

AtomWork Adv.

Inorganic Material Database

<https://atomwork-adv.nims.go.jp>



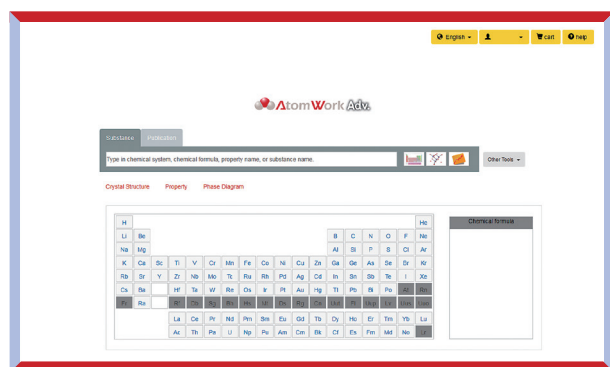
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National Institute for Materials Science

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: 409,723 X-ray diffractions: 746,888 Properties: 568,195 Type of properties: 512 Phase diagrams: 49,650 As of April 2026. To be upgraded and expanded further.
	Tools	Search functions Material matrix Property chart
How to use	Website access	
Contract type	Free trial use (Up to 72 hours, browsing only. Limited number of page views.) Fixed annual rate (Academic discounts available.)	

Search Function

Searchable by specifying chemical components, chemical formula, substance name, prototype, Pearson symbol, space group number, property name and various other methods.



Crystalline Structure 409,723

The detailed information in Table 1 is displayed along with the 3D image visually observable from any angle. Download data: CIF (Crystallographic Information File)

Table 1 Detailed Information (Crystal structure)

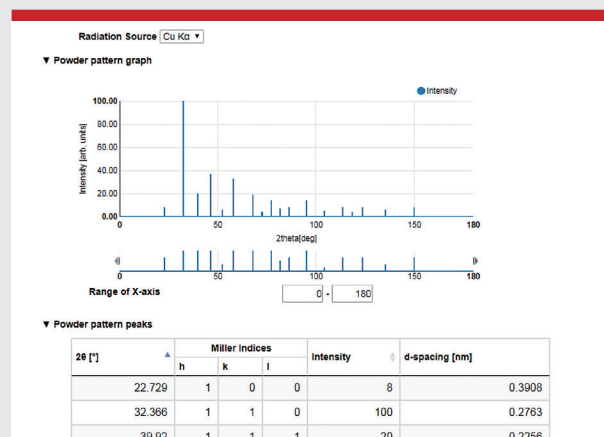
Substance information	Substance name and chemical composition, structure type, Pearson symbol, space group name and number
Sample information	Raw material, synthesis process
Structure determination	Sample condition, experiment method, temperature
Cell parameters determination	Sample condition, experiment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

X-ray Diffraction 746,888

Graphs and information related to the experimental and calculated data appear. On the graph, display range is changeable. In the table, entries are sortable.

Table 2 Detailed information (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

568,195

7 property categories are available: electronic and electrical, magnetic, mechanical, optical, phase transmission, super conductivity, thermal and thermodynamic. Properties can be searched by respective property names. In addition to the searched property values, detailed information of each substance is obtainable. Download data: TSV file contains the substance's properties.

Table 3 Detailed information (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

The screenshot displays the 'Property of Materials (electron concentration [m⁻³])' interface. It features a table with columns for 'No. System', 'electron concentration [m⁻³]', 'Lower Temperature [K]', 'Upper Temperature [K]', 'Name', and 'Publication'. Below the table, there are sections for 'Property of Substances' and 'List of Phase Diagrams'.

Phase Diagram

49,650

The image of phase diagram appears along with the list of phases and related information. Download data: graphics data (PNG file), list of phases (TSV file), summary and literature information (TSV file)

Table 4 Detailed information (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

The screenshot displays the 'List of Phase Diagrams' interface. It features a table with columns for 'No. Phase Diagram', 'Chemical System', 'Lower Temperature [K]', 'Upper Temperature [K]', 'Composition', and 'Year'. Below the table, there are sections for 'Detail of Phase Diagram' and 'Property of Substances'.

Convenient Tools

Property chart

Recorded matching substances' values are plotted when the items: properties, density, and the nearest atoms distance are selected for x, y and z axis. By clicking a point, you will reach to the crystal structure of the target substance. Also, its properties and related phase diagram are accessible.

The screenshot displays the 'Property chart' interface. It shows a scatter plot with axes for 'Density', 'Thermal interatomic Distance', and 'Property'. The plot contains numerous colored data points representing different substances.

Material matrix

A matrix is displayed that represents the number of substances of combinations of elements on the vertical axes by color. The composition ratio of the elements are changeable. In addition to number of substances, most frequent crystal structures, average values of the properties and number of phase diagrams can also be displayed.

The screenshot displays the 'Material matrix' interface. It shows a heatmap matrix with columns for 'All Compositions', 'AB₂', 'AB', 'AB₃', 'AB₃', 'AB₃', and 'AB₃'. The matrix cells are colored based on the number of substances.

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