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NWACC
c/o Reed College
3203 SE Woodstock Blvd.
Portland, OR 97202

Tel: (503) 777-7254
Email: nwacc@reed.edu

Outstanding Project Award Winners

2008 | Interactive Visualizations of Crystal Structures and Morphologies in the Wikipedia Approach
Peter Moeck, Portland State University

2007 | 3-D Avatar-Based, Virtual World Learning in a Second Life Educational Metaverse
Gregory Möller, University of Idaho

2006 | Using Digital Imaging and GPS/GIS Technologies to Map Biodiversity Patterns in Terrestrial and Aquatic Habitats
Joel Elliott, University of Puget Sound

2005 | The Nolli Map Project
James Tice, University of Oregon

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Year 2005

Project: "Nanocrystallography Visualizations"

Year 2007

Project: "Nanocrystal Structure and Morphology Visualization"

Year 2008

Project: "Interactive Visualizations of Crystal Structures and Morphologies in the Wikipedia Approach"

Project made possible by assistance from:
Portland State University NWACC ONAMI Research Corporation NanoMEGAS Advanced Tools for electron diffraction

Crystallographic database

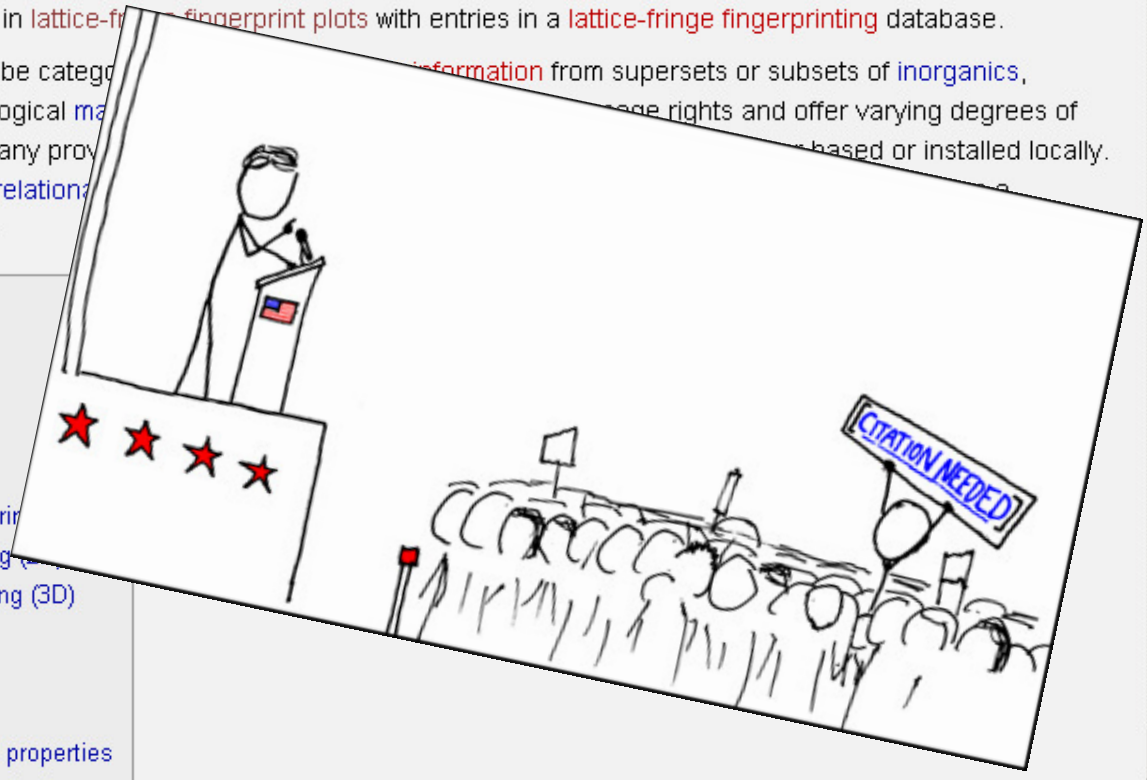
From Wikipedia, the free encyclopedia

A **crystallographic database** is a database specifically designed to store information about crystals and crystal structures. Crystals are solids having, in all three dimensions of space, a regularly repeating arrangement of atoms, ions, or molecules. They are characterized by symmetry, morphology, and directionally dependent physical properties. A crystal structure describes the arrangement of atoms, ions, or molecules in a crystal.

