INSTITUTE FOR COMPUTATIONAL PHYSICS

Universität Stuttgart

Einladung zum
ICP-Kolloquium (ICP Seminarraum + Hybrid via Zoom)

Bitte geänderte Uhrzeit beachten – 10:00 Uhr

Dr. Philip Loche
EPFL Lausanne

hält am

Donnerstag, 30.06.2022, 10:00 Uhr
ICP Seminarraum 1.079, Allmandring 3

und via zoom
https://us06web.zoom.us/j/87094806309?pwd=QzZlYWZxSUwxbVZNN0ZKTXNreC9MZz09
ID 870 9480 6309
Code **574486**

einen Vortrag über das Thema:

"Atomistic Machine Learning for Aqueous Solutions"

Abstract:
Accurate modeling of matter at the atomic scale requires to simultaneously account for the quantum nature of the chemical bond - that usually manifests itself on short time and length scales - and long-range interactions, such as electrostatics and dispersion, that occur on a large scale and often result in phenomena with a long characteristic time. Electronic structure calculations provide an accurate description of both quantum and long-range effects, but are computationally demanding, and scale poorly with system size. Machine learning (ML) approaches have emerged as a very effective strategy to build surrogate models that provide comparable accuracy at a fraction of the cost, but the most widespread techniques base their efficiency and transferability on a local description of atomic structure, which makes them ill-equipped to deal with long-range effects.

Here, we are going to connect local and long-range physics in a data driven ML approach by applying the current ML techniques to, condensed-phase systems, involving the characterization of aqueous systems. We show that a combination of a short and a long-range approach is necessary to predict appearing effects.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Apl. Prof. Dr. R. Hilfer
Dr. Rudolf Weeber
Dr. Alexander Schlaich