Digital Discovery

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Contributors to the *Digital Discovery* Emerging Investigators collection 2025

Milad Abolhasani is the ALCOA Professor, a University Faculty Scholar, and the Director of the Graduate Program in the Department of Chemical and Biomolecular Engineering at North Carolina State University. He also serves as the Director of Accelerated Technologies within NC State's Integrative Sciences Initiative. He received his PhD from the University of Toronto in 2014. Prior to joining NC State University, he was an NSERC Postdoctoral Fellow in the Department of Chemical Engineering at MIT (2014–2016). At NC State University, Dr Abolhasani leads a multidisciplinary research group that studies self-driving labs tailored toward accelerated discovery, development, and manufacturing of advanced functional materials and molecules using fluidic micro-processors.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00062A.

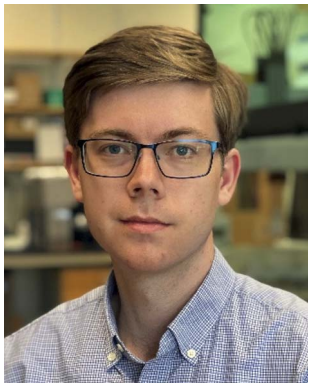
Fang Liu is an Assistant Professor in the Department of Chemistry at Emory University. She received her BS from the Department of Chemical Physics at the University of Science and Technology of China in 2011 and her PhD in Chemistry from Stanford University under the supervision of Professor Todd J. Martínez in 2017. She completed her postdoc at the Massachusetts Institute of Technology with Professor Heather J. Kulik, prior to joining Emory as a faculty member in 2020.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00012B.

Hessam Mehr obtained his BSc in electrical engineering from Sharif University of Technology in Iran, followed by a PhD in supramolecular chemistry with Prof Mark MacLachlan at the University of British Columbia. He is a Leverhulme Early Career Research Fellow at the University of Glasgow, leading a programme focused on next-generation discovery paradigms in experimental chemistry. At the interface of chemistry, automation and computational modelling, his group's goal is to derive frameworks to elicit new and unprecedented behaviours in chemical systems. His work has been supported by the Royal Society of Chemistry, Royal Society of Edinburgh and the Leverhulme Trust.

His contribution to the 2025 *Digital Discovery* Emerging Investigators

collection can be read at https://doi.org/10.1039/D5DD00100E.



Connor W. Coley is the Class of 1957 Career Development Professor and an Associate Professor at MIT in the Department of Chemical Engineering and the Department of Electrical Engineering and Computer Science. He received his BS and PhD in Chemical Engineering from Caltech and MIT, respectively, and did his postdoctoral training at the Broad Institute. His research group at MIT works at the interface of chemistry and data science to develop models that understand how molecules behave, interact, and react and use that knowledge to engineer new ones, with an emphasis on therapeutic discovery.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00233H.

Francesca Grisoni is an Associate Professor at Eindhoven University of Technology, where she leads the Molecular Machine Learning Team. She earned her PhD in the group of Prof. Roberto Todeschini at the University of Milano-Bicocca and conducted postdoctoral research with Prof. Gisbert Schneider at ETH Zurich after working for a year in industry. Her research blends chemistry, biology, and computer science to develop innovative AI approaches for molecule discovery. Prof. Grisoni's research has been recognized by several accolades, including the Early Career Award from the Dutch Royal Academy of Arts and Sciences, an NWO Vidi, and an ERC Starting Grant.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00028A.

Esther Heid received her PhD in Theoretical Chemistry from the University of Vienna in 2019. She subsequently held postdoctoral positions at MIT (2020–2022) and TU Wien (2022–2024), where she advanced her work at the interface of chemistry and machine learning. In 2024, she was awarded a prestigious ERC Starting Grant, which supported her promotion to tenure-track Assistant Professor at TU Wien. Her research group focuses on deep learning approaches for chemical reactions, with an emphasis on predicting reaction properties and pathways across gas-phase, organocatalytic, and biocatalytic systems.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00240K.

