Tools

- Fully automatic calculation system of electronic structure by First-principles
- nap (Nagoya Atomistic-simulation Package)
- Compound Prediction App
- Specific Heat Prediction App
- API Tools

LINK

- MateriApps
- Toki no Mori Wiki - Machine learning (Japanese only)

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Specific Heat Prediction App

Overview

In this web application, specific heat capacity is predicted by selecting chemical formula. Maximum temperature is also selectable and the minimum temperature is fixed at 10K. This prediction is based on machine learning and Neumann-Kopp rule which used collected data from literatures. Related information to specific heat capacity is also provided.

How to Use

- Anyone can use it by "Specific Heat Prediction App".