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xtal2png: A Python package for representing crystal structure as PNG files

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Summary

The latest advances in machine learning are often in natural language processing such as with long short-term memory networks (LSTMs) and Transformers, or image processing such as with generative adversarial networks (GANs), variational autoencoders (VAEs), and guided diffusion models. `xtal2png` encodes and decodes crystal structures via PNG images (see e.g. Figure 1) by writing and reading the necessary information for crystal reconstruction (unit cell, atomic elements, atomic coordinates) as a square matrix of numbers. This is akin to making/reading a QR code for crystal structures, where the `xtal2png` representation is an invertible representation. The ability to feed these images directly into image-based pipelines allows you, as a materials informatics practitioner, to get streamlined results for new state-of-the-art image-based machine learning models applied to crystal structures.

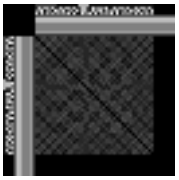

Figure 1: A real size 64×64 pixel `xtal2png` representation of a crystal structure.

Statement of need

Using a state-of-the-art method in a separate domain with a custom data representation is often an expensive and drawn-out process. For example, (Vaswani et al., 2017) introduced the revolutionary natural language processing Transformer architecture in June 2017, yet the application of Transformers to the adjacent domain of materials informatics (chemical-formula-based predictions) was not publicly realized until late 2019 (Goodall & Lee, 2019), approximately two-and-a-half years later, with peer-reviewed publications dating to late 2020 (Goodall & Lee, 2020). Interestingly, a nearly identical implementation was being developed concurrently in a different research group with slightly later public release (A. Wang et al., 2020) and publication (A. Y.-T. Wang et al., 2021) dates. Another example of a state-of-the-art algorithm domain transfer is refactoring image-processing models for crystal structure applications, which was first introduced in a preprint (Kipf & Welling, 2016) and published with application for materials' property prediction in a peer-reviewed journal over a year later (Xie

& Grossman, 2018). Similarly, VAEs were introduced in 2013 (Kingma & Welling, 2014) and implemented for molecules in 2016 (Gómez-Bombarelli et al., 2016), and denoising diffusion probabilistic models (DDPMs) were introduced in 2015 (Sohl-Dickstein et al., 2015) and implemented for crystal structures in 2021 (Xie et al., 2021). Here, we focus on state-of-the-art domain transfer (especially of generative models) from image processing to crystal structure to enable materials science practitioners to leverage the most advanced image processing models for materials' property prediction and inverse design.

`xtal2png` is a Python package that allows you to convert between a crystal structure and a PNG image for direct use with image-based machine learning models. Let's take Google's image-to-image diffusion model, Palette (**saharia**), which supports unconditional image generation, conditional inpainting, and conditional image restoration, which are modeling tasks that can be used in crystal generation, structure prediction, and structure relaxation, respectively. Rather than dig into the code and spending hours, days, or weeks modifying, debugging, and playing GitHub phone tag with the developers before you can (maybe) get preliminary results, `xtal2png` lets you get comparable results using the default parameters, assuming the instructions can be run without error. While there are other invertible representations for crystal structures (Ren et al., 2022; Xie et al., 2022) as well as cross-domain conversions such as converting between molecules and strings (Krenn et al., 2022; Weininger, 1988), to our knowledge, this is the first package that enables conversion between a crystal structure and an image file format.

