MONTAN UNIVERSITÄT LEOBEN

WO AUS FORSCHUNG ZUKUNFT WIRD

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MONTAN UNIVERSITÄT LEOBEN

EINLADUNG

zum

Schwerpunkt-Nachmittag zum Thema

Artificial Intelligence (AI) / Machine Learning in Materials Science

organisiert von
ReMET
“Responsible Materials for Energy Transition”

06. DEZEMBER 2023
13:30 – 17:00 UHR

Hörsaal Kupelwieser
(Erzherzog-Johann-Trakt, 1. OG)

MONTANUNIVERSITÄT LEOBEN
Erzherzog-Johann-Auditorium, 1. OG
FRANZ-JOSEF-STRASSE 18, 8700 LEOBEN

PROGRAMM

13:30 Uhr	Get-Toghether
14:00 Uhr	Univ.-Prof. Dr. Christoph Dellago – Universität Wien
	„Finding the needle in the haystack: machine learning for rare event simulations”
14:45 Uhr	Ass.-Prof. Dr. Stefan Kowarik – Universität Graz
	“Accelerating Experiment Analysis and Control: Neural Networks in Physics and Chemistry”
15:30 Uhr	Univ.-Prof. Dr. Lorenz Romaner – Montanuniversität Leoben
	"Application of machine learning techniques in computational materials design"
16:15 Uhr	Open Discussion / Networking
17:00 Uhr	End

ANMELDUNG

Aus organisatorischen Gründen
bitten wir Sie, sich bis spätestens 25. November 2023 unter
hannah.hochedlinger@unileoben.ac.at anzumelden.

Abstract

Univ.-Prof. Dr. Christoph Dellago – Universität Wien

The microscopic dynamics of many condensed matter systems occurring in nature and technology is dominated by rare but important barrier crossing events. Examples of such processes include nucleation at first order phase transitions, chemical reactions and the folding of biopolymers. The resulting wide ranges of time scales are a challenge for molecular simulation and numerous simulation methods have been developed to address this problem. Recently, machine learning methods have been proposed as a powerful way to further enhance such simulations. In my talk, I will discuss various machine learning approaches based on deep neural networks to sample rare reactive trajectories and identify the collective variable needed for the construction of low-dimensional models capturing the microscopic mechanism.

Ass.-Prof. Dr. Stefan Kowarik – Universität Graz

This talk delves into the transformative applications of Artificial Neural Networks (ANNs) in the fields of physics and chemistry, specifically focusing on data analysis and adaptive experiments.We present compelling results demonstrating the effectiveness of ANNs in analyzing diverse experimental data, encompassing x-ray diffraction, NMR, UV-vis NMR data fusion, and optical interferometry. ANNs outperform state-of-the-art methods like differentialevolution fitting, offering the unique ability to seamlessly integrate prior k nowledge and physical models. Moreover, they exhibit a remarkable speed advantage, surpassing established iterative algorithms by over a factor of 100. This accelerated processingspeed is instrumental for real-time analysis, enabling online experiment feedback and control. As an outlook, we discuss the potential of ANNs in steering fully autonomous experiments, leveraging adaptive scans for faster and more precise experimental outcomes.

Univ.-Prof. Dr. Lorenz Romaner – Montanuniversität Leoben

Development of future high-performance materials requires reliable process-structure-property relationships. Computational materials science has used physical laws for this purpose and many successful material calculation tools on different length scales are available nowadays. Recently, machine learning approaches have entered this research field providing new opportunities for computational design in several respects. First of all, machine learning methods can replace and accelerate physics-based simulations with surrogate models. In this talk this will be shown for atomistic simulations of grain boundary segregation to scan the periodic table in a particularly efficient manner. Second, it will be shown how Bayesian inference can be used to calibrate models to thermodynamic data for uncertainty quantification and guided acquisition of new experimental data points. As a last point, it will be discussed how active learning techniques can be used for targeted material optimization for the use case of bainitic steels.