

News Release

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Merck KGaA, Darmstadt, Germany, and Mulliken Center for Theoretical Chemistry Collaborate in Machine Learning Project

- **Three-year project to focus on molecular representations and computational tools**
- **Methods and code developed in the program will be open source**

Darmstadt, Germany, June 14, 2022– Merck KGaA, Darmstadt, Germany, a leading science and technology company, today announced a collaboration with the [Mulliken Center for Theoretical Chemistry](#) at the Rheinische Friedrich-Wilhelms-University of Bonn, Germany. The three-year collaboration will focus on the development of new tools for computational chemistry modelling as well as new molecular representations to advance the next generation of molecular machine learning.

“We are excited to work with Merck KGaA, Darmstadt, Germany, on this project, which will be beneficial for the company and the computational chemistry community in general. The close interaction with the company’s scientists will help us to give the project and the resulting tools the right focus,” said Professor Stefan Grimme, Head of the Mulliken Center for Theoretical Chemistry and an internationally distinguished leader in theoretical chemistry and a member of the German National Academy of Sciences Leopoldina. The group led by Grimme has developed a plethora of methods and tools that are now widely used far beyond the computational chemistry community.

Merck KGaA, Darmstadt, Germany, is leveraging machine learning and artificial intelligence (AI) along all stages of its value chain. Through numerous initiatives and collaborations, the company aims to accelerate the life cycle of its products,



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break up silos and harness the power of data and digital. "Recent advances have shown the impact that molecular machine learning and AI in general can have in all chemistry-related areas, especially simulation and data-driven drug discovery, materials design and prediction of new formulations. With this collaboration, together we want to develop new molecular representations and computational tools that will help us in making drug candidate screenings faster, discover new compounds and predict the performance of materials," said Jan Gerit Brandenburg, Head of Digital Chemistry at Merck KGaA, Darmstadt, Germany.

Over the next three years, several PhD students from the Mulliken Center for Theoretical Chemistry will work with the Digital Chemistry team at Merck KGaA, Darmstadt, Germany, to identify methods applicable to the company's entire portfolio of chemicals and pharmaceuticals that would benefit from molecular machine learning techniques. All methods and codes developed within the program will be open source and will thus also benefit the broader scientific community. The program is partly embedded in the German Research Foundation's (DFG) Priority Programme on Molecular Machine Learning ([SPP 2363](#)).

About MCTC

The Mulliken Center for Theoretical Chemistry (MCTC) is a globally recognized research center of the University of Bonn, Germany, which has been awarded three Leibniz prizes (most recently in 2015 for Stefan Grimme). Three professors and more than 50 scientists conduct research in an international team with a focus on quantum and atomistic simulations of challenging chemical, pharmaceutical and energy-related problems.

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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 60,000 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 advancing gene editing technologies and discovering unique ways to treat the most challenging diseases to enabling the intelligence of devices – the company is everywhere. In 2021, Merck KGaA, Darmstadt, Germany, generated sales of € 19.7 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.