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Equivariant Generative Models: Atomic-Scale Representations from Diffraction Patterns

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Understanding a material inexorably requires from the determination of its atomic structure by means of neutron and x-rays based diffraction techniques. However, although artificial intelligence has shown valuable help in property-prediction lately [1], previous machine learning characterizations of diffraction patterns often yield vague insights. This work introduces a groundbreaking framework built upon denoising probabilistic diffusion models, such as those in which ChatGPT or DALL-E are based [2, 3], offering a transformative approach to extracting realistic atomistic snapshots of materials directly from their diffractograms.

The proposed framework would transcend the limitations of conventional methods by not only discerning atomic species but also precisely determining their positions within the material. Remarkably, it would extend its capability to identify potential secondary phases present in the material, leveraging the rich structural information embedded in diffractograms.

To enhance the performance of the model, our approach allows the incorporation of a priori knowledge about the expected presence or absence of specific atoms. This feature is particularly beneficial when a high level of certainty exists regarding chemical composition.

In our ongoing research, we are applying this innovative methodology to the emerging class of chalcohalide-based solar cell absorbers, to which our experimental group is devoted. The wealth of x-ray diffraction patterns available for these materials serves as a robust testing ground. The results obtained thus far underscore the potential of our framework to provide unprecedented clarity on the atomic-scale structure of complex materials.

[1] C. López, A. Emperador, E. Saucedo, et al. Universal ion-transport descriptors and classes of inorganic solid-state electrolytes, Materials Horizons, 2023.
[2] OpenAI (2023) ChatGPT
[3] OpenAI (2023) DALL-E

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