, O. Engkvist, S.A. Frank, D.R. Greve, D.J. Griffin, X. Hou, J.W. Johannes, C. Kreatsoulas, B. Lahue, M. Mathea, G. Mogk, C.A. Nicolaou, A.D. Palmer, D.J. Price, R.I. Robinson, S. Salentin, L. Xing, T. Jaakkola, W.H. Green, R. Barzilay, C.W. Coley, and K.F. Jensen. Current and future roles of artificial intelligence in medicinal chemistry synthesis. *J. Med. Chem.*, *J. Med. Chem.* **63**, 8667–8682 (2020).
- 452 T.J. Struble, C.W. Coley, and K.F. Jensen, Multitask prediction of site selectivity in aromatic C–H functionalization reactions, *React. Chem. Eng.*, **5**, 896-902 (2020).
- 451 K.F. Jensen, Radial flow system decouples reactions in automated synthesis of organic molecules. *Nature* **579** (7799):346-348 (2020).
- 450 I. Lignos, H. Ow, J.P. Lopez, D. McCollum, H. Zhang, J. Imbrogno, Y. Shen, C. Sehoon, W. Wang, and K.F. Jensen, Continuous Multistage Synthesis and Functionalization of sub-100 nm Silica Nanoparticles in a 3D-printed CSTR Platform, *ACS Applied Materials & Interfaces*, **12**, 5, 6699-6706 (2020).
- 449 H. Gao, C.W. Coley, T.J. Struble, L. Li, Y. Qian, W.H. Green, K.F. Jensen, Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list, *React. Chem. Eng.*, **5**, 367-376 (2020).
- 448 M. Lusardi, T. Struble, A. R. Teixeira, and K.F. Jensen: Identifying the roles of acid-base sites in formation pathways of tolualdehydes from acetaldehyde over MgO-based catalysts, *Catal. Sci. Technol.*, **10**, 536-548 (2020).
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