Pre-Trained Large Language Model for Crystal Structures

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Machine learning has demonstrated its ability as a tool to filter through millions of possible crystal structures and discover new stable crystal structures [1]. Transformer based models have risen in popularity in natural language processing (NLP) due to its ability capture the correlation between words through the attention mechanism [2]. Recognizing correlations between atoms is crucial to determining the structure's properties. Advancements in graph-based neural networks have shown promised with high accuracy in predicting material properties [3, 4]. However, graph-based neural networks are not ideal in capturing long range interactions for its reliance on a cut-off radius or increased number of layers to accommodate long range interactions. In this work, introduce a transformer-based neural network model for representing crystalline materials and explore its ability to capture atomic-interactions through unsupervised pre-training on a large dataset of various materials. We examine the model's capability by fine-tuning the model on material property prediction task. Our model can be generalized to any property prediction task through fine-tuning, paving way for a more computationally efficient architecture for material predictions.

References:

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