NATIONAL ACADEMIES Sciences Engineering Medicine

CHEMICAL SCIENCES ROUNDTABLE | BOARD ON CHEMICAL SCIENCES AND TECHNOLOGY

AI + Limited Data

Hosted by the Chemical Sciences Roundtable

AI + Y 2024 Series

THURSDAY, NOVEMBER 21, 2024

About

This episode of AI + Limited Data will explore how to effectively use and analyze limited datasets to arrive at useful solutions. Before embarking on these conversations, speakers will discuss how they define “limited” or “small” data including the number of data points and variables considered. Discussions around data quality; trust and interpretability; and their integration into existing big-data workflow will be presented and speakers will share their strategies for picking chemistry problems that could be solved using the “limited data” approach. Members of the public are welcome to register and attend!

12:30PM–12:35PM **Introduction to the National Academies, The Chemical Sciences Roundtable, Webinar Planning Committee, and NAS Staff**

Michael Janicke, CSR Director, National Academies

12:35PM–12:40PM **Welcome from Moderator, Introduction to Panelists and Webinar Topic**

Carlos Gonzalez, Chief, Chemical Sciences Division – National Institute of Standards and Technology

12:40PM–01:20PM **Background and Perspectives from Academic and Chemical Industries**

Johannes Hachmann, Associate Professor, University of Buffalo - SUNY
Stephan Mohr, Scientific Director, Nextmol

01:20PM–01:40PM **Moderated Panel Discussion**

Carlos Gonzalez, Chief, Chemical Sciences Division – National Institute of Standards and Technology

Johannes Hachmann, Associate Professor, University of Buffalo - SUNY
Stephan Mohr, Scientific Director, Nextmol

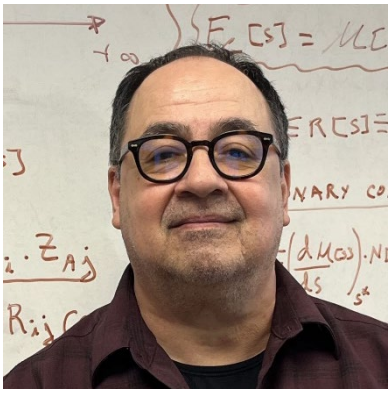
01:40PM–01:55PM **Q&A with the Audience**

Johannes Hachmann, Associate Professor, University of Buffalo - SUNY
Stephan Mohr, Scientific Director, Nextmol

01:55PM–02:00PM **Final Remarks**

Johannes Hachmann, Associate Professor, University of Buffalo - SUNY
Stephan Mohr, Scientific Director, Nextmol

BIOGRAPHIES ON SPEAKERS AND PLANNERS



Moderator and Planner- Carlos Gonzalez, Chief, Chemical Sciences Division – National Institute of Standards and Technology

Carlos Gonzalez has been the Chief of the Chemical Sciences Division of the National Institute of Standards and Technology (NIST) since 2012. Dr. Gonzalez joined NIST in 1997 as a member of the Computational Chemistry Group within the Physical and Chemical Properties Division. He was appointed to the position of Chief, Chemical and Biochemical Reference Data Division in 2008. Previously, Dr. Gonzalez was a Postdoctoral Scholar at Carnegie Melon University under the mentorship of Prof. John A. Pople, a 1998 Nobel Laureate in Chemistry. Dr. Gonzalez received his Ph.D. in Chemistry from Wayne State University.

Panelist - Johannes Hachmann, Associate Professor, Department of Chemical and Biological Engineering; Director, Engineering Science (Data Science Focus) Graduate Program, Institute for Artificial Intelligence and Data Science; University at Buffalo, The State University of New York

Johannes Hachmann is an Associate Professor of Chemical Engineering at the University at Buffalo (UB), the Director of the Engineering Science (Data Science Focus) graduate program, a Leadership Member of the UB Institute for Artificial Intelligence and Data Science, and a Faculty Member of the New York State Center of Excellence in Materials Informatics. He earned a Dipl.-Chem. degree (2004) after undergraduate studies at the universities of Jena and Cambridge, M.Sc. (2007) and Ph.D. (2010) degrees in Chemistry from Cornell University, and he conducted postdoctoral research at Harvard University before joining the UB faculty in 2014. The research of the Hachmann Group fuses (first-principles) molecular and materials modeling with virtual high-throughput screening and modern data science (i.e., the use of machine learning, artificial intelligence, and informatics) to advance a data-driven discovery and rational/inverse design paradigm in the chemical and materials disciplines. One of the centerpieces of the group's efforts is the creation of an open, general-purpose software ecosystem for the data-driven design of chemical systems and the exploration of chemical space. This work was recognized with a 2018 NSF CAREER Award

Panelist - Stephan Mohr, Scientific Director, Nextmol

Stephan Mohr is co-founder and Chief Scientific Officer at Nextmol. Previously, he worked as as researcher at Barcelona Supercomputing Center (Spain), CEA Grenoble (France) and University of Basel (Switzerland). He holds a PhD in Physics,and is an expert in molecular simulations and chemicals informatics, both with respect to algorithmic developments and applications. Moreover, he has also a large experience in code development and High-Performance Computing. During his career he has authored 27 peer-reviewed papers and has been the principal investigator of several supercomputing projects on Tier-0 supercomputers. He has supervised numerous students and led R&D teams in multidisciplinary and fast-paced environments.

Planner - Jonathan Wylde, Technical Director, Assured Flow Solution

Jonathan Wylde serves as the Technical Director for Assured Flow Solution, a specialist chemical flow assurance laboratory servicing the oil and gas industry. Based in Houston, Dr. Wylde is responsible for overseeing the entire laboratory operation including direct customer interaction, project coordination and supervision of the laboratory staff. Prior to this Dr. Wylde worked for Clariant Oil and Mining Services for 20 years where he spent 10 of those years as Global Innovation Head where he oversaw the innovation and development advancement across multiple Clariant Oil and Mining Services channels, including technical, operational, sales and business development. As an Honorary Associate Professor at Heriot Watt University in Edinburgh, Scotland, Dr. Wylde has authored over 200 papers and patents and has served on the Society of Petroleum Engineers (SPE) committees for the International Scale Conference and Oilfield Chemical Conference and is actively serving as an Associate Editor for SPE Production and Operations and as a Technical Editor for the SPE Journal of Petroleum Technology, SPE Production and Operations and the SPE Journal.