

Mi²i Data Infrastructure

Data Platform Group

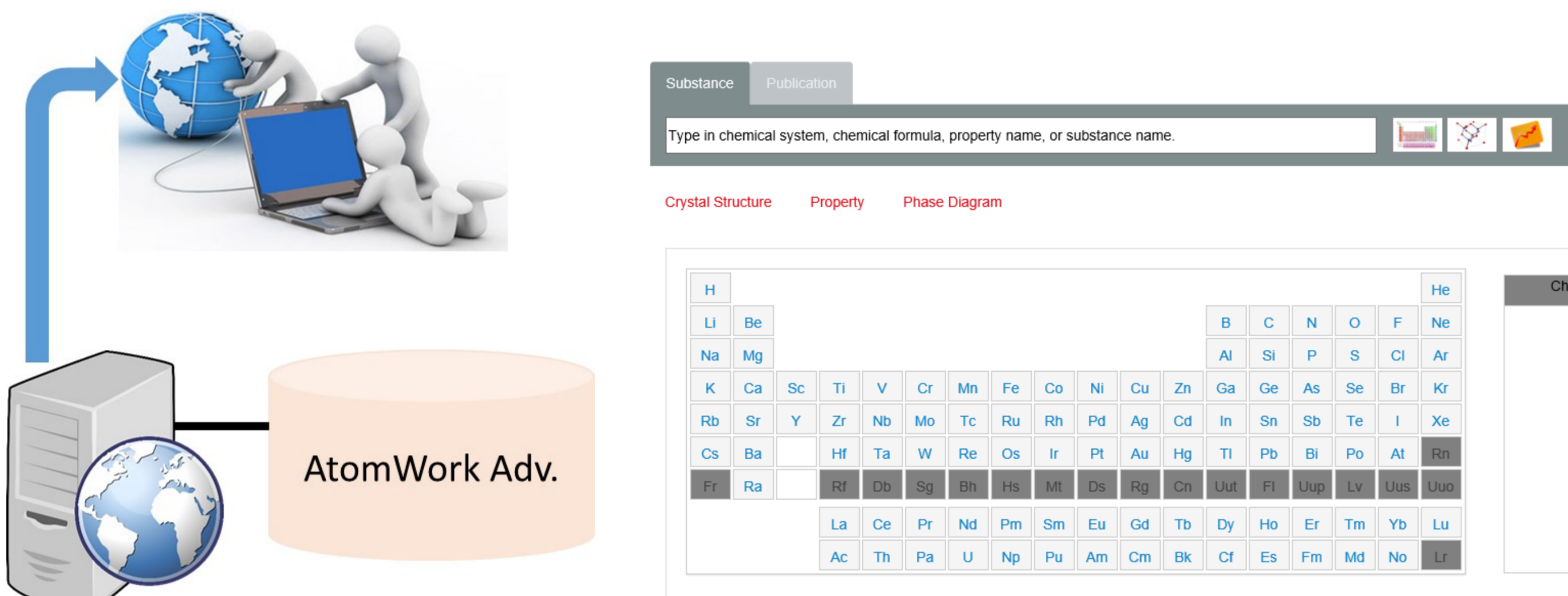
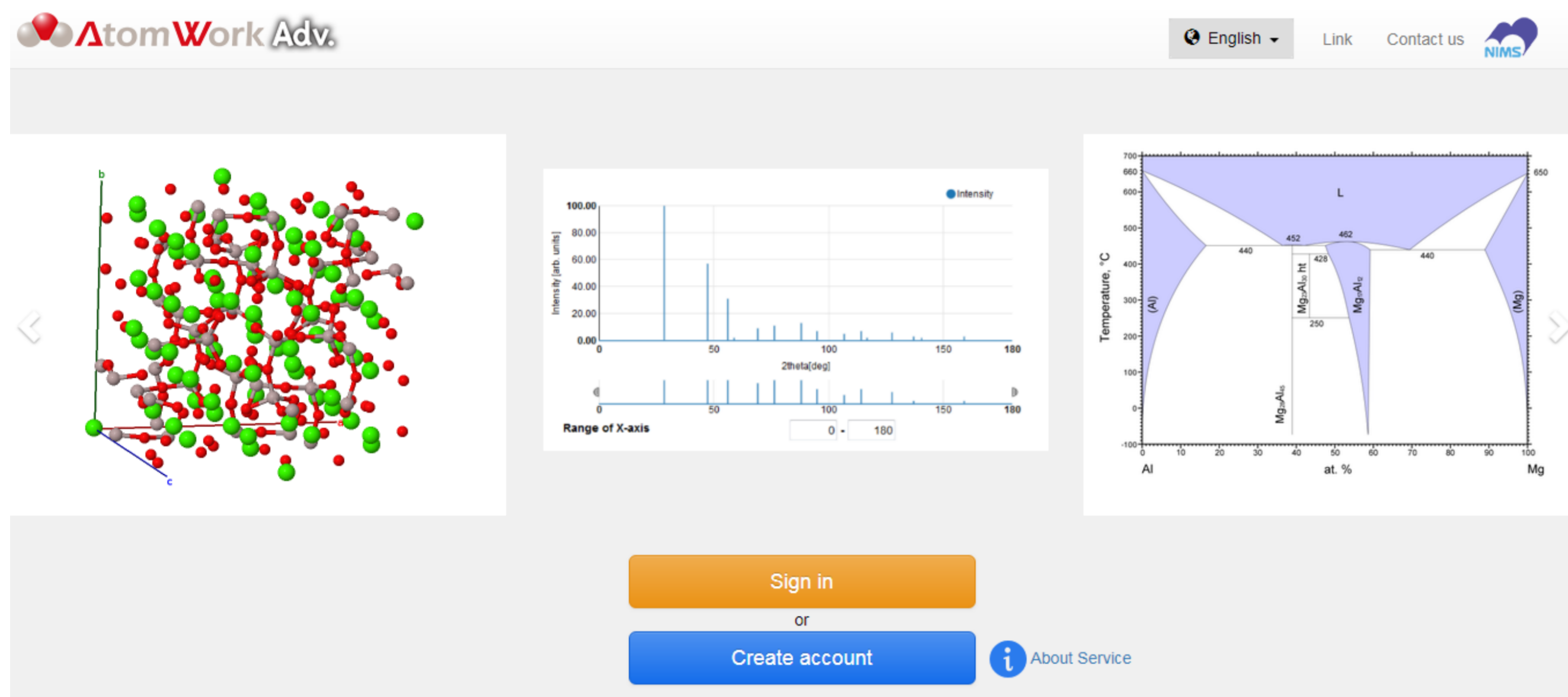
