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FIZnews

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40 years of ICSD – from an archive on paper to a digital gold treasure

When the first crystal structures were collected in the late 1970s, the vision was clear: to create a reliable collection of inorganic structures that would support researchers worldwide. What started out as stacks of paper is now one of the most important databases in materials research - the Inorganic Crystal Structure Database (ICSD).

In 1980, FIZ Karlsruhe joined as technical host, five years later also as content partner. From the very beginning, the highest standards and maximum reliability applied. The path led from the paper archive to complete digitization, and later to the great leap into the Internet - suddenly ICSD was available worldwide and at any time.

Since then, the database has been continuously developed. New data types such as organometallic or theoretically calculated structures have been added. Collaborations with international partners - such as the National Institute of Standards and Technology or the Cambridge Crystallographic Data Center - have made ICSD even more versatile. With the introduction of an API in 2020, the database is now directly integrated into research workflows and a driver for automated materials research.

Despite this dynamic, one point remains as important as ever: quality. Around 16,000 new structures are added every year and each one is checked - automatically and manually. Artificial intelligence provides support, for example in the assignment of structure types, while older data is continuously revised. ICSD is therefore not only growing, but is constantly being improved.

Today, the database is indispensable for many fields of research. Whether semiconductors, energy storage or other high-tech applications - anyone who wants to develop new materials needs high-quality, consistent data. ICSD is closely networked, for example with the Materials Project or OQMD. Data flows in both directions: Structures from ICSD form the basis for new calculations, the results of which are then fed back into the database.

For the 40th anniversary, we are not only looking back, but also forward. The search interface is being modernized, new tools for direct data processing are in the works, and issues surrounding the responsible use of AI are being actively addressed. The aim is to network ICSD even more closely, make it even more user-friendly - and perhaps one day be able to offer full open access.

In four decades, a pile of paper printouts has become a digital gold treasure that is shaping materials research worldwide. And the story still goes on.

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