

Salon on machine learning for materials science (ML4MS)

When & Where:

Time: Dec 2 (Wednesday), 2020 13:00 — 18:00+ via zoom

<https://tu-darmstadt.zoom.us/j/84883163867?pwd=dU5PU09ubXd4THN4YTdvYUplN0INZz09>

Meeting ID: 848 8316 3867

Passcode: 601717

For those with busy schedules, here is what you can keep in mind about the program:

- 13:00 — 15:00: Microstructure and multiscale modelling
- 15:00 — 16:00: STEM+APT+
- 16:00 +: Theory

Program:

Subject 1: Microstructure and Multiscale Modeling (13:00 — 15:00)

- **Multiscale** modelling in computational mechanics enhanced by ML approaches
Shahed Rezaei, MFM/TUDA
- ML for modelling **swaging**
Fansun Chi, PtU/TUDA
- ML in the **metal forming branch**
Christian Kubik, PtU/TUDA
- Data-Driven **Microstructure** Sensitivity Study in Paper Materials
Binbin Lin, MFM/TUDA
- Estimating **Permeabilities** from 2D Images: A Machine Learning Approach
Rainer Niekamp, IfM/UDE

Subject 2: STEM + APT Characterization (15:00 — 16:00)

- **4D-STEM**: ML-based phase and orientation identification in electron diffraction maps at nanometer resolution
Alex Zintler, AEM/TUDA
- Consistent **atom probe** representation for machine learning and data mining
Ye Wei, APT/MPIE
- Tentative strategies for **impedance** evaluation
Till Frömling, NAW/TUDA

- - continues on the next page - -

Subject 3: Materials by Design (16:00 – 16:50)

- Accelerated discovery of novel **INVAR** alloy with active learning
Ziyuan Rao + Ye Wei, APT/MPIE
- Finding new **antiferroelectric** materials: A classification study
Binbin Lin + Zhen Liu, MFM/TUDA

Subject 4: Lattice Dynamics (17:00 – 18:00)

- Gaussian Approximation Potentials: Increasing the accuracy of **interatomic potential** modelling by Machine Learning
Linus Erhard, MM/TUDA
- Compressive sensing **lattice dynamics**
Yixuan Zhang, TMM/TUDA
- Enhancing the **thermal conductivity** of nano-composite with Bayesian method
Binbin Lin + Mozdeh Fathidoost, MFM/TUDA

Subject 5: Deep Learning (18:00 – 18:50)

- Particle/Fiber **segmentation** using Deep Learning
Binbin Lin, MFM/TUDA
- **Inverse design** of crystal structures
Teng Long, TMM/TUDA

Notes:

- (1) Each talk is supposed to be 20 (talking) + 5 (discussion) = 25 minutes. Therefore, please (speakers) include more background and technical details and (audience) ask more questions.
- (2) The subjects (microstructure and experimental characterizations) of general interest are put at the beginning. In this way, we hopefully will get inspired and learn also the pending problems before diving into theoretical modelling.
- (3) We will start with Subject 2 at 15:00, when Till can join. If there is time left from Subject 1, we can have a break or shift one or two talks from Subject 3 before 15:00.
@Zhiyuan @Ye @Binbin @Zhen: I hope you are okay with this.
- (4) Do we need breaks? I am sure not all talks will last 25 minutes...