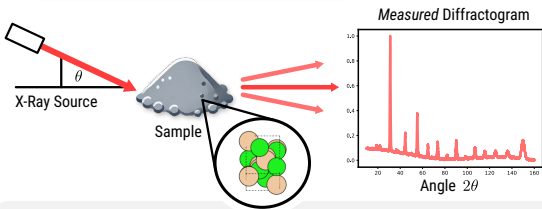


## Powder X-Ray Diffraction (pXRD)



PSL  
UNIVERSITÉ PARIS

KIT  
Karlsruhe Institute of Technology

香港科技大学 (广州)  
THE HONG KONG  
UNIVERSITY OF SCIENCE AND  
TECHNOLOGY (GUANGZHOU)

USC

Empa  
MOLECULAR  
FOUNDRY

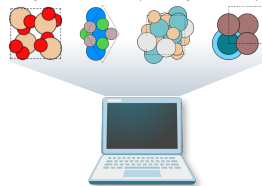
## opXRD Database



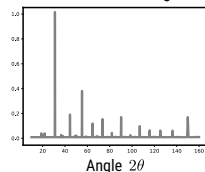
~XX Patterns from YY Contributors

## pXRD Simulation

Crystal Structures (ICSD, Synthetic, ...),



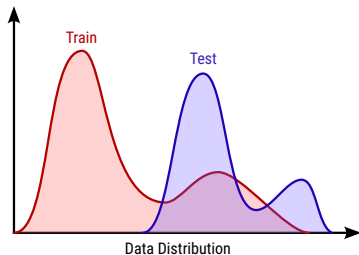
Simulated Diffractogram



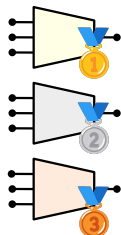
Improving Physics Simulations

## Benchmarking/Evaluation

Realistic Test Distribution



Model Comparison



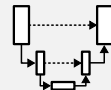
Realistic Evaluations on Real-World Data

## Model Training

Architecture



Convolutional Network



U-Net Network

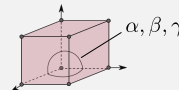
$$\text{sm}(\begin{bmatrix} K \\ Q \end{bmatrix} \times V)$$

Transformer

Downstream



Space Group Classification



Lattice Parameter Regression



Joint Learning using Real and Simulated Patterns, Transfer Learning, ...