CanSAS 2023

Collective action for nomadic Small Angle Scatterers

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Autonomous Materials Discovery using X-ray Scattering

Monday, 16 October 2023 16:30 (30 minutes)

Autonomous experimentation (AE) holds enormous promise for accelerating scientific discovery. This paradigm leverages machine-learning methods to construct experimental loops where the machine selects and conducts experiments, liberating the human scientist to focus on high-level goals and understanding. This talk will discuss autonomous experiments (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 AE.

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Session Classification: Automation & software