

## Workshop

### Machine Learning in Scanning Transmission Electron Microscopy

**Monday June 3<sup>rd</sup>:**

#### **Atomic Resolution STEM, Deep Convolutional Neural Networks, and Variational Auto Encoder**

8:30 – 9:00 Welcome

9:00-10:00 Principles of Electron Optics and Aberration Correction in STEM (Duscher)

10:00-10:50 Remote Aberration Correction in STEM (Duscher, Houston)

11:10-12:00 Simulation of Ronchigrams [Participant computer] (Duscher)

**Commented [SK1]:** What do you mean, Gerd?

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Remote Atomic Resolution Imaging (Duscher)

2:00-2:50 Methods of Atom Position Determination [Participant computer] (Duscher, Kalinin, Houston)

3:20 -4:00 Training datasets and Neural Networks (Kalinin, Houston, Pratijs)

4:00-5:00 Advanced Machine Learning of Atomically Resolved Images (Kalinin)

**Tuesday June 4<sup>th</sup>:**

**Electron Diffraction, 4D-STEM, Differential Phase Contrast, and Variational Auto Encoder**

9:00-10:00 Introduction to Diffraction (Duscher)

10:00-10:50 Remote Diffraction Acquisition and DPC in STEM (Duscher, Houston)

11:10-12:00 Simulation of Diffraction Pattern (Duscher)

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Analyzing Diffraction Pattern [Participant computer] (Duscher, Houston)

2:00-2:50 Live Remote Acquisition of 4D STEM and DPC (Houston)

3:20 -4:00 Training Datasets and Neural Networks for Diffraction (Kalinin, Houston, Pratiis)

4:00-5:00 Advanced Machine Learning for 4D-STEM and Diffraction (Kaliin, Pratiis)

**Wednesday June 5<sup>th</sup>:**

**Energy Dispersive X-Ray Spectroscopy, Principal Component Analysis, and Non-Negative Matrix Factorization**

9:00-10:00 Introduction to Energy Dispersive X-ray Spectroscopy (Duscher)

10:00-10:50 Live Remote Acquisition of EDS spectra in STEM (Duscher, Houston)

11:10-12:00 Analysis of EDS [Participant computer] (Duscher)

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Introduction to Electron Energy Loss spectroscopy (Duscher)

2:00-3:50 Live Remote Acquisition of EELS Spectra in STEM (Duscher, Houston)

3:20-4:00 Analysis EELS [Participant computer] (Duscher)

4:00- 5:00 Clustering in Spectroscopy (Duscher, Kalinin)

**Thursday June 6<sup>th</sup>:**

**Advanced Machine Learning**

9:00-10:00 Introduction to Principles of Machine Learning

10:00-10:50 Principles of Neural Networks for Spectroscopy [Participant computer]  
(Kalinin, Houston, Pratijs)

11:10-12:00 Advanced Machine Learning for Spectroscopy

12:00-1:00 Lunch (provided for onsite participants)

1:00-2:00 Convolutional Neural Network

2:00-2:50 Deep Kernel Neural Networks

3:20 -4:00 Principles of Neural Networks for Spectroscopy II [Participant computer]  
(Kalinin, Houston, Pratijs)

4:00-5:00 Pycroscopy Ecosystem and Machine Learning Tools (Rama Vasudevan, ORNL)

**Friday June 7<sup>th</sup>:**

**Imaging, EELS, Deep Kernel Learning, Automation, and human-in the loop automated experiment (hAE)**

9:00-10:00 Introduction to Remote Access to STEM (Duscher)

10:00-10:50 Remote Acquisition of data with remote computers (Pratius, Houston)

11:10-12:00 Introduction to sparse matrices in acquisition

12:00-1:00 Lunch (provided for onsite participants)

1:00-2:00 Principles of Bayesian Optimization

2:00-2:50 New methods enabled by remote computer-controlled acquisition (Kalinin)

3:20 -4:00 Advanced Machine Learning

4:00-5:00 Conclusion