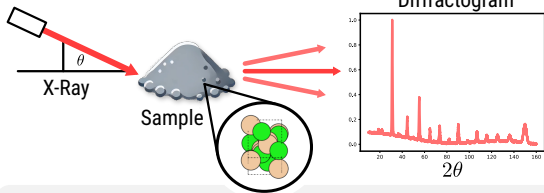


opXRD Database

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

MOLECULAR
FOUNDRY

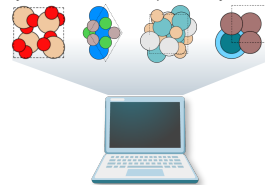
Empa

~XX Patterns from YY Contributors

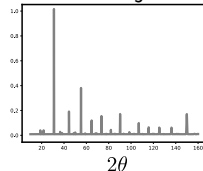


pXRD Simulation

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



Simulated
Diffractogram

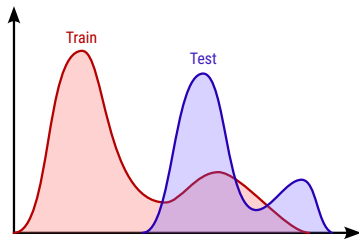


Improving Physics Simulations

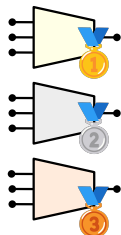
Benchmarking/Evaluation

Realistic Test Distribution

Model Comparison



Data Distribution



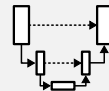
Realistic Evaluations on Real-World Data

Model Training

Models



Convolutional Network



U-Net

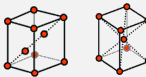
$$\text{sm}(\begin{bmatrix} K \\ Q \end{bmatrix}) \times V$$

Transformer

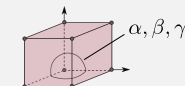
Tasks



Space Group Classification



Lattice Parameter Regression



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