

Integrating structure solution by deep learning in Olex2

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PhAI [1], [2], [3] is a recently developed deep learning approach to solve the phase problem in crystallography. Being trained on a set of millions of artificial but physically sound structures, the neural net “learned” diffraction, becoming able to interpret even diffraction patterns with low completeness or resolution (i.e. data reaching only up to approximately 2 Å or having wedges missing). PhAI employs a convolutional, multilayer perceptron architecture and can interpret 3D but also 1D diffraction data.

In this contribution we will present our progress on implementing this approach as a pipeline solution into the popular structure solution, refinement and analysis program Olex2 [4], [5]. Furthermore, recent developments and improvements for electron and powder diffraction data will be addressed.

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