

Chemistry 2050: A Roadmap to the Future - A Workshop

Committee

T. Daniel Crawford

Chair

Professor T. Daniel Crawford is the University Distinguished Professor and Ethyl Chair of Chemistry at Virginia Polytechnic Institute and State University (Virginia Tech), as well as the Director of the Molecular Sciences Software Institute in Blacksburg, Virginia. He held joint postdoctoral positions at University of Georgia and University of Texas before joining the Virginia Tech faculty in 2000. Professor Crawford's research focuses on the development of accurate quantum mechanical models for simulating the optical and vibrational spectra of chiral molecules. He has given more than 250 lectures in 27 countries. Professor Crawford is the winner of 2010 Dirac Medal of the World Association of Theoretical and Computational Chemists (WATOC), winner of the 2023 Cottrell STAR Award from the Research Corporation for Science Advancement, and a Fellow of the American Chemical Society, as well as an elected member of the International Academy of Quantum Molecular Science and WATOC. He is a Fellow of the American Chemical Society and, from 2021-2026, the Deputy Editor of the Journal of Physical Chemistry A. He received his bachelor's degree in chemistry and mathematics in 1992 from Duke University and his Ph.D. in 1996 from the University of Georgia's Center for Computational Quantum Chemistry under the direction of Professor Henry F. Schaefer.

Thao T. Tran Dominy

Member

Dr. Thao T. Tran Dominy is the Dean's Associate Professor in the Departments of Chemistry, Physics and Astronomy at Clemson University, South Carolina. She is deeply committed to shaping the chemical sciences to elevate people's lives. Her research team at the Materials Chemistry Whisperers Laboratory studies quantum and functional materials, with a particular focus on leveraging electronic structure and physical principles to address key challenges in quantum information science and energy technology. Her research program has been supported and recognized by the Beckman Foundation, the National Science Foundation, the Research Corporation for Science Advancement, the Dreyfus Foundation, the Kavli Foundation, and the US National Academy of Sciences. She serves as an executive member of the APS Quantum Materials Synthesis Topical Group, the Structural Science Panel at Argonne National Laboratory, and the Neutron User Group at Oak Ridge National Laboratory, and as an associate editor of Nature-Communications Materials. With these functions, she brings strong connections, thoughtful insight, and a forward-looking perspective to contribute and shape the future direction of chemical sciences. Dr. Tran Dominy earned her Ph.D. from University of Houston and completed postdoctoral research at Johns Hopkins University. As noted above, she is also a US National Academy of Sciences Kavli Fellow.

Carlos Alberto Gonzalez

Member

Dr. Carlos Gonzalez is the Senior Strategic Advisor on Material Data, Machine Learning, and AI in the Material Measurement Laboratory, at the National Institute of Standards and Technology (NIST). He previously served as the Chief of the Chemical Sciences Division for over 15 years until February 2026. Prior to that tenure, he held the position of Chief of the Chemical and Biochemical Reference Data Division and was the founding Director of NIST's Center for Theoretical and Computational Nanosciences. His primary research expertise focuses on the development and implementation of modern ab initio quantum chemical methodologies, particularly their application to conceptual DFT, chemical Information Theory, chemical reactivity, nanotechnology, materials at the nano-scale, and data-driven AI for chemistry. A co-author of the Gaussian suite of programs, Dr. Gonzalez has published over 100 peer-reviewed papers in quantum chemistry. His professional honors include the 2024 Allen V. Astin Award, the 2013 HENAAC Professional Achievement Level II Award and the 2005 Department of Commerce Bronze Medal. He is an active member of the American Chemical Society and the American Physical Society. Dr. Gonzalez earned his Ph.D. in Theoretical Chemistry from Wayne State University in 1990. He subsequently completed a postdoctoral fellowship at Carnegie Mellon University under the supervision of Nobel Laureate Prof. John A. Pople.

