

Machine learning of transferable implicit solvation models

Projektgruppe “Praxis der Forschung”
Sommersemester 2025

1 Project

In this project, a team of up to three students will work on a proof of principle study that combines machine-learning accelerated molecular simulations with latest developments in VR technology - haptic gloves. The overall goal is the development of an VR environment, in which simulations of molecules become tangible and interactive. Challenges include the integration of molecular simulations in unity for visualization and haptic feedback; real-time feedback from haptic gloves back into the simulation to make it interactive; and integration of machine learning models to enable real-time simulations at quantum-mechanical accuracy.

2 Supervision

- Henrik Schopmans <henrik.schopmans@kit.edu>, room 105 (bldg. 40.28)
- Jonas Teufel <jonas.teufel@kit.edu>, room 320 (Geb. 40.28)
- Pascal Friederich <pascal.friederich@kit.edu>, room 123 (bldg. 40.28)