Brookhaven National Laboratory

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Tuesday, May 31st, 2022
12:00 PM – 1:00 PM

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Host: Meifeng Lin, CSI

Autonomous Materials Discovery using X-rays

Abstract: This talk will discuss the ongoing development of autonomous experimentation at a synchrotron x-ray scattering beamline. Deep learning (convolutional neural network) methods are used to classify x-ray detector images, with performance improving when domain-specific data transformations are exploited. These methods can be combined with customized data healing algorithms. To enable fully autonomous experiment control, we deploy a general-purpose decision-making algorithm based on Gaussian Process (GP) methods. Using this, experiments can be conducted in modes that minimize uncertainty and experimental cost, or that target desired outcomes. Tailoring models to system physics improves performance. Examples from recent autonomous experiments will be presented, demonstrating how these AI/ML methods can accelerate the discovery of novel materials.

Biography: Kevin Yager is the group leader for Electronic Nanomaterials in the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL). He obtained his Ph.D. from McGill University in 2006, worked at the National Institute of Standards and Technology (NIST) from 2006-2009, and joined BNL in 2010. His research focuses on engineering new nanomaterials, especially by exploiting self-assembly methods; and the development of new measurement methods, especially using x-ray scattering.