Inorganic Material Database “AtomWork-Adv”

Data Platform Group

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Outline

Inorganic Material Database

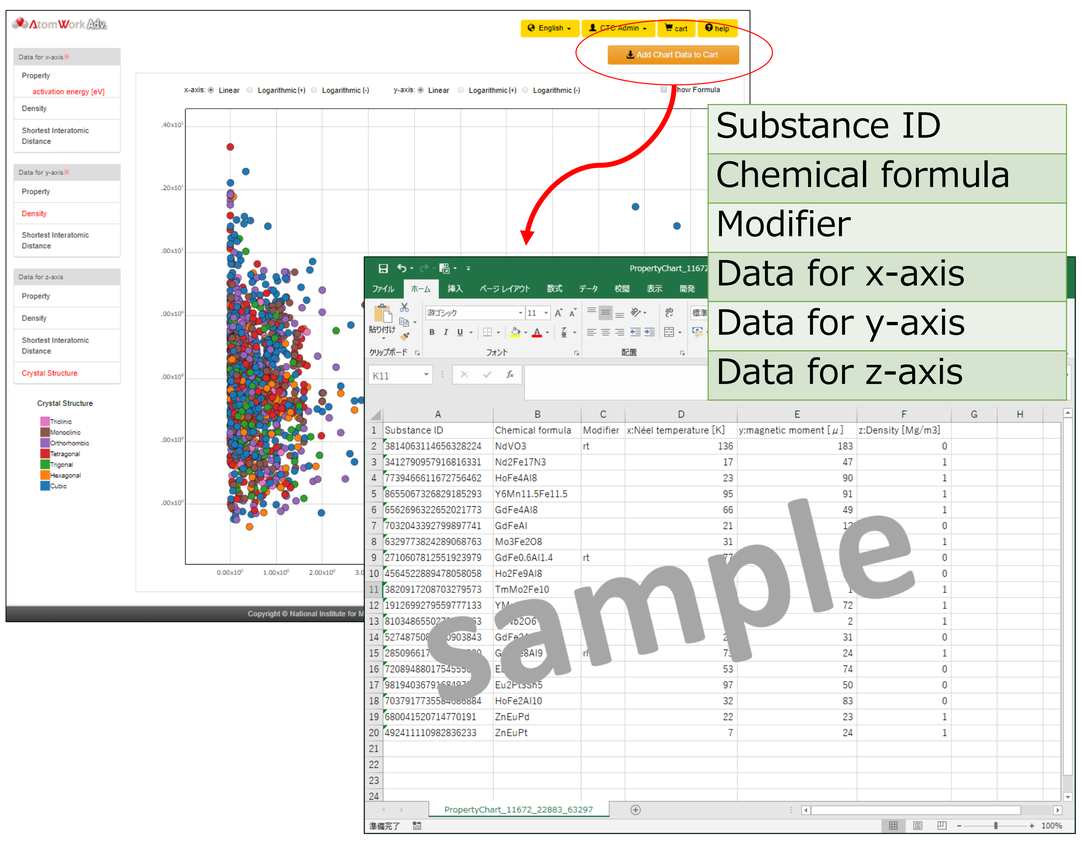
AtomWork Adv.

This database offers crystal structure, X-ray diffraction, material properties and phase diagrams extracted from approx. 1,000 of science and technology journals.

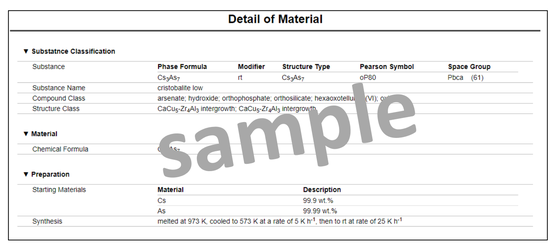
Contents	Data	Crystalline structures: 318,837 X-ray diffractions: 577,449 Properties: 390,263 Type of properties: 480 Phase diagrams: 43,498 As of Sep. 2019. To be upgraded and expanded.
	Tools	Search functions Material matrix Property chart
How to use	Website access	
Contact type	**Free trial use** **(72 hours, browsing only.)** Fixed annual rate (Academic discounts available.)	

