Machine Learning Conference for X-Ray and Neutron-Based Experiments, Munich 2024



Contribution ID: 63 Type: Invited talk

Autonomous Soft Matter Discovery using X-ray Scattering

Tuesday 9 April 2024 11:00 (30 minutes)

Autonomous experimentation (AE) holds enormous promise for accelerating scientific discovery, by leveraging machine-learning to drive experimental loops where the machine selects and conducts experiments. This talk will discuss AE at synchrotron x-ray scattering beamlines. Deep learning is used to classify x-ray detector images, with performance improving when domain-specific data transformations are applied. To close the autonomous loop, we deploy a general-purpose algorithm based on gaussian processes. Several examples of successful autonomous experiments in polymer science will be presented, including the use of AE to explore the non-equilibrium self-assembly of block copolymer thin films into non-native morphologies. Finally, we discuss the intersection of large language models (LLMs) with material discovery.

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