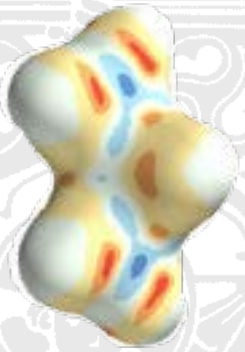
Physikalisches Institut
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg

PHYSIKALISCHES KOLLOQUIUM

AM 3. FEBRUAR 2020 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



MACHINE LEARNING MEETS QUANTUM PHYSICS

PROF. DR. KLAUS-ROBERT MÜLLER
TECHNISCHE UNIVERSITÄT BERLIN

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.