Thijs Stuyver is a Junior Professor at Ecole Nationale Supérieure de Chimie de Paris, a constituent college of PSL University. He received his PhD from the Vrije Universiteit Brussel in 2018, under the supervision of Prof. P. Geerlings and Prof. F. De Proft. He subsequently did postdoctoral research at the Hebrew University of Jerusalem (2018–2021), working with Prof. S. Shaik, and at the Massachusetts Institute of Technology (2021–2023), working with Prof. Connor Coley. His research interests lie at the interface between computational chemistry and artificial intelligence. He is one of the coordinators of the ChemAI initiative, which aims to bring PSL University to the forefront of the on-going data science revolution in chemistry.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00256G.

Dr Nicola Bell is an EPSRC Open Fellow in Digital Inorganic Chemistry at the University of Glasgow, where she leads the Bell Group. Nicola obtained her PhD from the University of Edinburgh in 2013 and has a background in organometallic

and catalytic chemistry. Founded in 2022, the Bell Group addresses the unique challenges of air-sensitive, highly reactive, and hazardous chemistries through the use of digital and remote-handling strategies. By combining automation with the practical demands of sensitive synthetic chemistry, the group aims to redefine how such systems are discovered, studied, and controlled—opening new frontiers beyond our reactive atmosphere.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00305A.

Fernanda Duarte, born in Santiago, Chile, earned her PhD in 2012 from the Pontificia Universidad Católica de Chile. She was a postdoctoral researcher at Uppsala, Newton Fellow at Oxford, and Chancellor's Fellow and lecturer at Edinburgh. Returning to Oxford in 2018 as an associate professor, she leads a team developing computational tools to explore (bio)chemical reactivity, optimise synthesis, and guide molecular design, connecting computational developments with practical applications. Her awards include L'Oreal–UNESCO Women in Science (2009), MGMS Frank Blaney (2020), OpenEye Outstanding Junior Faculty (2021), Harrison–Meldola (2021), Novartis Early Career (2022), and finalist for the 2024 UK Blavatnik Awards.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00261C.

Tim Cernak obtained a BSc in Chemistry from University of British Columbia Okanagan and there studied the aroma profile of Chardonnay wines. Following PhD training in total synthesis with Prof. Jim Gleason at McGill University, Tim was a FQRNT Postdoctoral Fellow with Tristan Lambert at Columbia University. From 2009–2018, Tim worked with the Medicinal Chemistry team at Merck Sharp & Dohme in Rahway and Boston. In 2018, Dr Cernak joined the Department of Medicinal Chemistry at the University of Michigan in Ann Arbor as an Assistant Professor. The Cernak Lab is exploring an interface of chemical synthesis and AI for drug discovery. Tim is developing research in conservation chemistry, where chemists engage in preventing species extinction.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00310E.

Dr Mingjie Liu received her PhD in Materials Science and Nanoengineering from Rice University. After doing a postdoc at Brookhaven National Laboratory and Massachusetts Institute of Technology, she joined the University of Florida in 2022 as an Assistant Professor in Chemistry. Dr Liu's research interests center on leveraging materials informatics, data-driven methodologies and generative AI to advance high-impact research in the realms of materials design and chemical discovery.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00241A.

Laia Vilà-Nadal started her independent research group at the University of Glasgow in June 2019, where she is a Lecturer. She completed her PhD in February 2011 at the Universitat Rovira i Virgili (URV) in Tarragona, followed by postdoctoral research at Glasgow. A materials scientist by training, Laia describes herself as a biochemist who somehow found her way into chemistry and computational modelling. Her group blends computational and experimental approaches, using theory, modelling, and digital tools to design molecular metal oxides—focusing on redox properties, countercation effects, and sustainable nitrogen fixation. Her current efforts explore data-driven catalyst discovery and hybrid biochemical–inorganic systems. This is her first step into digital chemistry—and the first of many.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00453E.

Jakob S. Kottmann is a professor of quantum algorithmics at the Computer Science Institute at the University of Augsburg (Germany). His research lies in the intersection of quantum algorithmics (physically automatically differentiable circuits, grid-based representations, sparse data structures), quantum chemistry (system-adapted quantum circuits, multiwavelet-based orbital representation, efficient qubit encodings) and scientific software development (Tequila, FrayedEnds, Sunrise, PauliEngine). In 2025, he was awarded a Quantum Future Young Investigator grant from the Federal Ministry of Research, Technology and Space.