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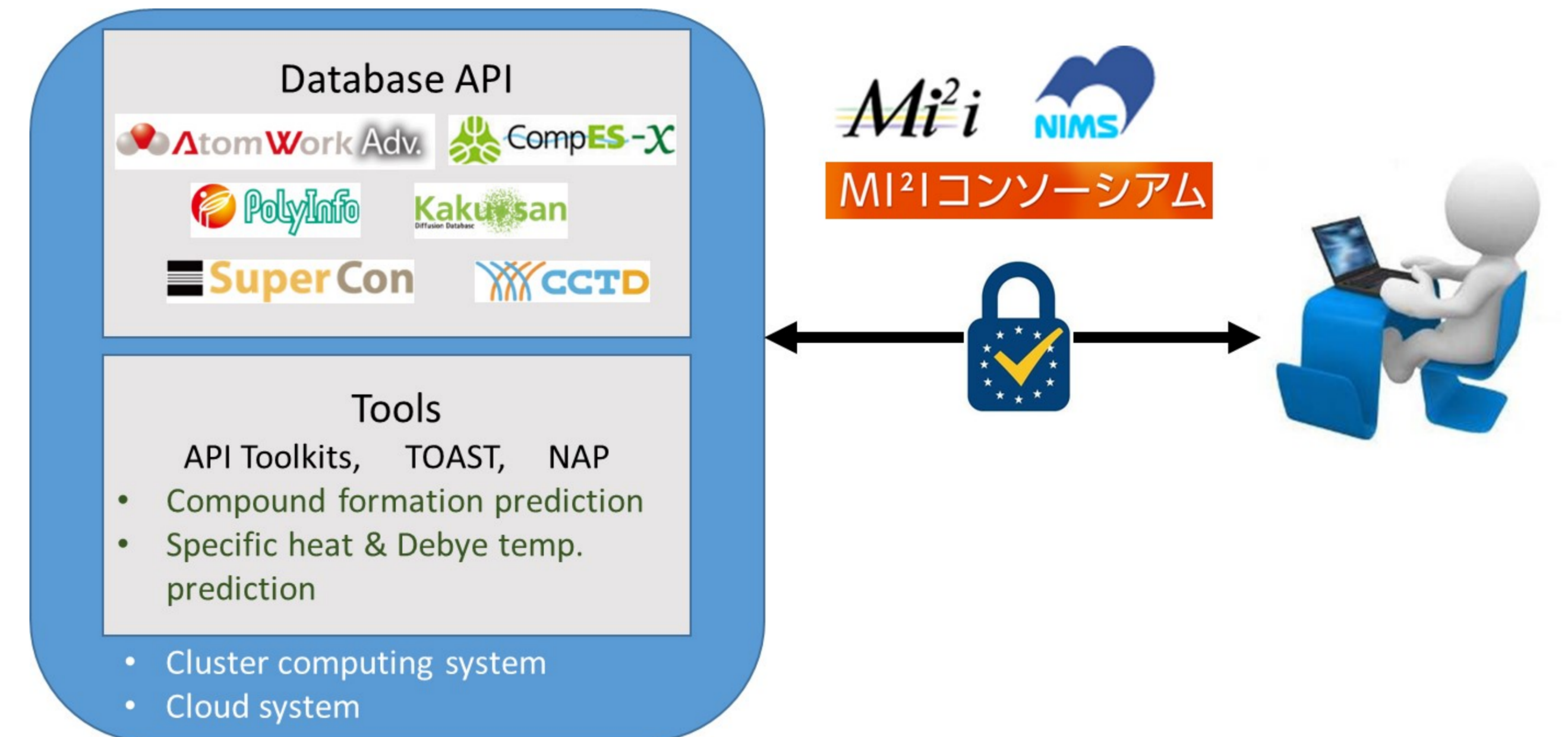
Inorganic Materials Database AtomWork-adv.