Crystal structures of crystalline material are typically determined from X-ray or neutron single-crystal diffraction data and stored in crystal structure databases. They are routinely identified by comparing reflection intensities and lattice spacings from X-ray powder diffraction data with entries in powder-diffraction fingerprinting databases.

Crystal structures of nanometer sized crystalline samples can be determined via structure factor amplitude information from single-crystal electron diffraction data or structure factor amplitude and phase angle information from Fourier transforms of HRTEM images of crystallites. They are stored in crystal structure databases specializing in nanocrystals and can be identified by comparing zone axis subsets in lattice-fr fingerprint plots with entries in a lattice-fringe fingerprinting database.

Crystallographic databases can be catego information from supersets or subsets of inorganics, metals/alloys, organics, and biological ma age rights and offer varying degrees of search and analysis capacity. Many prov based or installed locally. Newer versions are built on the relationa universal data exchange format.



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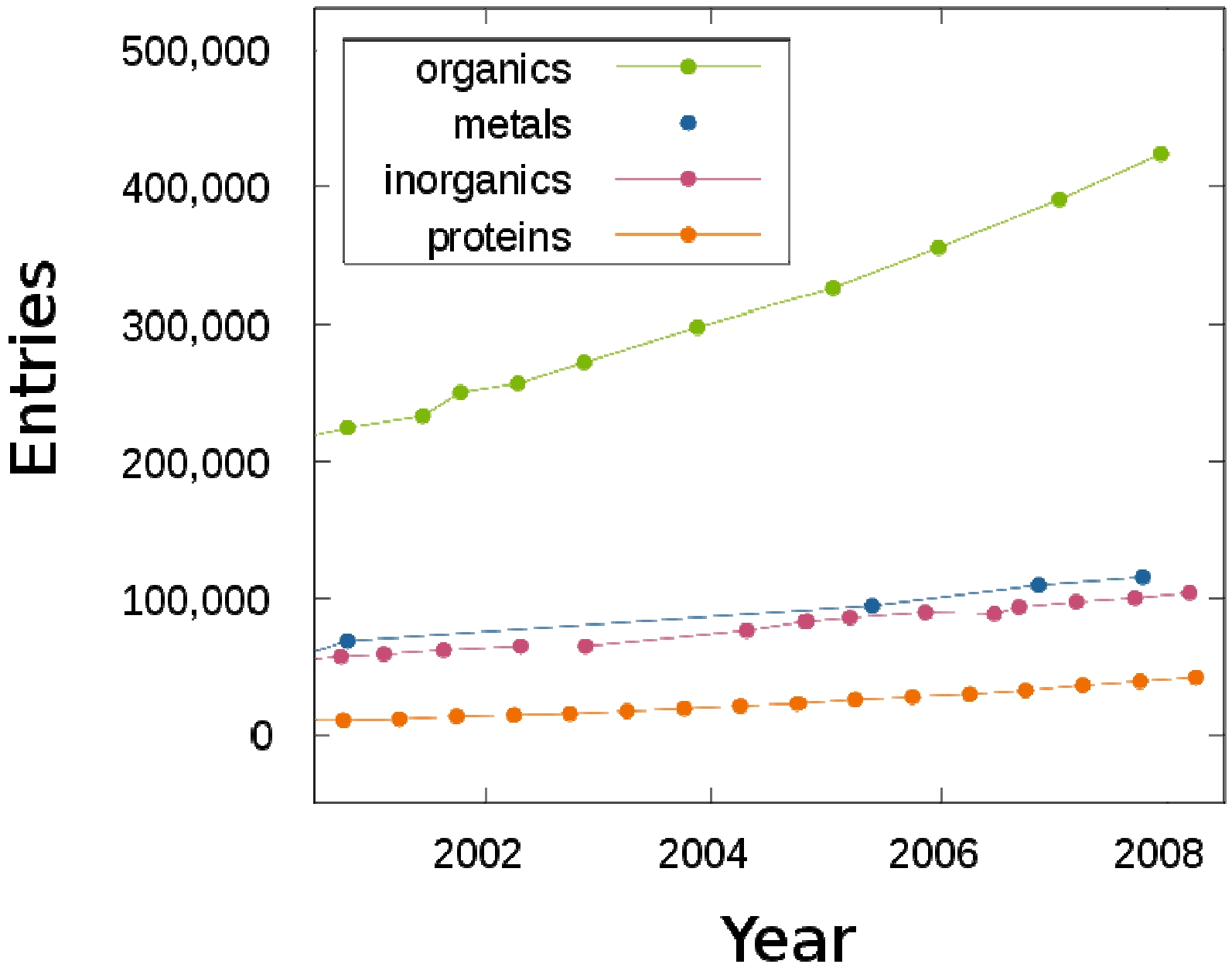
organics
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Entries
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2006
2008
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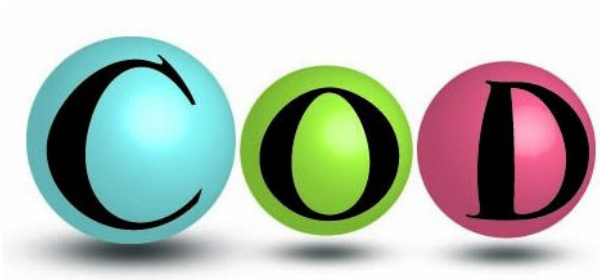
Crystallography Open Database



