



Database API

Tools

Cluster system

Cloud system

Usage guide

Reference

## 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)

[Home](#) > [Tools](#) > Fully automatic calculation system of electronic structure by First-principles


## Fully automatic calculation system of electronic structure by First-principles

## Overview

- A tool of automated first-principles electronic structures calculations for high-throughput computational screening of materials;
- A tool to generate data contents of CompES-X database;
- Python language used as runtime environment.

## Framework

Template Oriented Atomic Simulation Toolkit (TOAST) is a python-based automated framework for high-throughput electronic structure calculations.

TOAST supports three first-principles (FP) electronic structure calculation packages. The unified setup of computational environment, job manager, calculation parameters and workflows are predefined in several template files. TOAST implements a customized Python library for the conversion of CIF file to input files of FP calculations, the generation of job script, the job launching and the data parsing and post-processing.

## Requirements of runtime environment

- Linux OS system;
- Python 3.x or 2.x, numpy 1.x;
- FP electronic structures calculations packages: VASP (5.3.5 and 5.4.1), Quantum Espresso (6.0) and ABINIT (8.0.8b) Gniplot for band structure, density of states and Brillouin zone visualization;
- Jmol, VESTA, or Xcrysden for structure, charge density, Brillouin zone and Fermi surface visualization;
- Support PBS Pro/Torque, and GridEngine job scheduling systems

## Download

for Python 3.x

- TOAST: Template Oriented Atomic Simulation Toolkit : [toast-0.6.0.tar.gz](#)
- [toast-0.6.0 usage manual \(PDF\)](#)

for Python 2.x

- TOAST: Template Oriented Atomic Simulation Toolkit : [toast-0.5.4.tar.gz](#)
- [toast-0.5.4 usage manual \(PDF\)](#)

## Licence

This software is released under the MIT License, see [LICENSE.txt](#).