

Poster

Semi and self-supervised approaches to space group and Bravais lattice determination**W. Ratcliff^{1,2}, S. Lolla¹, I. Takeuchi^{1,2}, Aaron Kusne^{1,2}, Haotong Liang^{1,2}**¹*National Institute of Standards and Technology, Gaithersburg, Maryland, USA*²*University of Maryland, College Park, Maryland, USA**william.ratcliff@nist.gov*

During this talk, I will discuss our work [1] to use neural networks to automatically classify Bravais lattices and space-groups from neutron powder diffraction data. Our work classifies 14 Bravais lattices and 144 space groups. The novelty of our approach is to use semi-supervised and self-supervised learning to allow for training on data sets with unlabelled data as is common at user facilities. We achieve state of the art results with a semi-supervised approach. Our accuracy for our self-supervised training is comparable to that with a supervised approach.

[1] Satvik Lolla Et al, Journal of Applied Crystallography **55** (2022) <https://doi.org/10.1107/S1600576722006069>

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