THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 19: Contextual Bandits and ML Agents

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Definitions:

- **Objective:** overall goal that we aim to achieve. Not available during or immediately after experiment.

- **Reward:** the measure of success available at the end of experiment

- **Value:** expected reward. Difference between reward and value is a feedback signal for multiple types of active learning

- **Action:** how can ML agent interact with the system

- **State:** information about the system available to ML agent

- **Policy:** rulebook that defines actions given the observed state

Agriculture

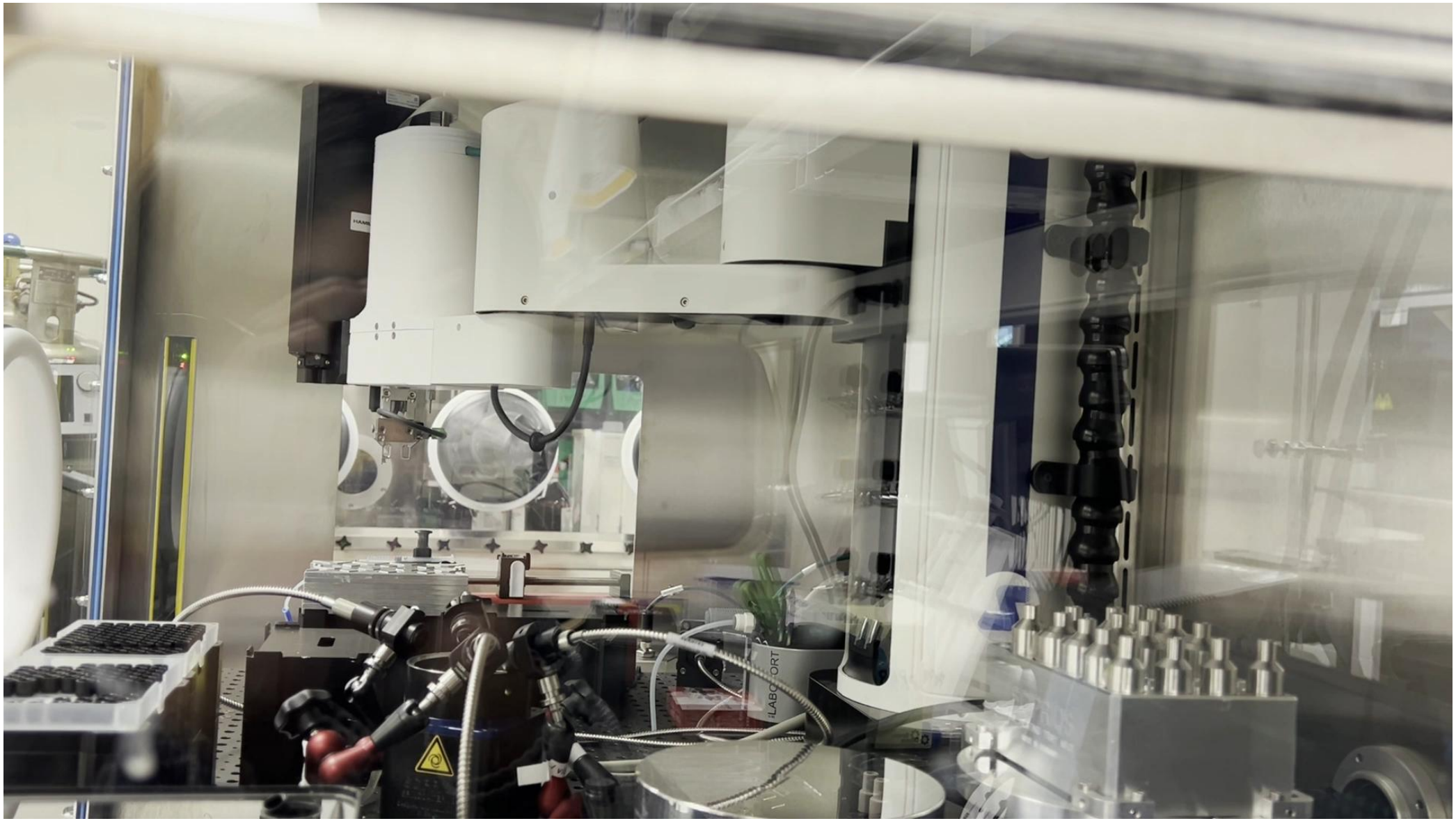
Agriculture

Winemaking

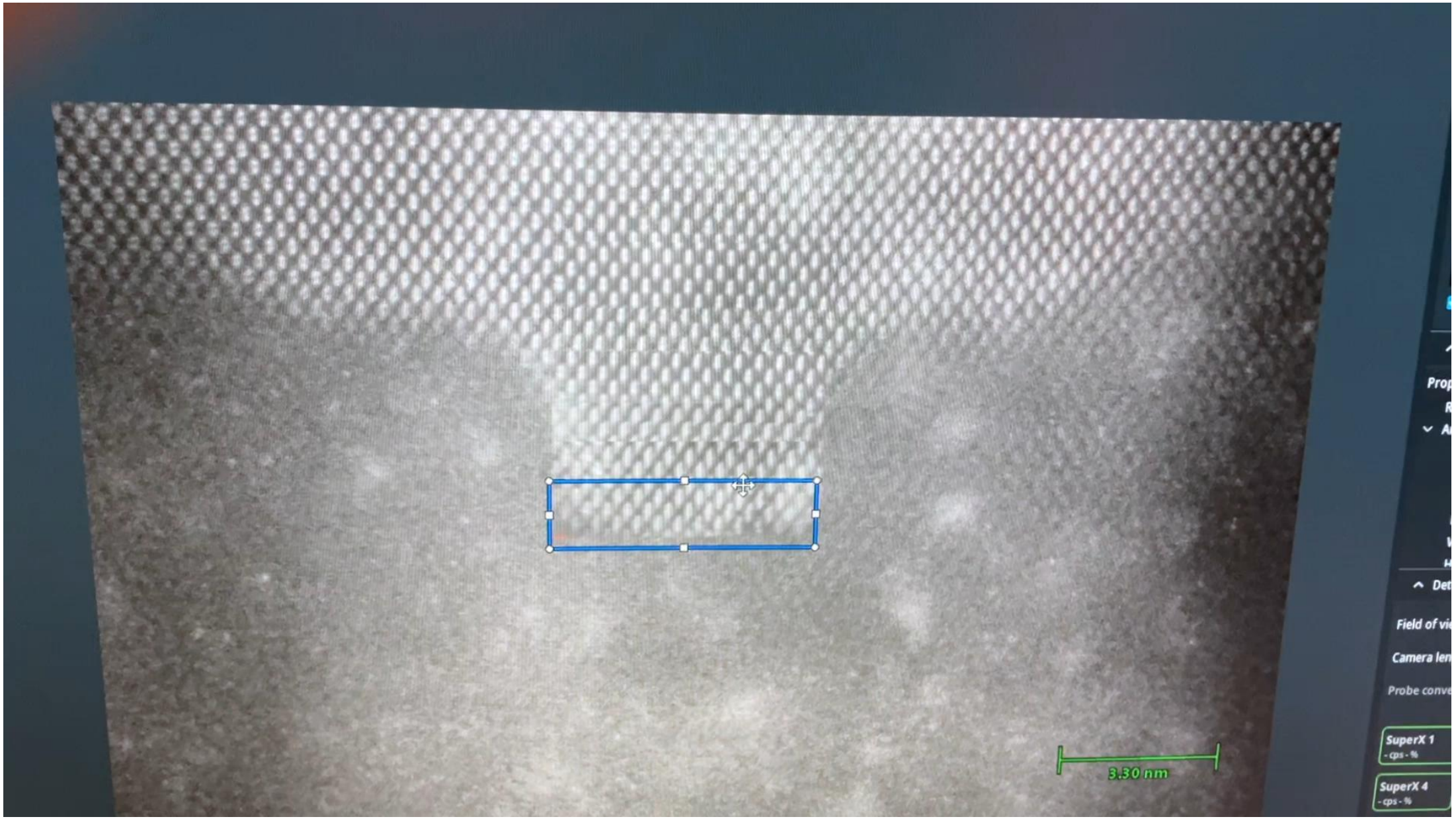
Manufacturing

ML/AI in experimental materials research

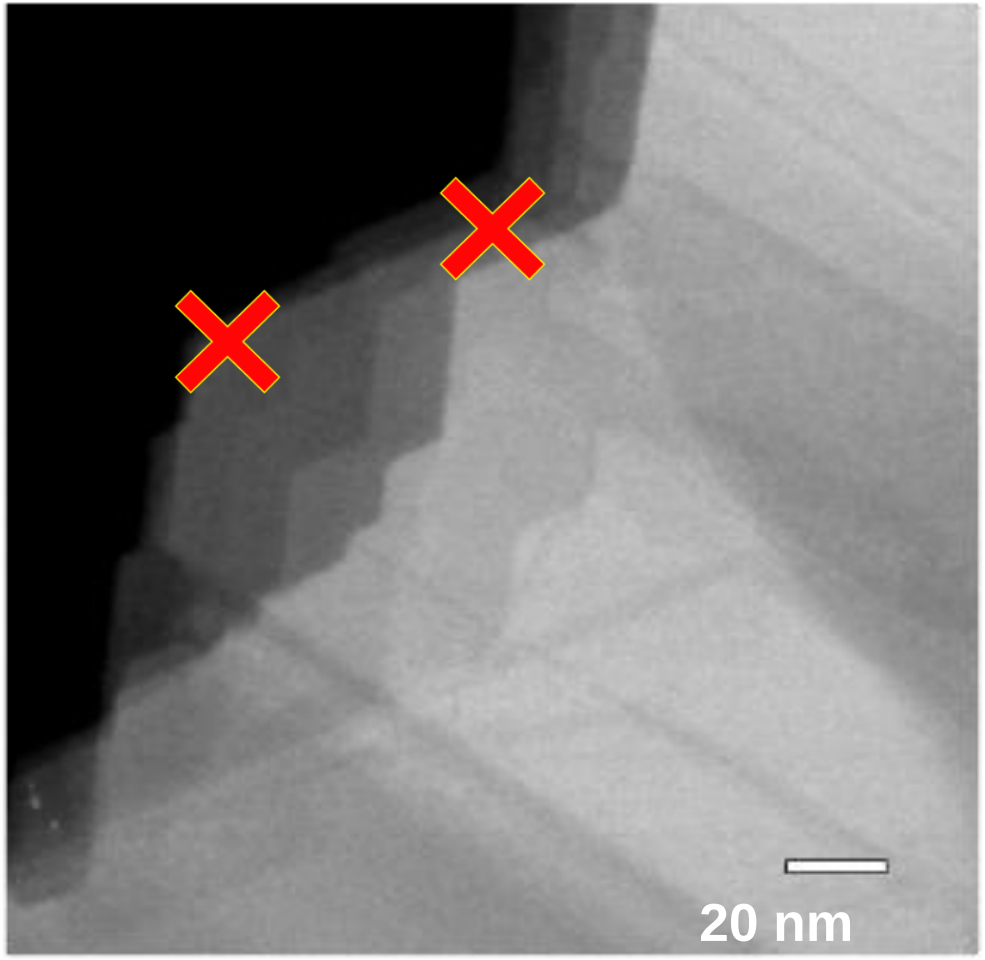
Automated Experiment At UT Knoxville

