

Contribution ID: 188

Type: Invited talk

Methods and Prospects of Machine Learning applied to Challenges in Crystallography

Tuesday, 15 March 2022 11:00 (1 hour)

We show how to design an automated phase-analysis model based on a Convolutional Neural Networks (CNN). A framework for the efficient generation of simulated diffraction scans is developed, since real measured and labeled scans are hardly available. Using this synthetic database, a CNN is parameterized, trained and compared against the manual analysis. As a supportive approach, a denoising autoencoder is presented, to be used to eliminate background and other disturbing effects from the signal

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Session Classification: Plenary Talk

Track Classification: Main conference: Theory, simulation, modeling, computational crystallography