Inorganic Materials Database for Exploring the Nature of Material

Yibin Xu National Institute for Materials Science

An inorganic materials database system, AtomWork, has been developed and released on the Internet. It includes the phase diagram, crystal structure, X-ray powder diffraction, and property data of more than 80,000 inorganic materials extracted from scientific literature. The feature of this database is that the information of the synthesis, identification, and property of materials is organically linked, which enables the data reported in different papers to be grouped and compared at four different levels: chemical system, compound, substance, and material. The database can

provide users with a comprehensive overview of substances and necessary information to understand the relationships among chemical component, structure, and property.

Keywords: materials data, database system, crystal structure, phase diagram, material property