

Plenary Talk

PV XVIII Fri 9:00 Audimax 2

Machine Learning meets Quantum Physics — •KLAUS-ROBERT MÜLLER — TU Berlin, Germany, Korea University, Seoul, Korea and MPII, Saarbrücken, Germany

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.