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Learning self-supervised representations of powder diffraction patterns

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Determining an unknown crystal structure from powder diffraction may be considered an ill-defined problem that requires experienced users to make strategic choices. Therefore, investigating the viability of the Machine Learning (ML) models for inferring structural information from powder-diffraction patterns is a highly coveted goal. Due to the limited availability of labeled experimental data, self-supervised representation learning pipelines are designed to evaluate the efficacy of using simulated diffraction patterns of known structures from crystallographic databases for training. Detailed simulation pipelines are developed that follow the evolution of constant-wavelength X-ray diffraction (XRD) while extensively modeling sample and instrumental effects. Several training and testing standards are introduced to ensure that the model learns representations obeying both invariances and equivariances attributable to instrumental and sample effects, respectively. The initial focus is to use these representations to make accurate predictions of the space group and lattice parameters of phase-pure XRD measurements. Subsequently, these representations shall be used as feature embeddings for training generative models, and they shall also be extended to accommodate neutron-diffraction measurements.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Instrumentation & Data Management