
pumml Documentation

Release 0.0.1

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Positive and Unlabeled Materials Machine Learning (pumml) is a code that uses semi-supervised positive and unlabeled (PU) machine learning to classify materials when data is incomplete and only examples of “positive” materials are available.

CHAPTER 1

Citing pumml

If you use pumml in your research, please cite the following work:

Nathan C. Frey, Jin Wang, Gabriel Iván Vega Bellido, Babak Anasori, Yury Gogotsi, and Vivek B. Shenoy.
Prediction of Synthesis of 2D Metal Carbides and Nitrides (MXenes) and Their Precursors with Positive and Unlabeled Machine Learning. ACS Nano 2019 13 (3), 3031-3041.

DOI: 10.1021/acsnano.8b08014 <https://pubs.acs.org/doi/abs/10.1021/acsnano.8b08014>

CHAPTER 2

Features

- Predict a “synthesizability score” between 0 and 1 for theoretical materials.
- Consider interactions between parent layered phases and child 2D phases.
- Easily inspect model outputs and performance.

CHAPTER 3

Contribute

- Issue Tracker: github.com/ncfrey/pumml/issues
- Source Code: github.com/ncfrey/pumml

CHAPTER 4

Support

If you are having issues, please let us know through [github](#).

CHAPTER 5

License

The project is licensed under the MIT license.

6.1 Project Modules

This page contains the list of project's modules

`pumml.learners`

6.1.1 pumml.learners

CHAPTER 7

Indices and tables

- `genindex`
- `modindex`
- `search`