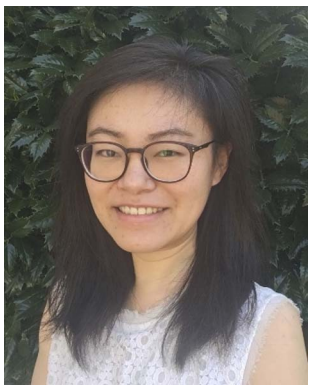
His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00251F.

Zhongyue John Yang is an Assistant Professor of Chemistry at Vanderbilt University. He graduated from the inaugural Chemistry Po-Ling class at Nankai University in 2013, earned his PhD in Theoretical and Computational Chemistry with Ken Houk at UCLA in 2017, and undertook postdoctoral training with Heather Kulik in the Department of Chemical Engineering at MIT from 2018 to 2020. Since fall 2020, he has started his independent research group at Vanderbilt. His research emphasizes establishing "Mutexa", a physics-informed, AI-assisted framework for "intelligent" protein engineering that generates testable hypotheses and mechanistic insight simultaneously.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00307E.

Luke Baldwin is a Senior Research Chemist at the Air Force Research Laboratory (AFRL), leading research at the interface of polymer chemistry and laboratory automation. He earned his PhD in Chemistry from The Ohio State University after completing his BSc at Carroll University. Since 2018, his independent research has focused on the development and understanding of high-performance materials, including vitrimers, elastomers, and 2D polymers. Alongside this materials work, he continues to refine and implement digital chemistry methods, such as continuous flow chemistry and Bayesian optimization. Dr Baldwin is currently bridging these disciplines by building modular, experimentalist-led platforms and custom workflows to better connect automated data generation with the creative investigation of structure–property relationships. His work is recognized by the ACS-PMSE Early Investigator Award (2025), the AFRL Early Career Award (2025), and two OUSD Fellowships (2021, 2026).

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00477B.



Shuwen Yue is an Assistant Professor in the R. F. Smith School of Chemical and Biomolecular Engineering at Cornell University. Her research focuses on machine learning–enabled molecular simulation, with an emphasis on electrolyte microenvironments, catalyst materials, and electrochemical interfaces. Her group develops physically informed machine learning models to understand and predict transport, thermodynamics, and reactivity in complex molecular systems. She received her PhD in Chemical Engineering from Princeton University and completed postdoctoral training at MIT.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00414D.

Carolin Müller is an Assistant Professor for the Theory of Electronically Excited States at FAU Erlangen-Nürnberg and head of the CPC group since November

2023. She previously held postdoctoral positions at the University of Luxembourg (2022–2023) and Friedrich Schiller University Jena (2021–2022). Carolin earned her BSc and MSc in chemistry from Friedrich Schiller University Jena and Dublin City University and completed her PhD at Friedrich Schiller University Jena. Her research focuses on unravelling molecular mechanisms through the synergy of quantum chemistry and chemoinformatics, complemented by spectroscopy. Current investigations explore phenomena such as photocatalysis and photoswitching.

Her contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00299K.

Mohamad Moosavi is an Assistant Professor of Chemical Engineering & Applied Chemistry at the University of Toronto and a Faculty Member of the Vector Institute. Mohamad directs the Artificial Intelligence for Chemical Science (AI4ChemS) research group, focusing on leveraging AI and computational methods for the discovery of advanced materials. His team's current research focuses on developing MOFs and nanoporous materials for carbon capture and conversion, aiming to advance technology development for sustainable technologies. Mohamad's academic journey began with an undergraduate degree in Mechanical Engineering from Sharif University of Technology, Iran, followed by a PhD in Chemistry and Chemical Engineering from EPFL, Switzerland, and a Postdoctoral Fellowship in Mathematics and Computer Science at the Free University of Berlin, Germany.

His contribution to the 2025 *Digital Discovery* Emerging Investigators collection can be read at https://doi.org/10.1039/D5DD00489F.