The world largest scale database for inorganic materials. At present, 318,837 crystals, 43,497 phase diagrams and 390,263 properties are available.

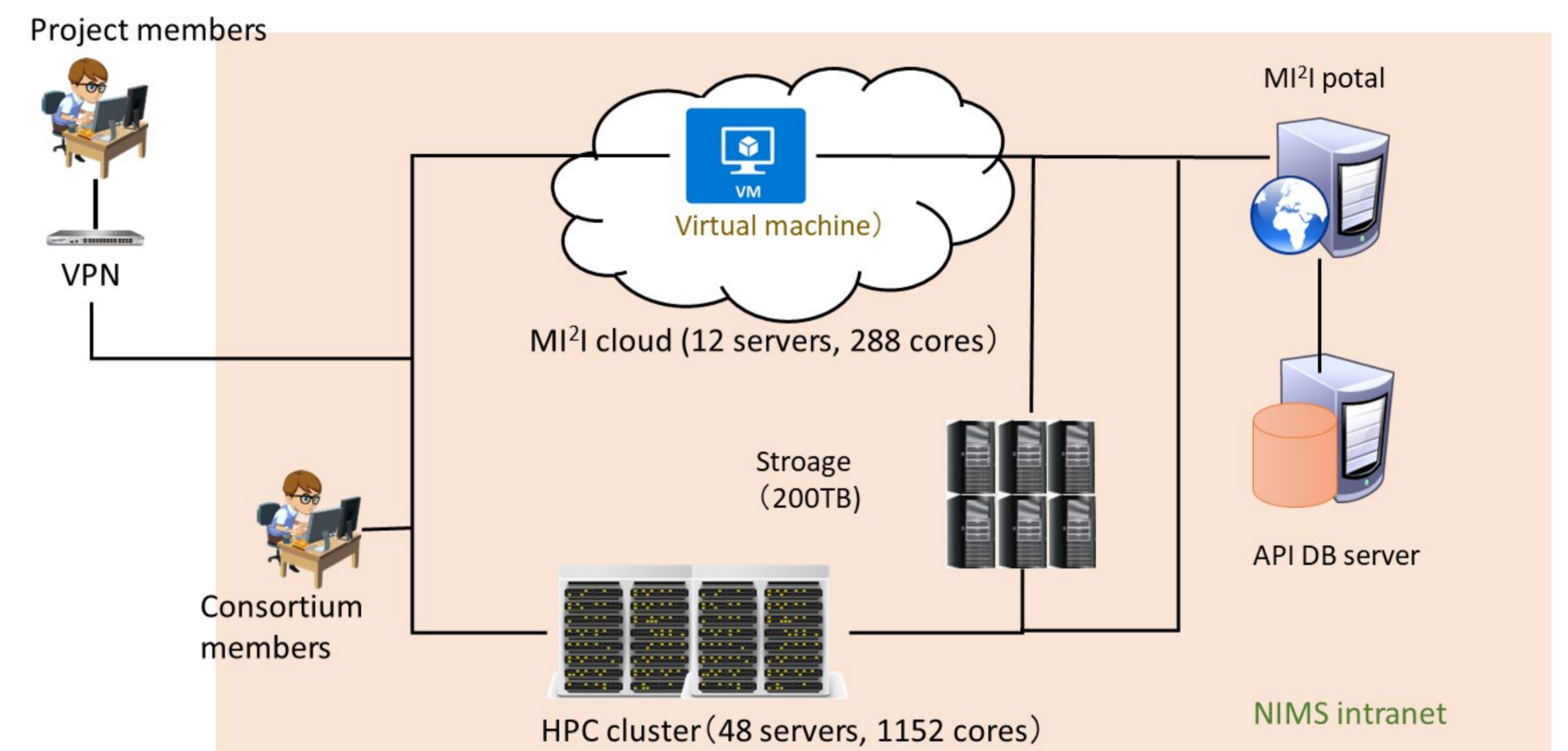


Mi²i Data Platform

API service of MatNavi and AtomWork-Adv. data

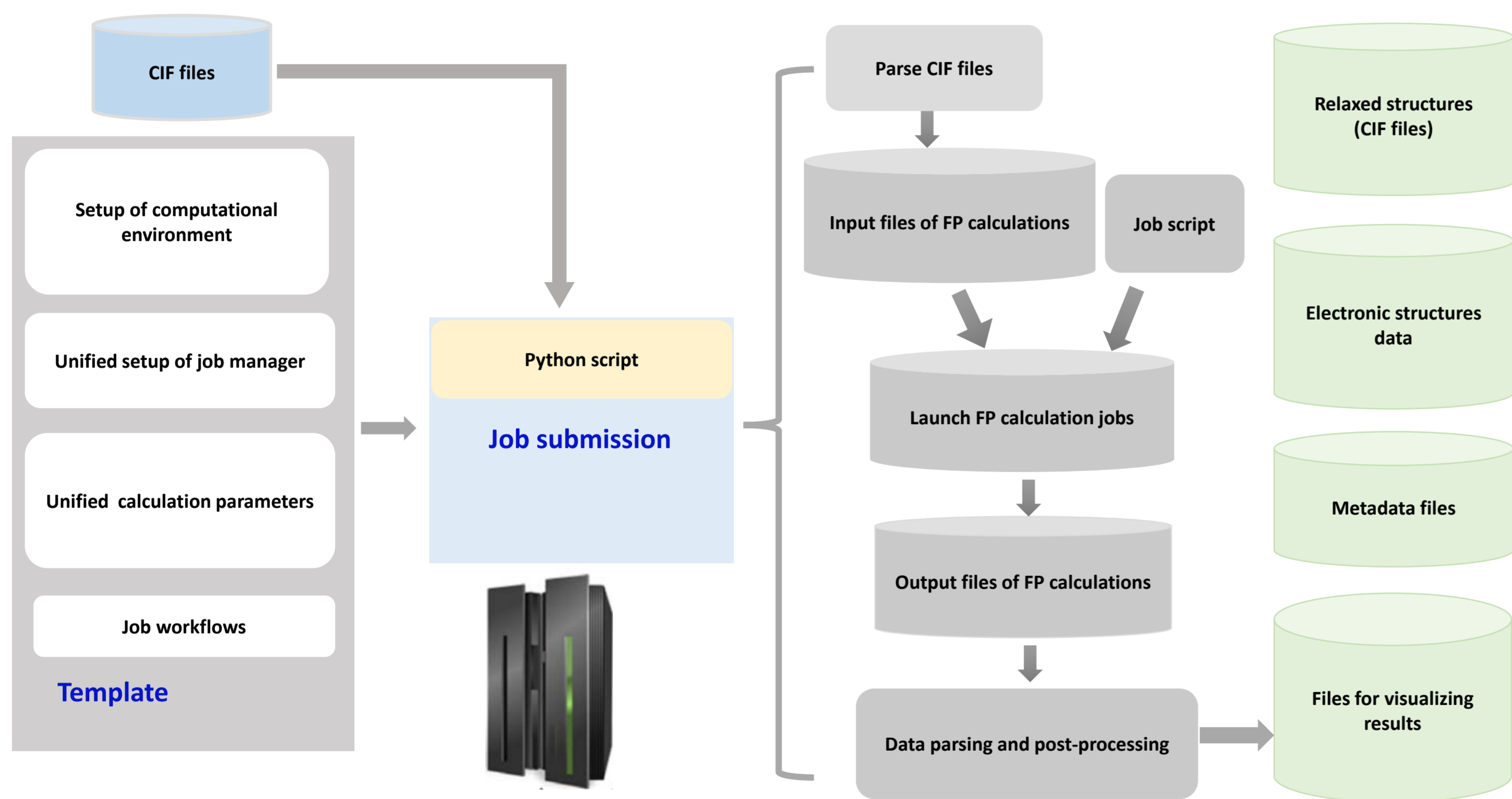


Computational platform of HPC cluster and cloud

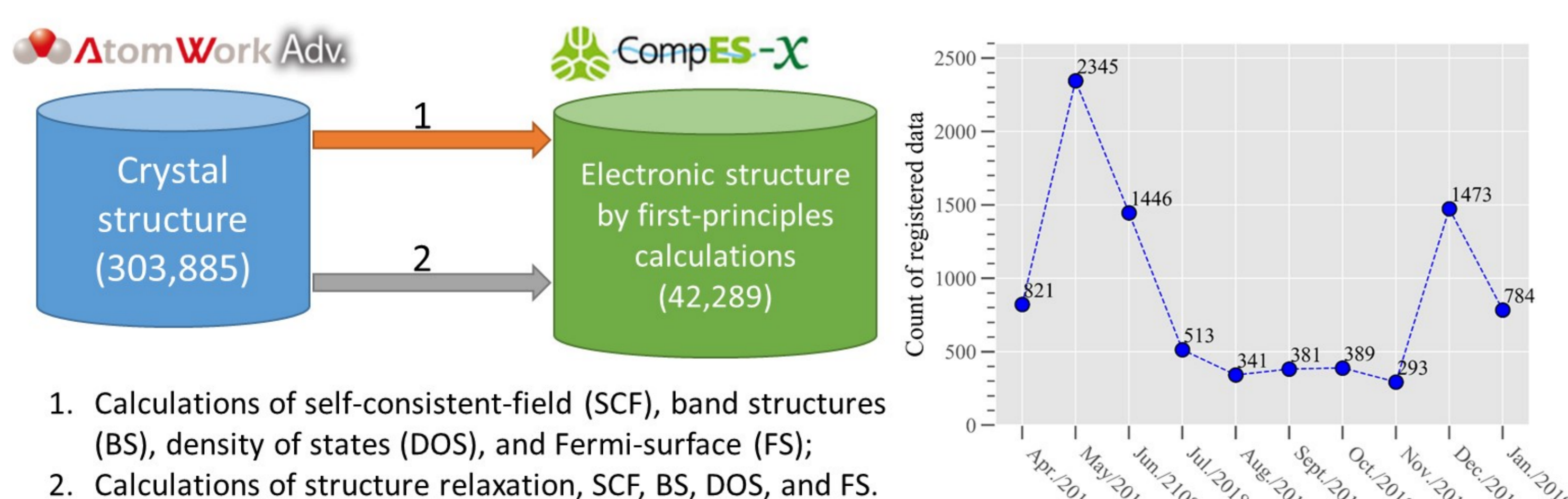


Data Applications

Framework of Template Oriented Atomic Simulation Toolkit (TOAST)



Electronic Structure Data Generation



1. Calculations of self-consistent-field (SCF), band structures (BS), density of states (DOS), and Fermi-surface (FS);
2. Calculations of structure relaxation, SCF, BS, DOS, and FS.

Mi²i Portal Site

<https://mi2i.nims.go.jp/>

Structure of portal site :

- Page for the public**
 - Outline of services
 - Download of tool
 - Usage guide
- Page for specified users (Only accessible from NIMS LAN and MI²i-DPF)**
 - Details of services
 - Download of usage manual
 - Download of API manual & sample codes
- Page for DPF users (User authentication needed)**
 - Changing password
 - Display of API token
 - Display of API call count

Specific Heat Prediction Tool. Predict specific heat and Debye temperature by Neumann-Kopp's law and machine learning based on experts evaluated data.