Kaytlin Henderson

Member

Kaytlin Henderson is the Analytics and AI Leader in Enterprise Data and Analytics at Dow. In her 14 years at Dow, she has held leadership positions in data and analytics, Dow's digital manufacturing transformation, and roles in reaction engineering R&D and manufacturing operations. Her expertise bridges applied chemical engineering and AI, with deep experience in reactor optimization, predictive analytics for manufacturing reliability, digital tools deployment, and enterprise data strategy. She has led large-scale AI deployment programs across Dow's manufacturing footprint, including predictive maintenance, third-party data integration, and enterprise-wide AI adoption. She now shapes and implements Dow's enterprise AI strategy across areas including sustainability, energy, and materials, with strategic priorities in Responsible AI frameworks, generative AI, and emerging agentic AI capabilities. Dr. Henderson is an active member of the American Institute of Chemical Engineers (AIChE), recently serving as Chair of the Career and Education Operating Council and the Membership Committee. She chairs Dow's Insight Scientist Community, focused on data application in materials development and the process industries. She received a Frost and Sullivan Manufacturing Leadership Award (2014) for engineering and manufacturing innovation. Dr. Henderson holds a BS in Chemical Engineering from Lafayette College and a PhD in Chemical Engineering from Carnegie Mellon University.

Yiguang Ju

Member

Yiguang Ju is the Robert Porter Patterson Professor in Mechanical and Aerospace Engineering, Associated Faculty of Princeton Plasma Physics Laboratory, and is the Director of DOE Energy Earthshot Research Center (EERC) for plasma assisted hydrogen production. Dr. Ju's research interests include combustion, green fuels, plasma, and electrified manufacturing. Dr. Ju is a Fellow of the American Institute of Aeronautics and Astronautics (AIAA), the American Society of Mechanical Engineers (ASME), and The Combustion Institute. He has received many awards such as the Friedrich Wilhelm Bessel Research Award from the Alexander von Humboldt Foundation, the AIAA propellant and combustion award, the Alfred C. Egerton Gold Medal from the Combustion Institute, and the 2025 R&D 100 Award. He is Co-founder of HiTNano Inc, Princeton NuEnergy Inc, Polymer-X Inc, and USPlasma Inc. to develop innovative technologies for electrified and plasma aided manufacturing for energy decarbonization. Dr. Ju received his BSE in 1986 and an MSE in 1988 in mechanical engineering from Tsinghua University and his PhD in 1994 in mechanical engineering from Tohoku University, respectively.

Laurel Royer

Member

Laurel Royer, PhD, is the Founder and Chief Scientific Officer of Carinalis Consulting and Research. Dr. Royer has more than 15 years of combined research, scientific, technical advising expertise. She has developed and built an inter- and trans-disciplinary consultancy focused on evaluating the balance between innovation and detrimental impact. She applies the fundamentals of the chemical and related sciences to evaluate manufacturing/production and application, disposal, contamination, and exposure issues via the use cycle to support stakeholders in achieving an overall positive impact. To that cause, she supports clients and partners across a myriad of sectors addressing both proactive and reactive responses at the intersection of the built and natural environments. Dr. Royer is keenly aware that the consequences of chemical contamination and exposure unequally impact communities across the globe. To that end, she works with these communities in technical advisory roles and is an ardent advocate of addressing the disproportionate burdens and consequences of our anthropogenic footprint. She holds a PhD in Environmental Organic Chemistry and a MS in Medicinal Chemistry and Molecular Pharmacology from Purdue University, a BS in Chemistry from the University of the Virgin Islands.

Hye Kyung C. Timken

Member

Dr. Hye Kyung Timken retired from Chevron Corporation in October 2025 after 25 years, where she was a Principal Scientist and Chevron Fellow; before that she worked for Mobil Corporation for 13 years. Her roles spanned technical team leadership and R&D project management. Dr. Timken's expertise spans novel refining and petrochemical process development and catalyst innovation for petrochemicals, base oil, and fuels. Her work employed solid catalysts including zeolites and other adsorbents, as well as ionic liquids, for hydrocarbon conversion processes. Her current interests include technologies supporting the energy transition toward a lower carbon future, particularly manufacturing technologies for new fuels and plastics recycling, and processes for efficient carbon capture. She received the University of Illinois LAS Alumni Award in 2020, National Academy of Sciences Award for Chemistry in Service to Society in 2023 for development of a safer fuel manufacturing process, and was inducted into the National Academy of Engineering in 2024. She holds 163 US patents and has published 20 scientific journal articles. Dr. Timken received a Ph.D. degree in Physical Chemistry from the University of Illinois, Urbana-Champaign, and MS and BS degrees in Chemistry from Yonsei University, Seoul, Korea.

Elizabeth Zeitler

Staff Officer