Advisory Board

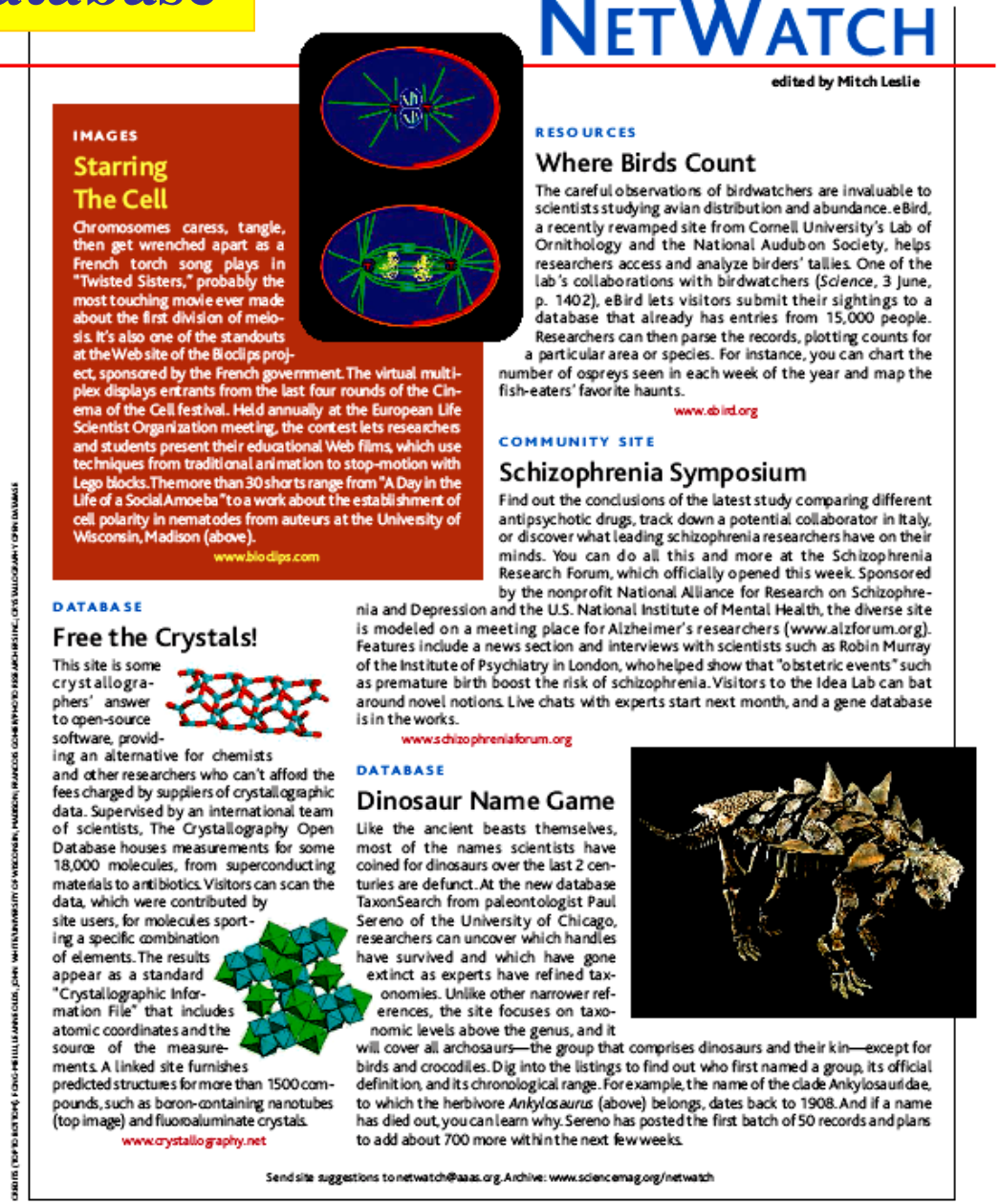
Daniel Chateigner, Xiaolong Chen, Marco Ciriotti, Robert T. Downs, Saulius Gražulis, Armel Le Bail, Luca Lutterotti, Yoshitaka Matsushita, Peter Moeck, Miguel Quirós Olozábal, Hareesh Rajan, Alexandre F.T. Yokochi

