

## News Release

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### **Merck KGaA, Darmstadt, Germany, Collaborates with Research Groups Based in Berkeley, California, on Digital Design of Catalysts**

- **Partners are the Hartwig Group at University of California, Berkeley and Lawrence Berkeley National Laboratory jointly led by John Hartwig**
- **Three-year collaboration in computational catalysis science**
- **Aim is to predict novel catalysts using machine learning (ML) and artificial intelligence (AI) techniques**

Darmstadt, Germany, May x, 2023– Merck KGaA, Darmstadt, Germany, a leading science and technology company, today announced a three-year collaboration with the research group of [John Hartwig](#) at University of California, Berkeley and [Lawrence Berkeley National Laboratory](#), Berkeley, California. The primary focus of this collaboration between the public research institutes associated with the University of California and the Digital Chemistry Team of Merck KGaA, Darmstadt, merGermany, will be on understanding the underlying mechanisms for catalysis innovation using machine learning and high-throughput experimentation.

“The application of artificial intelligence to catalysis is a deeply interdisciplinary topic ripe for collaboration. I am excited for the opportunity to assemble the intellect and expertise of researchers at Berkeley and Merck KGaA, Darmstadt, Germany, me to create new approaches to predict and imagine new catalysts and catalytic reactions for the synthesis of high-value compounds relevant to our partner’s portfolio,” said John F. Hartwig, Henry Rapoport Professor of Organic Chemistry at the University of California, Berkeley and Senior Faculty Scientist at Lawrence Berkeley National Laboratory.



## News Release

“Our commitment to exploring disruptive technologies that have the potential to impact our pioneering businesses is unwavering, and this collaboration on digital design of catalysts represents a significant step forward. I am excited to see what groundbreaking advancements will emerge from this partnership,” said Philipp Harbach, Global Head of Group Digital Innovation of Merck KGaA, Darmstadt, Germany.

The collaboration is funded through the company’s 2022 Research Grant “[Chemistry in the cloud](#) – Rapid synthesis through automation”. This annual research grant program was developed in 2018 to explore potentially disruptive technologies that impact the businesses of Merck KGaA, Darmstadt, Germany.

The research of the three partners aims to enhance the process of creating novel catalysis materials by implementing new machine learning representations of catalysts and advanced algorithms to determine the optimal catalysts for a process when given limited reaction data. The machine learning algorithms will be combined with high-throughput experimentation to create optimized predictions using real-world results. Outcomes will include new algorithms and software as well as novel catalysis materials.

John F. Hartwig is the Henry Rapoport Professor of Organic Chemistry at the University of California, Berkeley and Senior Faculty Scientist at Lawrence Berkeley National Laboratory. Hartwig’s research focuses on the discovery and understanding of new reactions catalyzed by transition metal complexes. He is well known for his contributions to widely practiced cross-coupling chemistry that form arylamines, aryl ethers, aryl sulfides, and  $\alpha$ -aryl carbonyl compounds as well as for the discovery of practical C-H bond functionalization reactions. He has received numerous awards and was elected to the National Academy of Sciences in 2012. Hartwig was awarded the [Emanuel Merck Lectureship](#) in 2022.

The Digital Chemistry Team at Merck KGaA, Darmstadt, Germany, concentrates on bringing digital tools and applications to chemistry-related business bottlenecks within the three business sectors of the company. The group aims to enhance productivity and increase innovation within the current product portfolio of Merck

## News Release

KGaA, Darmstadt, Germany, as well as open new opportunities in expanding digital businesses within the organization.

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### **About Merck KGaA, Darmstadt, Germany**

Merck KGaA, Darmstadt, Germany, a leading science and technology company, operates across life science, healthcare and electronics. More than 64,000 employees work to make a positive difference to millions of people's lives every day by creating more joyful and sustainable ways to live. From providing products and services that accelerate drug development and manufacturing as well as discovering unique ways to treat the most challenging diseases to enabling the intelligence of devices – the company is everywhere. In 2022, Merck KGaA, Darmstadt, Germany, generated sales of € 22.2 billion in 66 countries.

The company holds the global rights to the name and trademark "Merck" internationally. The only exceptions are the United States and Canada, where the business sectors of Merck KGaA, Darmstadt, Germany, operate as MilliporeSigma in life science, EMD Serono in healthcare and EMD Electronics in electronics. Since its founding in 1668, scientific exploration and responsible entrepreneurship have been key to the company's technological and scientific advances. To this day, the founding family remains the majority owner of the publicly listed company.