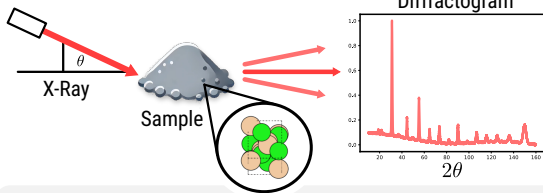


# opXRD Database

## Powder X-Ray Diffraction (pXRD)



PSL  
UNIVERSITÉ PARIS

KIT  
Karlsruhe Institute of Technology

THE HONG KONG  
UNIVERSITY OF SCIENCE AND  
TECHNOLOGY (GUANGZHOU)

USC

Empa

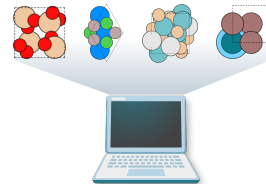
MOLECULAR  
FOUNDRY



92,552 patterns from  
19 contributors

## pXRD Simulation

Crystal Structures (ICSD, Synth., ...)



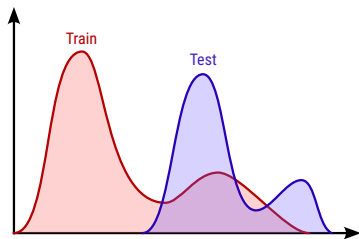
Simulated  
Diffractogram

Improving Physics Simulations

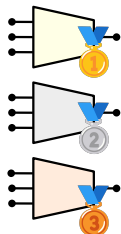
## Benchmarking/Evaluation

Realistic Test Distribution

Model Comparison



Data Distribution



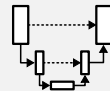
Realistic Evaluations on Real-World Data

## Model Training

Models



Convolutional Network



U-Net

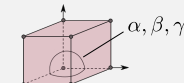
$$\text{sm}(\begin{bmatrix} K \\ Q \end{bmatrix}) \times V$$

Transformer

Tasks



Space Group Classification



Lattice Parameter Regression

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