## Workshop on MBE for Emerging Emitter Technologies
## Room Tamaya ABC - Session WME2-SaA

### AI/ML Techniques for MBE
**Moderator: Kurt Eyink**, Air Force Research Labs

4:15pm **WME2-SaA-12 Invited Paper***, **Remi Dingreville,*** Sandia National Laboratories **INVITED**

4:45pm **WME2-SaA-14 Machine Learning Methods for MBE Growth Optimization***, Mingyu Yu,* University of Delaware*; Isaiah Moses,* Pennsylvania State University, United States Minor Outlying Islands (the)*; Ryan Trice, Wesley Reinhart, **Stephanie Law,*** Pennsylvania State University **INVITED**

Machine learning models hold the potential to explore parameter space autonomously, quickly establish process-performance relationships, and diagnose material synthesis in real time. This reduces reliance on manual intervention in parameter space exploration, enabling more precise and efficient mechanistic control. For molecular beam epitaxy (MBE), despite its breakthroughs in materials synthesis, its stringent growth conditions and complex epitaxial mechanisms make the process of optimizing growth process time-consuming and expensive. Therefore, leveraging machine learning to develop autonomous MBE growth platforms presents a highly promising prospect. In this talk, I will discuss efforts to synthesize two material systems using machine learning and Bayesian optimization. We begin with a comprehensive high-quality dataset of GaSe thin films grown on GaAs (111)B substrates. GaSe is an emerging two-dimensional semiconductor material with intriguing properties, including thickness-tunable bandgaps, nonlinear optical behaviors, and intrinsic p-type conductivity. We were interested in leveraging machine learning to analyze the relationships between growth conditions (Ga flux, Se:Ga flux ratio, and substrate temperature) and the resulting sample quality, as well as the correlations among various characterization results including in situ RHEED patterns and ex situ x-ray diffraction rocking curve full-width at half maximum (FWHM) and atomic force microscopy (AFM) root mean square (RMS) roughness. In this talk, I will discuss how unsupervised learning, mutual information analysis, and supervised learning can be used to understand the influence of different growth parameters on GaSe film quality. I will then move on to discussing our efforts to use Bayesian optimization along with machine learning to quickly find optimal growth parameters for the various polytypes of In2Se3. The techniques and code can be easily adapted to other materials and other MBE systems, making this approach broadly applicable to a wide range of problems.

# Author Index

## Bold page numbers indicate presenter

**— D —**
Dingreville, Remi: WME2-SaA-12, **1**
**— L —**
Law, Stephanie: WME2-SaA-14, **1**
**— M —**
Moses, Isaiah: WME2-SaA-14, 1
**— R —**
Reinhart, Wesley: WME2-SaA-14, 1
**— T —**
Trice, Ryan: WME2-SaA-14, 1
**— Y —**
Yu, Mingyu: WME2-SaA-14, 1