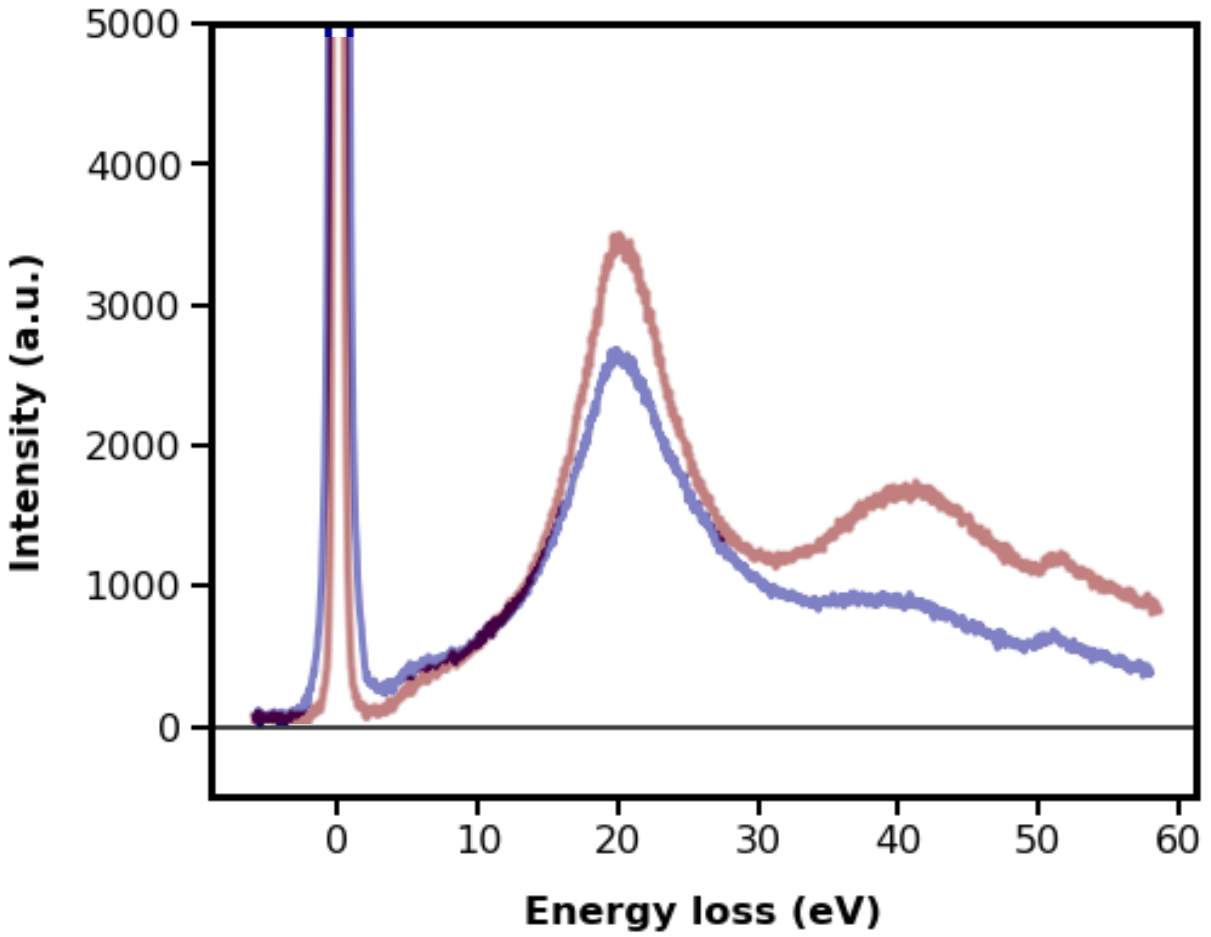


Automated Experiment At UT Knoxville



From Static to Active Learning

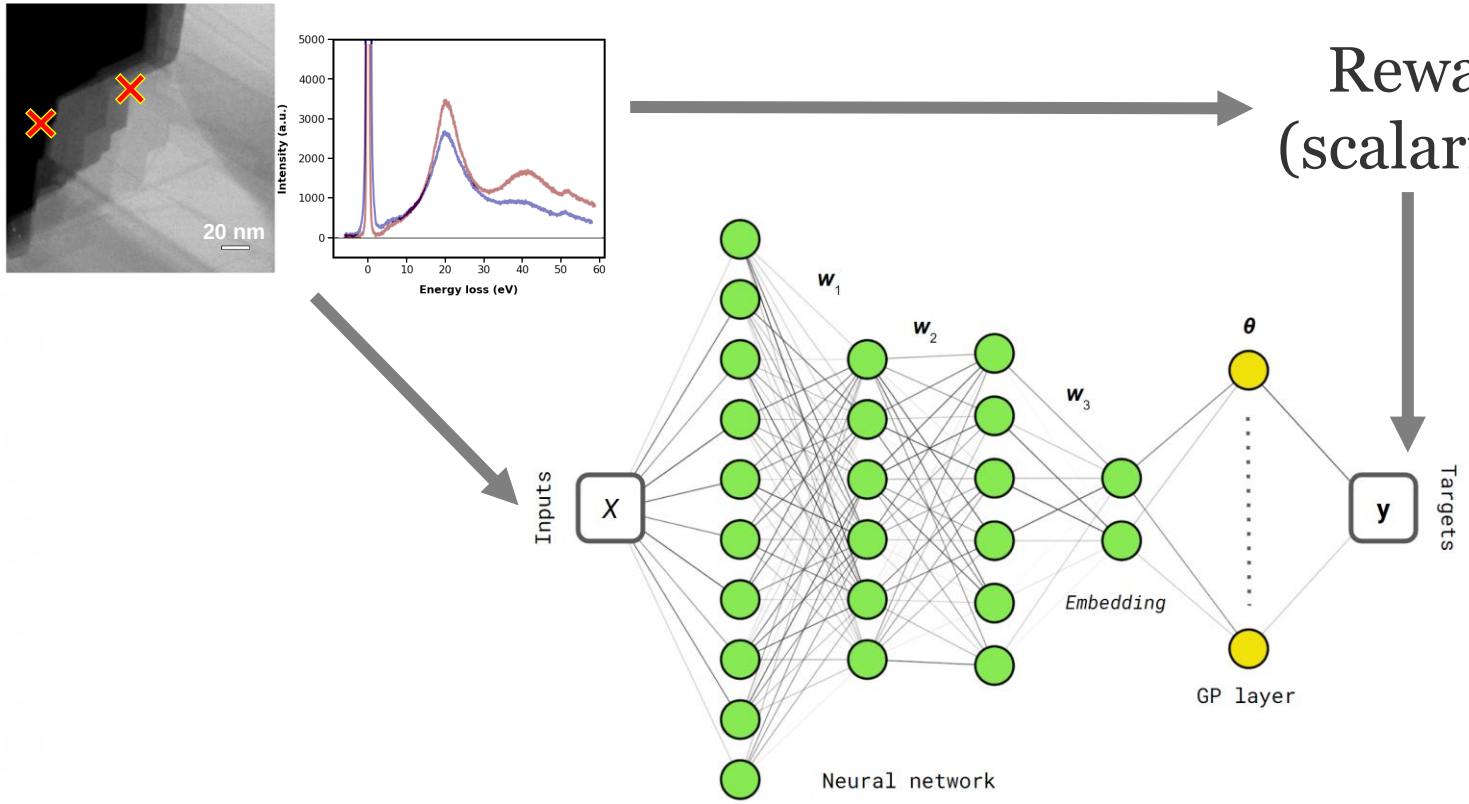




1. What if we have full access to structural information
2. And want to choose locations for (EELS, 4D STEM, CL, EDX) measurements
3. So as to **learn** relationship between structure and spectrum fastest
4. Or **discover** which microstructural elements give rise to specific **desired** spectral features?