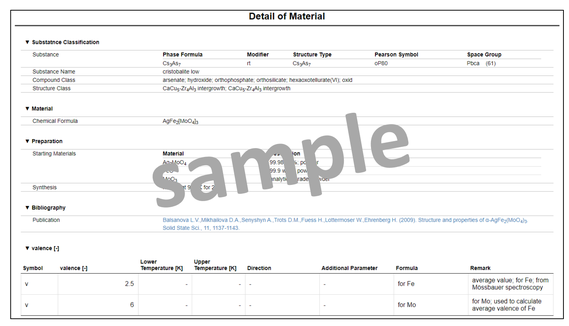
New features (planned)

1. Download the data list displayed by "Property Chart“



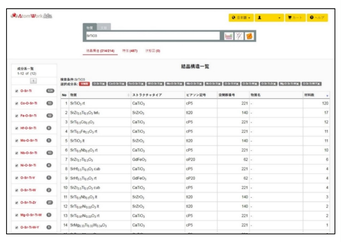
2. Added display items on the detail page

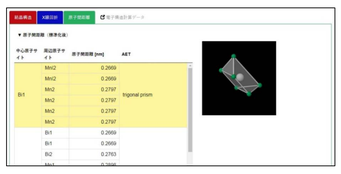


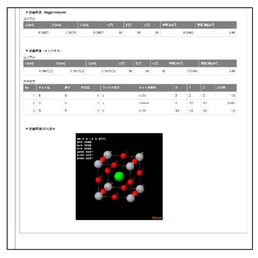


Data details

Crystalline Structure

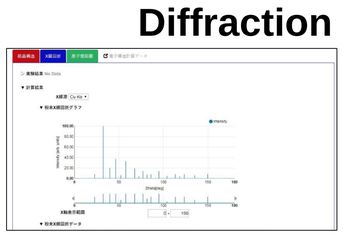






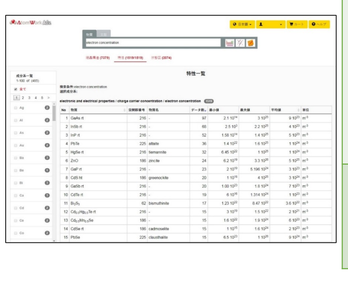
Substance information	Substance name and chemical composition, structure type, Pearson symbol, space group name and number
Sample information	Raw material, synthesis process
Cell parameters determination	Sample condition, experiment method, temperature
Cell parameters determination	Sample condition, experiment method, spectrum
Cell structure information (Standardized)	Lattice constant, atomic configuration
Other information	Interatomic distance, literature

X-ray Diffraction



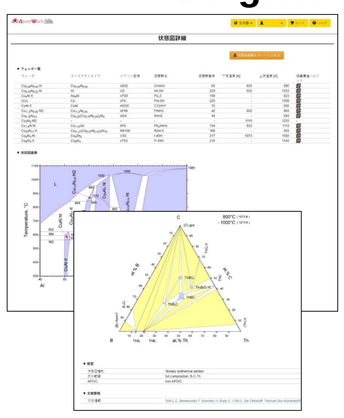
X-ray diffraction graph with specified X-ray source	x axis: 2θ, y axis: intensity
X-ray diffraction data (Tabular form)	2θ, Miller index, diffraction intensity, lattice spacing

Properties



Substance information	Substance name, chemical composition, structure type, space group name, space group No., link to crystal structure
Property data	Property values, temperature, literature

Phase Diagram



Summary	Type of phase diagram, composition range, temperature range, generation method
Phase information	Phases, structure type, Pearson symbol, space group name, space group number, maximum and minimum temperature, link to crystal structure data
Other information	Literature

User support: atomwork-adv@ml.nims.go.jp
Website : https://atomwork-adv.nims.go.jp