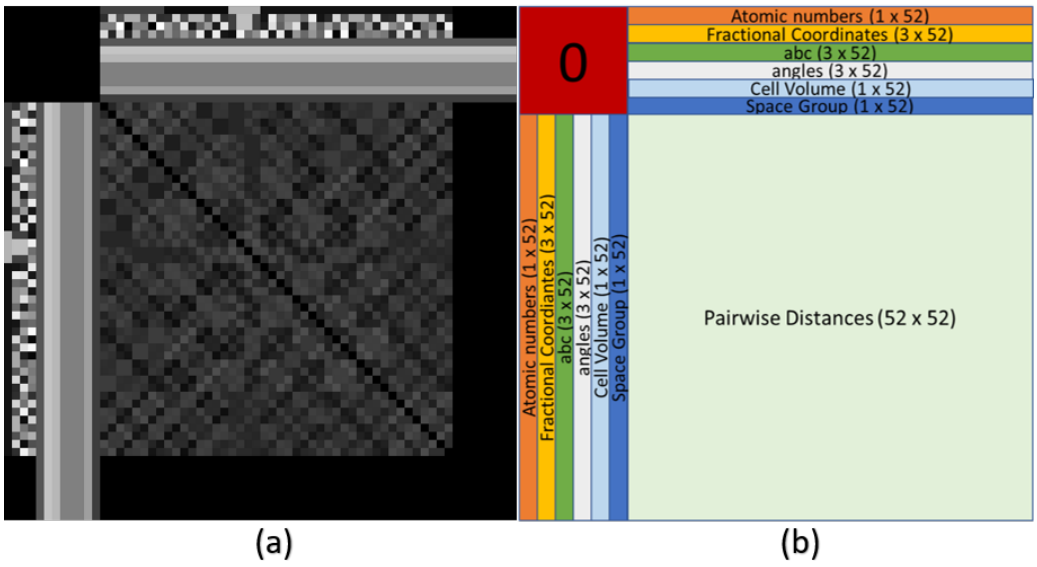

Figure 2: (a) upscaled example image and (b) legend of the `xtal2png` encoding.

`xtal2png` was designed to be easy to use by both "Pythonistas" and entry-level coders alike. `xtal2png` provides a straightforward Python application programming interface (API) and command-line interface (CLI). `xtal2png` relies on `pymatgen.core.structure.Structure` (Ong et al., 2013) objects for representing crystal structures and also supports reading crystallographic information files (CIFs) from directories. `xtal2png` encodes crystallographic information related to the unit cell, crystallographic symmetry, and atomic elements and coordinates which are each scaled individually according to the information type. An upscaled version of the PNG image and a legend of the representation are given in Figure 2. Due to the encoding of numerical values as PNG images (allowable values are integers between 0 and 255), a round-off error is present during a single round of encoding and decoding. An example comparing an original vs. decoded structure is given in Figure 3.

There are some limitations and design considerations for `xtal2png` that are described in `xtal2png`'s documentation in the Overview section. At this time, it is unclear to what extent deviation from the aforementioned design choices will affect performance. We intend to use hyperparameter optimization to determine an optimal configuration for crystal structure generation tasks using the `xtal2png` representation.

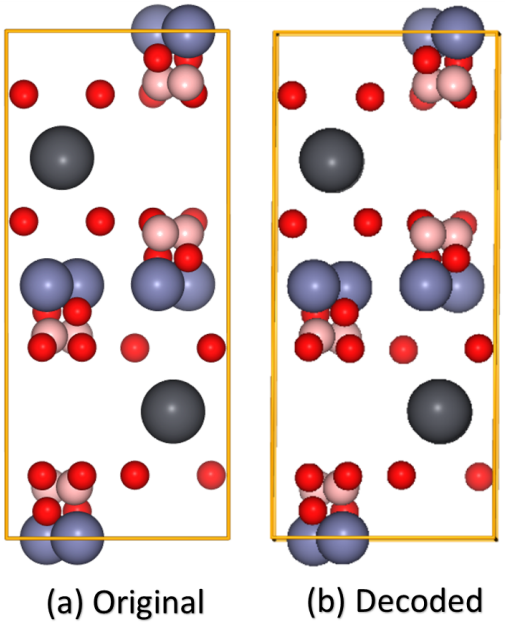

Figure 3: (a) Original and (b) `xtal2png` decoded visualizations of `mp-560471` / $Zn_2B_2PbO_6$. Images were generated using ase visualizations.

The significance of the representation lies in being able to directly use the PNG representation with image-based models which often do not directly support custom dataset types. We expect the use of `xtal2png` as a screening tool for such models to save significant user time of code refactoring and adaptation during the process of obtaining preliminary results on a newly released model. After obtaining preliminary results, you get to decide whether it's worth it to you to take on the higher-cost/higher-expertise task of modifying the codebase and using a more customized approach. Or you can stick with the results of xtal2png. It's up to you!

We plan to apply `xtal2png` to a probabilistic diffusion generative model as a proof of concept and present our findings in the near future.

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