pumml Documentation

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Contents

1 Citing pumml **3**

2 Features **5**

3 Contribute **7**

4 Support **9**

5 License **11**

6 Contents **13**

6.1 Project Modules 13

7 Indices and tables **15**

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.

CHAPTER 6

Contents

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