Universität Basel

Research Project

QML/Quantum Machine Learning: Chemical Reactions with Unprecedented Speed and Accuracy

Third-party funded project

Project title QML/Quantum Machine Learning: Chemical Reactions with Unprecedented Speed and Accuracy
Principal Investigator(s) von Lilienfeld, Anatole ;
Organisation / Research unit
Departement Chemie / Physikalische Chemie (Lilienfeld)
Department
Project start 01.06.2018
Probable end 31.05.2023
Status Completed

Large and diverse property data sets of relaxed molecules and crystals, resulting from compu- tationally demanding quantum calculations, have recently been used to train machine learning models of various energetic and electronic properties. We propose to advance these techniques to a level where they can also describe reaction profiles, i.e. reactive non-equilibrium processes which traditionally would require quantum chemistry treatment. The resulting quantum ma- chine learning (QML) models will provide reaction profiles for new reactants in real-time and with quantum accuracy. The overall goal is to develop a predictive computational tool which allows chemists to easily optimize reaction conditions, develop new catalysts, or even plan new synthetic pathways.

Financed by
Commission of the European Union