Template Oriented Atomic Simulation Toolkit (TOAST): A python-based automatic framework for high-throughput electronic structure calculations

Data Platform Group

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Mi²i

Template Oriented Atomic Simulation Toolkit

Introduction

Aim of TOAST:

- A tool to generate data contents of CompES-X database;
- A tool of automated first-principles electronic structures calculations for high-throughput computational screening of materials;
- A tool of MI²I data platform;
- Python language used as runtime environment.

Framework of TOAST

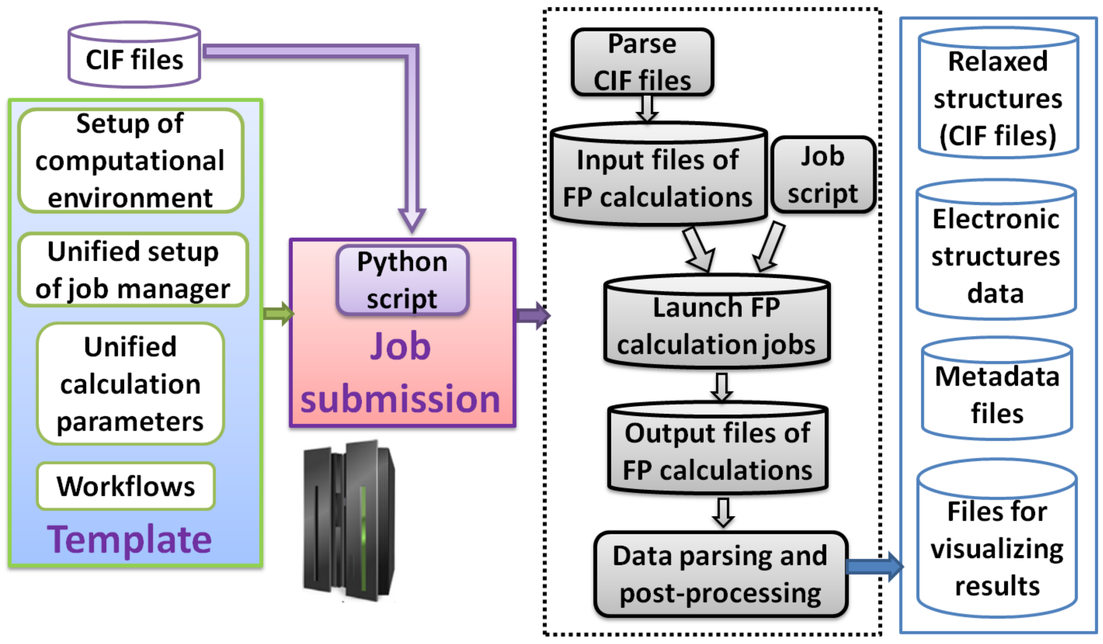

Figure 1. Framework of TOAST. It supports three first-principles (FP) electronic structure calculations packages. The unified setup of computational environment, job manager, calculation parameters and workflows are predefined in several template files. A customized Python library implements the conversion of CIF file to input files of FP calculations, the generation of job script, the job launching and the data parsing and post-processing.

Overview of TOAST

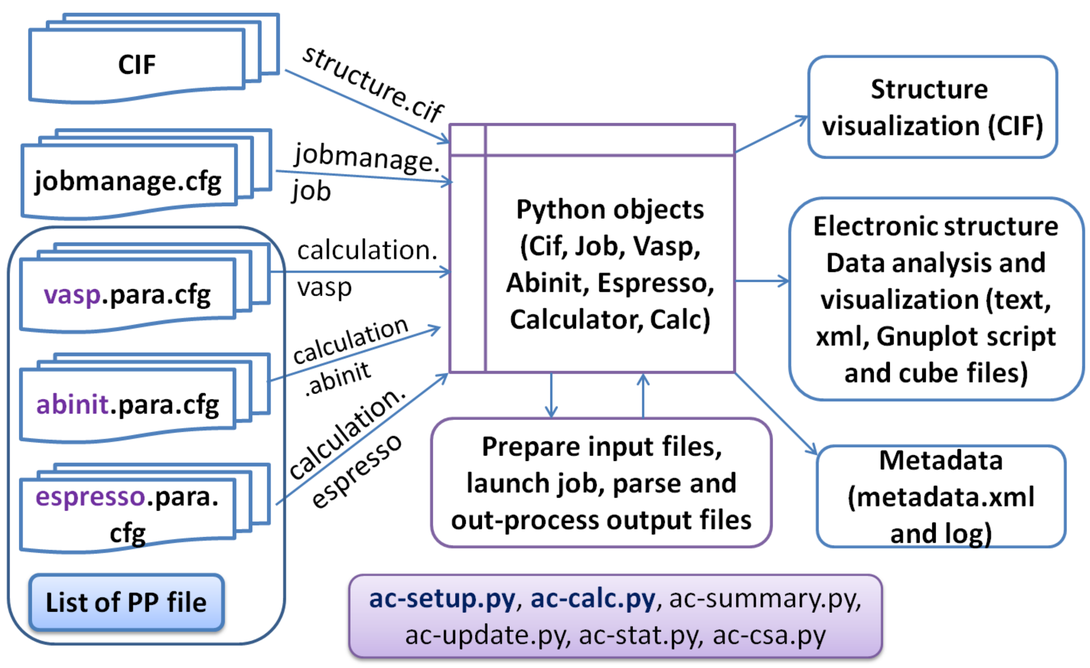

Figure 2. Overview of TOAST. The python script files: **ac-setup.py** and **ac-calc.py** for job submission of the calculations of many and single compound(s), respectively.

