



Friedrich-Alexander-Universität
Research Center for
Mathematics of Data | MoD

FAU MoD Lecture Series



Exemplary applications of machine learning and optimization in quantum chemistry

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FAU



WWW.MOD.FAU.EU

#FAUMoDLecture

WHEN

Monday **July 7, 2025**
16:00H (Berlin time)

WHERE

On-site / Online

Friedrich-Alexander-Universität
Erlangen-Nürnberg (FAU)
Room **H12**
Felix-Klein building
Cauerstraße 11, 91058
Erlangen. Bavaria, Germany

Live-streaming:
www.fau.tv/fau-mod-livestream-2025

Two exemplary applications of machine learning and optimization in quantum chemistry are presented:

- (i) The use of machine-learned force fields in molecular dynamics simulation.
- (ii) The calculation of properties of atoms, molecules, and surfaces in chemistry, physics, or materials sciences requires a quantum mechanical treatment of electrons.