(5) ポスター発表

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# XenonPy：材料設計を加速する機械学習プラットフォーム

## XenonPy: a machine learning platform for accelerating materials design

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### 1. Introduction

There has been a growing need for using machine learning (ML) to derive ultrafast prediction models on materials properties. In recent years, various kinds of machine learning (ML) algorithms have been applied to material science and achieved lots of outstanding successes. However, introduce these methods into a new project often to be hard works. Firstly, almost all of these ML methods are in general-purpose, and their developers are not professional software engineers. When using these packages, you have to customize them for your using case and face lots of bugs. Additionally, in most cases, these packages are just built for paper submission, which means they will never be maintained after the paper publication. We realize that these instabilities will be the considerable risks for the ML applications in industry and further researches. To facilitate these problems fundamentally, we decided to build new software that focuses on material informatics using yet keep it user-friendly.

### 2. XenonPy

XenonPy is a Python open-source platform for materials informatics. It provides an easy-to-use and extensible platform that allows users to build tailored workflows of machine learning in various tasks of designing materials, including high-throughput screening across extensive virtual libraries of candidate materials. A common workflow consists of two steps; the first step is to train a machine learning model that predicts forwardly properties of input materials with high level of accuracy. The second step is solving the inverse mapping of the forward model. After step 2, a diverse set of highly probable materials exhibiting arbitrary given desired properties are computationally explored. In this presentation, we focus on a set of modules related to transfer learning, which has been shown to have great potential to overcome the problem of limited amounts of materials data (Yamada & Liu et al. ACS Cent Sci. 2019). XenonPy currently provides 140,000 pre-trained neural networks for the prediction of various properties of small organic molecules, polymers, and inorganic crystalline materials. Along with this pre-trained model library, we demonstrate outstanding successes of transfer learning in various tasks of predicting materials properties with exceedingly small data.

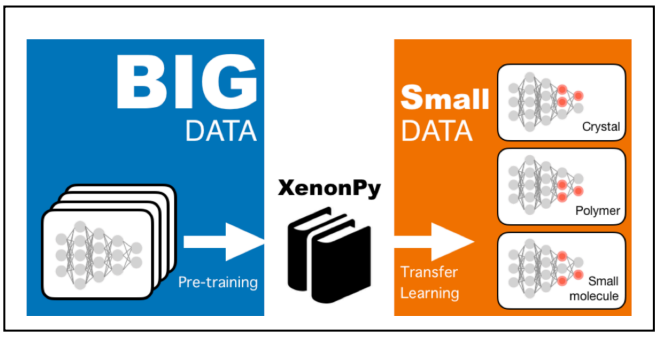


Fig. 1 Along with the XenonPy.MDL model library, we describe the great potential of transfer learning to break the barrier of limited amounts of data in materials property prediction using machine learning.

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**[関連プロジェクト]**
(情報統合型物質・材料研究イニシアティブ>物質・材料記述基盤グループ

**[参考文献]**

[1] Yamada, H., Liu, C., Wu, S., Koyama, Y., Ju, S., Shiomi, J., & Yoshida, R. (2019). ACS Central Science, acscentsci.9b00804.
[2] Wu, S., Lambard, G., Liu, C., Yamada, H., & Yoshida, R. (2019). Molecular Informatics, 1900107, minf.201900107.

**[関連 WEB]**(最大 2 本)

[1] https://xenonpy.readthedocs.io/en/stable/
[2] https://github.com/yoshida-lab/XenonPy