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Calculations workflows in TOAST

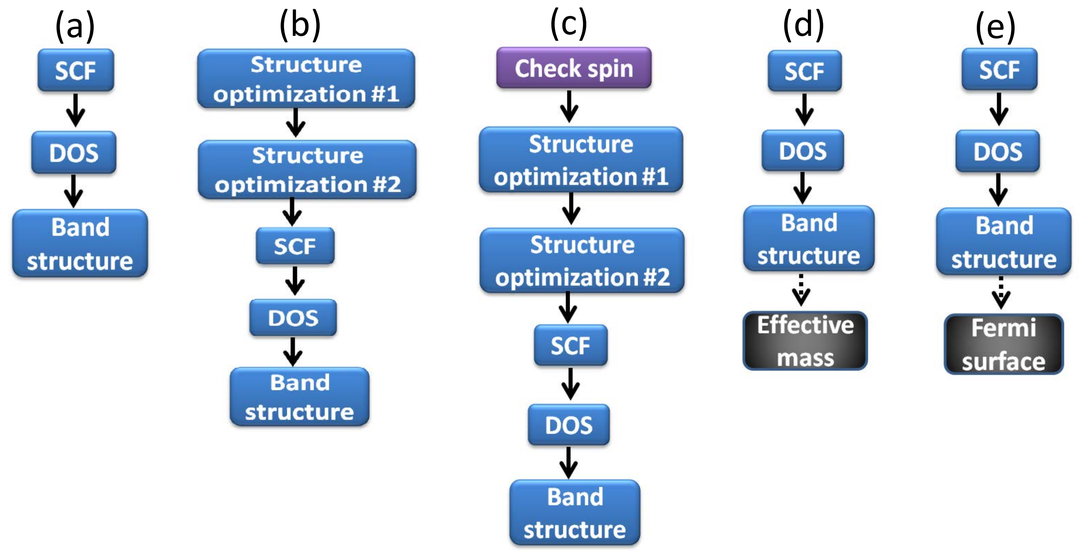

Figure 3. Examples of predefined workflows of FP calculations in TOAST. In the self-consistent field (SCF) calculation, the total energy and charge density will be obtained.

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)**
- **Gnuplot** 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

Application example of TOAST

- Generate electronic structure data for CompES-X database.
- High-throughput calculations of ternary borides to search superhard ultra-incompressible materials.

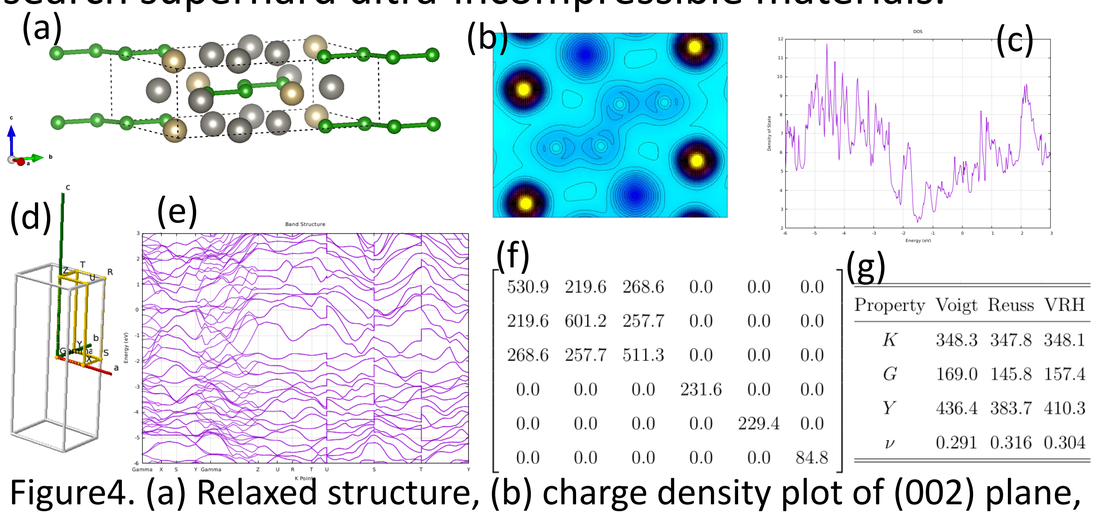

Figure4. (a) Relaxed structure, (b) charge density plot of (002) plane, (c) total density of states, (d) Brillouin zone, (e) band structure, (f) elastic constants (C_{ij} in GPa) and (g) bulk modulus *K*, shear modulus *G*, Young's modulus *Y* and isotropic Poisson ratio *v* of OsW_2B_2.