Materials Science and Engineering

4TU.HTM

Joint Workshop on the role of

Machine Learning in Molecular Discovery & Scientific Understanding

Theatre Hall X, TU Delft, Thursday 21 March 2024

Programme

Keynote lecture by

Prof.dr. Max Welling (UvA)

Relating Non-Equilibrium Thermodynamics to Machine Learning: what can we learn?

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Aim of the workshop

The exponential growth of computational power combined with the emergence of innovative machine learning (ML) algorithms offers a revolutionary paradigm in the realm of molecular discovery and scientific understanding. This workshop aims to create a dialogue between pure ML researchers, and scientists using cutting-edge models for data-centric scientific molecular and material discovery.

Together we will focus on exploring theoretical machine learning research and delve into real-world applications in molecular and material discovery. The emphasis will be on integrating small scale experimental data and quantum mechanical calculations into machine learning frameworks, forming collaborative networks, and addressing key challenges.

TU Delft Delft University of Technology

TU/e Eindhoven University of Technology

University of Twente.

Wageningen University & Research

4TU.

university of groningen / faculty of science and engineering / zernike institute for advanced materials

Machine Learning in Molecular Discovery

university of groningen

4TU.HTM

Programme

9.30	**Walk-in and coffee**
10.00 - 10.05	Welcome and introduction **Prof.dr.ir. Arjan Mol, Scientific Director 4TU.HTM, TU Delft (ME, MSE)**
	Chair: Sid Kumar
10.05 – 11.00 *(40 min + Q&A)*	**Keynote speaker - Prof.dr. Max Welling (UvA)** *Relating Non-Equilibrium Thermodynamics to Machine Learning: what can we learn?*
11.00 – 11.30 *(20 min + Q&A)*	**Dr. Jana Weber (TU Delft)** *Towards generative design of molecular ensembles with machine learning*
11.30 – 11.55 *(20 min + Q&A)*	**Dr. Nong Artrith (Utrecht University)** *Machine Learning (ML) for Simulating Complex Energy Materials with Non-Crystalline Structures*
11.55 – 12.00	**Dr. Kevin Rossi (TU Delft)** *Introducing DAEMON COST, the European network on ML for materials design*
12.00 – 13.30	**Lunch**
	Chair: Kevin Rossi
13.30 – 14.00 *(20 min + Q&A)*	**Pim de Haan, MSc (UvA, Qualcomm)** *Scientific Machine Learning with the Geometric Algebra Transformer*
14.00 – 14.30 *(20 min + Q&A)*	**Dr. Sid Kumar (TU Delft)** *Inverse design of materials with generative modeling: from molecules to meta-molecules*
14.30 – 15.00 *(20 min + Q&A)*	**Dr. Menno Bokdam (UTwente)** *Looking inside 'dynamic solids' using on-the-fly machine learning force fields*
15.00 – 15.30	**Break**
	Chair: Can Özkan
15.30 – 16.00 *(20 min + Q&A)*	**Prof. dr. Vedran Dunjko (Leiden University)** *Towards quantum machine learning for quantum physical systems with provable advantages*
16.00 – 16.30 *(20 min + Q&A)*	**Dr. Will Robinson (Radboud University)** *Machine Learning's role in understanding chemical reaction systems*
16.30 – 17.00 *(20 min + Q&A)*	**Dr. Jakub Tomczak (Eindhoven University of Technology)** *Generative AI with Decision Making for Drug Design*
17.00	**Closure, drinks & bites**