INSTITUTE FOR COMPUTATIONAL PHYSICS

Universität Stuttgart

Einladung zum ICP-Kolloquium (online)

via zoom
https://us06web.zoom.us/j/84589852698?pwd=ZUFZVkt1SFY4U2RTbW1XZ05rdXpOdz09
Meeting-ID: 845 8985 2698
Kenncode: 199063

Prof. Michele Ceriotti
Laboratory of Computational Science and Modelling (COSMO)
EPFL Lausanne

hält am

Donnerstag, 28.10.2021, 14:00 Uhr

einen Vortrag über das Thema:

"Machine learning at the atomic scale"

Abstract:
When modeling materials and molecules at the atomic scale, achieving a realistic level of complexity and making quantitative predictions are usually conflicting goals. Data-driven techniques have made great strides towards enabling simulations of materials in realistic conditions with uncompromising accuracy. In particular, statistical regression techniques have become very fashionable as a tool to predict the properties of systems at the atomic scale, sidestepping much of the computational cost of accurate quantum chemical calculations, and making it possible to perform simulations that require thorough statistical sampling without compromising on the accuracy of the electronic structure model.

In this talk, I will argue how data-driven modelling can be rooted in a mathematically rigorous and physically-motivated symmetry-adapted framework, and discuss the benefits of such a principled approach. I will present several examples demonstrating how the combination of machine-learning and atomistic simulations can offer useful insights on the behavior of complex systems, and discuss the challenges towards an integrated modeling framework in which physics- and data-driven steps can be combined to improve the accuracy, the computational efficiency and the transferability of predictions, from interatomic potentials to electronic-structure properties.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Apl. Prof. Dr. R. Hilfer
Apl. Prof. Dr. M. Fyta