INSTITUTE FOR COMPUTATIONAL PHYSICS

Universität Stuttgart

Einladung zum ICP-Kolloquium

(ICP Seminarraum und online)

PD Dr. Jens Smiatek
Boehringer Ingelheim Pharma GmbH & Co. KG

hält am

Montag, 19.06.2023, 16:30 Uhr
ICP Seminarraum 1.079, Allmandring 3

und via zoom
https://zoom.us/j/2840750354?pwd=T2VQUG5KL1IxWkg4M1pneGhlQ3Q0dz09
Meeting ID: 284 075 0354
Passcode: 6mZY10

einen Vortrag über das Thema:

"Molecular Theories meet Scientific Machine Learning - Novel Concepts for Pharmaceutical Applications"

Abstract:
Pharmaceutical processes and drug formulations are based on a variety of molecular mechanisms and principles. Significant advances have been made in recent years in terms of basic understanding. Despite these advances, a large number of mechanisms are not yet fully understood, which would be of great advantage, especially for the optimization of development processes as well as the quality and stability of drugs.
In the first part of this talk I will present fundamental molecular theories of electronic interactions in solutions. Due to the large number of components and the complexity of the interactions, these theories can only be used for a qualitative understanding. However, by combining it with explainable machine learning, the basic molecular mechanisms can be identified and the corresponding thermodynamic properties of the solutions can be predicted. I will present some examples and discuss the underlying benefits and additional challenges for future developments. In the second part of the talk, I will present recent applications and extensions of physics-informed neural networks for the study and prediction of chemical reaction kinetics.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Dr. Rudolf Weeber
Dr. Alexander Schlaich