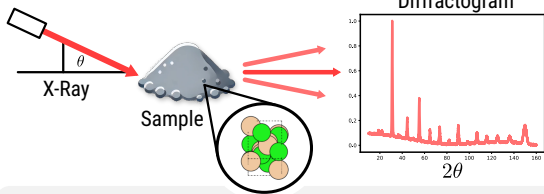


## Powder X-Ray Diffraction (pXRD)

PSL  
UNIVERSITÉ PARISKIT  
Karlsruher Institut für Technologie香港科技大学 (广州)  
THE HONG KONG  
UNIVERSITY OF SCIENCE AND  
TECHNOLOGY (GUANGZHOU)

USC

MOLECULAR  
FOUNDRY

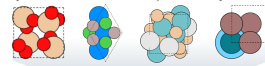
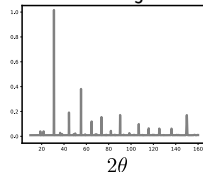
Empa



~XX Patterns from YY Contributors

## pXRD Simulation

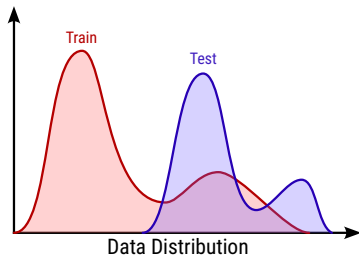
Crystal Structures (ICSD, Synth., ...)

Simulated  
Diffractogram

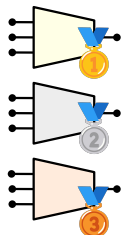
Improving Physics Simulations

## Benchmarking/Evaluation

Realistic Test Distribution



Model Comparison



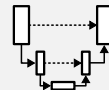
Realistic Evaluations on Real-World Data

## Model Training

Models



Convolutional Network



U-Net

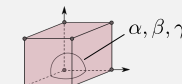
$$\text{sm}(\begin{bmatrix} K \\ Q \end{bmatrix}) \times V$$

Transformer

Tasks



Space Group Classification



Lattice Parameter Regression



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