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Semi-supervised approaches to determining space groups and Bravais Lattices

Monday 8 April 2024 11:30 (20 minutes)

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 unlabeled 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. *Support for Satvik Lolla was provided by the Center for High-Resolution Neutron Scattering, a partnership between the National Institute of Standards and Technology and the National Science Foundation under Agreement No. DMR-2010792

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