

3rd UniSysCat Annual General Assembly

Start Time: Wednesday, November 24, 2021 05:00 pm

End Time: Wednesday, November 24, 2021 07:00 pm

Zoom Meeting
Online Meeting

We kindly invite you to the **3rd UniSysCat Annual General Assembly** taking place on **Wednesday, November 24, 2020 at 5 pm**. We will meet online via Zoom. The link will be sent around by email - if you didn't receive it, please ask for it by email to info@unisyscat.de

The Annual General Assembly will be opened by a meet & greet at 5 pm. Then, shortly after, the cluster's spokesperson Prof. Dr. Arne Thomas will give the annual report. Like in the last few years, there will be a lecture afterwards. This year, [Prof. Dr. Klaus-Robert Müller](#) from the Machine Learning group at TU Berlin will give a talk about "Machine Learning meets Quantum Chemistry".

Machine Learning meets Quantum Chemistry

Prof. Dr. Klaus-Robert Müller

Technische Universität, Institute of Software Engineering and Theoretical Computer Science
Machine Learning

The talk will first briefly introduce machine learning (ML) concepts, before applying them in Quantum chemistry and materials. This will include kernel-based learning methods and deep neural networks. A particular focus will lie on the challenge of interpreting nonlinear machine learning models. In other words, given that we have an excellent predictor of quantum chemical properties, how can we gain an understanding of the physics or chemistry that this learning machine has implemented? I will show selected examples of ML applied for predicting properties of small molecules and also for materials.