



The National
Academies of

SCIENCES
ENGINEERING
MEDICINE

NIST
National Institute of
Standards and Technology

The US National Committee for Crystallography

Exploring Structural Database Use in Crystallography: Workshop Series

The U.S. National Committee for Crystallography (USNC/Cr) of the National Academies of Sciences, Engineering, and Medicine is providing an online workshop series for students and researchers on the use, development, and maintenance of crystallographic and structural databases. Encompassing macromolecular, small molecule, and powder diffraction information, the series will include 11 modules each meeting for one or two days:

[Opening Keynote](#) - John Helliwell - The Exemplary Crystallography and Structural Databases

[ICSD](#) Searching and using the Inorganic Crystal Structure Database (2 days)

[ICDD](#) The International Center for Diffraction Data Powder Diffraction File™: Database Concepts And Applications (2 days)

[PDB](#) Introducing the Protein Data Bank: 3D Macromolecular Structure Data Deposition, Validation, Biocuration, Archiving, and Delivery for Researchers, Educators, and Students Worldwide (2 days)

[EMDB](#) Introducing the Electron Microscopy Data Bank (EMDB) -- a public repository for electron cryo-microscopy volume maps and tomograms of macromolecular complexes and subcellular structures

[SBGrid](#) Using the SBGrid Software Installer, AppCiter, and SBGrid Data Bank on PCs, HPC clusters and AWS cloud

[COD](#) Searching and getting data from the Crystallography Open Database (COD)

[IRRMIC](#) Access to experimental data is crucial for scientific reproducibility (Integrated Resource for Reproducibility in Macromolecular Crystallography)

[COD](#) Depositing and managing data in the Crystallography Open Database (COD)

[CSD](#) Working with the Cambridge Structural Database (CSD): searching, analyzing and depositing data using Cambridge Crystallographic Data Centre (CCDC) tools (2 days)

[COD](#) Under the hood: Building your own scientific database

Graduate students, postdoctoral fellows, faculty members and researchers in any of the crystallographic, diffraction, and imaging sciences affiliated with the International Union of Crystallography (IUCr) are encouraged to register and participate in the training sessions that interest them.

Registration for this online series is free. To register, please visit:

<https://www.nationalacademies.org/our-work/exploring-structural-database-use-in-crystallography-a-usnccr-workshop-series> The details about each session can be found by clicking the event pages along with a [registration link](#) allows one to register for any combination of the sessions.

Undergraduate students with appropriate research experience will be considered.

Exploring Structural Database Use in Crystallography: A USNC/Cr Workshop Series

2022

	Sun	Mon	Tue	Wed	Thur	Fri	Sat
M A R C H	20	21 - Keynote John Helliwell 11a-12:15p EDT 16-17:15 CET	22	23 - ICSD Inorganic Crystal Structure Day 1 11a-1p EDT 16-18 CET	24 - ICSD Inorganic Crystal Structure Day 2 11a-1p EDT 16-18 CET	25	26
	27	28 - ICDD Powder Diffraction File Day 1 11a-2p EDT 17-20 CEST	29 - PDB Macromolecular Structure Day 1 11a-1p EDT 17-19 CEST	30 - ICDD Powder Diffraction File Day 2 11a-2p EDT 17-20 CEST	31 - PDB Macromolecular Structure - Day 2 11a-1p EDT 17-19 CEST	1	2
A P R I L	3	4 - EMDB Electron Microscopy DB 11a-2p EDT 17-20 CEST	5 - SBGrid Structural Biol Software and DataBank 11a-2p EDT 17-20 CEST	6 - COD Search Cryst. Open DB 10a-2p EDT 16-20 CEST	7 - IRRMC Protein Crystal Raw data archive 11a-2p EDT 17-20 CEST	8	9
	10	11 - COD Deposit and Manage Cryst. Open DB data 10a-2p EDT 16-20 CEST	12 - CSD Cambridge Structure DB Day 1 11a-2p EDT 17-20 CEST	13 - CSD Cambridge Structure DB Day 2 11a-2p EDT 17-20 CEST	14 - COD Building your own Scientific Database 10a-2p EDT 16-20 CEST	15	16

The workshop is sponsored by the National Institute of Standards and Technology (NIST).

For more information please contact Ana Ferreras, Telephone: (202) 334-1697 Email: aferreras@nas.edu

Workshop website

<https://www.nationalacademies.org/our-work/exploring-structural-database-use-in-crystallography-a-usnccr-workshop-series>

Registration form

<https://docs.google.com/forms/d/e/1FAIpQLSezswwokQ5Yn2meCjqlomV-8swqqQkpuUxywWLZwGiGwT2vA/viewform>