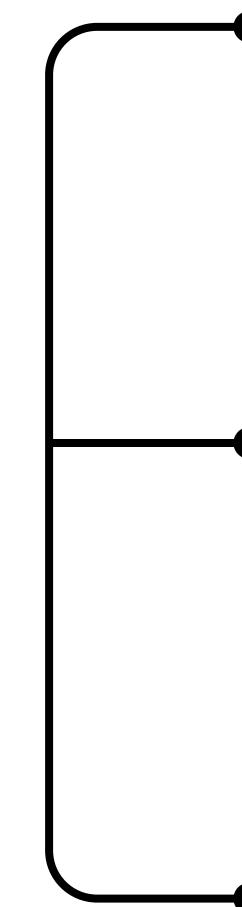


# **Machine Learning-Based XRD Analysis for Nanostructure Characterization**

Nguyen Khac Huy  
Faculty of Science

# Problem statement



- High-throughput XRD produces hundreds/thousands of diffractograms
- Traditional methods (CMWP, WPPM) are accurate but slow and computationally intensive
- Manual analysis is a bottleneck in materials discovery

# ML-Based Solution (ML-XLPA)

## What is ML-XLPA

- Uses machine learning to predict microstructural parameters directly from XRD patterns.
- Fast: reduces analysis time from hours/days to second.

## How it works

### Combines:

1. Physical diffraction modeling (for training data)
2. Background subtraction (e.g., ARPLS)
3. ML regression (e.g., XGBoost)

# Limitations & Goals

## Limitations

- Current ML-XLPA works only for cubic (FCC) materials.
- Not yet extended to hexagonal (HCP) structures.
- Real data challenges: noise, peak shifts, overlapping peaks.

## Goals of project

- Extend ML-XLPA to HCP and multiphase materials.
- Improve preprocessing for noisy/real data.
- Enable fast microstructure mapping for combinatorial libraries.

# Working Plan

## This semester

- Focused on theoretical understanding of ML-XLPA foundations.
- Studied diffraction modeling, background correction, ML methods.
- No implementation yet—groundwork laid for next phase.

## Next semester

- Implement ML-XLPA for HCP structures.
- Improve handling of experimental artifacts and multiphase systems
- Test on synthetic and experimental datasets

# Why it matters?

- Enables high-throughput microstructure mapping
- Supports accelerated materials discovery (e.g., composition–property links).

# Future impacts

- Can be applied to complex alloy, ceramics, batteries, etc
- Bridges XRD experiments with ML-driven analysis.



**Thank You**

## References

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