CRYSTALLOGRAPHY EDUCATION NOTE

ICDD® InSession: Mastering the PDF® Database and JADE® Software

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In January 2021, ICDD launched a new, monthly webinar series titled, *ICDD® InSession: Mastering the PDF® Database and JADE® Software.* Once a month, registered attendees come together to take a deep dive into the PDF database or JADE software, depending on the chosen topic. ICDD's goal is to give current and potential users the opportunity to learn more about the database and software, directly from the experts. With the COVID-19 pandemic continuing to affect our face-to-face meetings, ICDD adapted and found a new way to reach scientists globally. Each webinar is about - one-hour long, with 45 min spent on instruction, and 15 min for Questions & Answers with ICDD staff members. This new opportunity has allowed ICDD to reach many new or potential users and allow everyone to learn more about the power of the Powder Diffraction File™ Database and JADE Software.

Below is a brief summary of the first four *InSession* webinars of 2021:

January 2021 – Navigating a Powder Diffraction File Entry with Tom Blanton, ICDD

A Powder Diffraction File (PDF) entry, also referred to as a PDF card, contains all of the scientific and bibliographic data available for a particular crystalline phase of a material. Information for each entry is organized into over 20 categories; some include 3D structure viewing, ring pattern simulations, and correlation graphs for entries within a temperature series. Attendees learned how to locate and access a PDF entry, navigate through the comprehensive content available, utilize simulation tools, and perform an elemental search and combine search criteria for phase data-mining applications.

If you are interested in watching ICDD's first *InSession* webinar, you can watch the recording on the ICDD website – https://www.icdd.com/in-session/#navigating.

February 2021 – Navigating JADE with Steffen Weber, Materials Data

JADE is a powerful, all-purpose powder XRD pattern viewer, processing, and analysis program with great emphasis on phase ID, quantitative analysis, Whole Pattern Fitting (WPF), and Rietveld refinement tools. JADE makes the task of processing and understanding your collected data simple and your results concise and easy to understand. Participants learned how to navigate the information rich JADE interface, quickly do a Search/Match and Whole Pattern Fitting/Rietveld Refinement of their pattern, view and create structures, and create publication worthy reports.

This *InSession* recording is currently not available for on-demand viewing. We will hold additional JADE webinars in the future.

March 2021 – Data Mining in PDF-4+ with Justin Blanton, ICDD

PDF-4+ combines the world's largest sources of diffraction data from inorganic crystals and powders into a single database, as well as a large collection of organic diffraction data. All entries to the PDF are processed and editorially evaluated by ICDD before entry into the database. The result is a comprehensive collection of inorganic materials and industrially useful organic materials, produced in a standardized format that can be rapidly searched for unknown phase identification. Extensive data mining is facilitated with 131 display fields coupled with 77 searches. This allows the user to find PDF entries of interest based on a large number of user-defined search criteria. Viewers tuned-in to learn how to perform searches based on elemental data, crystallographic data, physical properties, classifications, and more. They also learned how to combine multiple searches using Boolean logic, customize their search results by adding display fields and sorting table columns, and create X–Y graphs, category graphs, and histograms based on their search results.

If you are interested in watching ICDD's *InSession* webinar on Data Mining, you can watch the recording on the ICDD website – https://www.icdd.com/in-session/#datamining.

April 2021 – Phase Identification Using JADE with Rongsheng Zhou, Materials Data

JADE makes the task of processing and understanding your collected data simple and your results concise and easy to understand. During the fourth *InSession* webinar, attendees learned how to create index files for phase identification from the PDF database, create a custom database for phase identification, import and prepare data for phase identification, use chemistry filters and other search criteria, and identify major, minor, and trace phases.

This *InSession* recording is currently not available for on-demand viewing. We will hold additional JADE webinars in the future.

We hope you can join us for a webinar in the future. Please visit the ICDD website to stay informed of upcoming topics – https://www.icdd.com/in-session/.

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