Deep Kernel Learning

- All image patches are available in the beginning of the experiment
- We measure spectra one by one
- And are interested in some specific aspect of spectra
- We aim to learn the relationship between structure and this aspect



Specify physics criteria

Acquire **structural data**

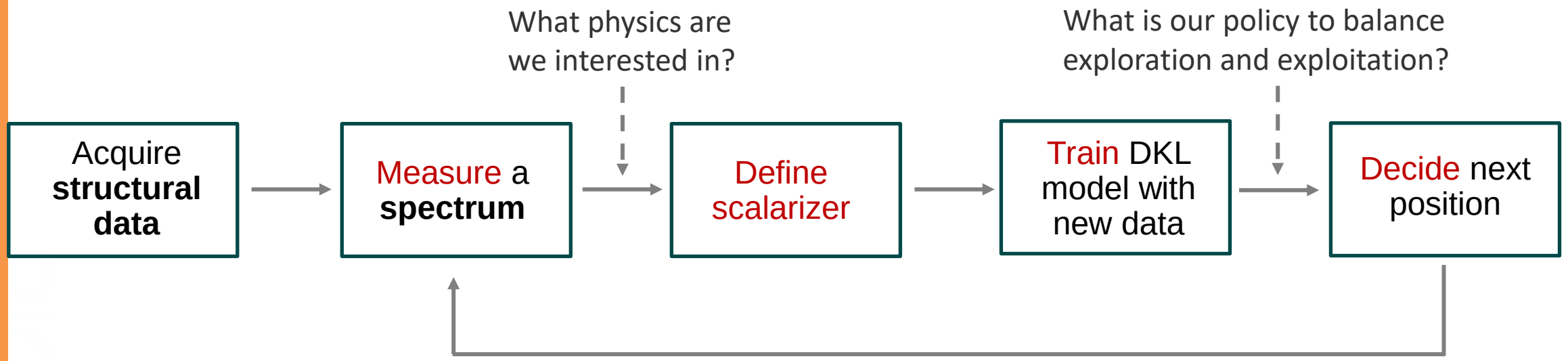
Measure a **spectrum**

Train DKL model with new data

Decide next position (optimize physics criteria)

Allows navigation of the system to search for physics

Deep Kernel Learning based BO



Key concepts:

- **Scalarizer:** (any) function that transforms spectrum into measure of interest. Can be integration over interval, parameters of a peak fit, ration of peaks, or more complex analysis
- **Experimental trace:** collection of image patches and associated spectra acquired during experiment. Note that we collect spectra, not only scalarizers