http://cod.ibt.lt

mirrors worldwide

http://nanocrystallography.org
http://www.crystallography.net
http://cod.ensicaen.fr/

more than 80,500 entries and 50,000 hits per month



NETWATCH

edited by Mitch Leslie

IMAGES

Starring The Cell

Chromosomes caress, tangle, then get wrenched apart as a French torch song plays in "Twisted Sisters," probably the most touching movie ever made about the first division of meiosis. It's also one of the standouts at the Web site of the Bioclips project, sponsored by the French government. The virtual multiplex displays entrants from the last four rounds of the Cinema of the Cell festival. Held annually at the European Life Scientist Organization meeting, the contest lets researchers and students present their educational Web films, which use techniques from traditional animation to stop-motion with Lego blocks. The more than 30 shorts range from "A Day in the Life of a Social Amoeba" to a work about the establishment of cell polarity in nematodes from auteurs at the University of Wisconsin, Madison (above).

www.bioclips.com

RESOURCES

Where Birds Count

The careful observations of birdwatchers are invaluable to scientists studying avian distribution and abundance. eBird, a recently revamped site from Cornell University's Lab of Ornithology and the National Audubon Society, helps researchers access and analyze birders' tallies. One of the lab's collaborations with birdwatchers (*Science*, 3 June, p. 1402), eBird lets visitors submit their sightings to a database that already has entries from 15,000 people. Researchers can then parse the records, plotting counts for a particular area or species. For instance, you can chart the number of ospreys seen in each week of the year and map the fish-eaters' favorite haunts.

www.ebird.org

COMMUNITY SITE

Schizophrenia Symposium

Find out the conclusions of the latest study comparing different antipsychotic drugs, track down a potential collaborator in Italy, or discover what leading schizophrenia researchers have on their minds. You can do all this and more at the Schizophrenia Research Forum, which officially opened this week. Sponsored by the nonprofit National Alliance for Research on Schizophrenia and Depression and the U.S. National Institute of Mental Health, the diverse site is modeled on a meeting place for Alzheimer's researchers (www.alzforum.org). Features include a news section and interviews with scientists such as Robin Murray of the Institute of Psychiatry in London, who helped show that "obstetric events" such as premature birth boost the risk of schizophrenia. Visitors to the Idea Lab can bat around novel notions. Live chats with experts start next month, and a gene database is in the works.

www.schizophreniaforum.org

DATABASE

Free the Crystals!

This site is some crystallographers' answer to open-source software, providing an alternative for chemists and other researchers who can't afford the fees charged by suppliers of crystallographic data. Supervised by an international team of scientists, The Crystallography Open Database houses measurements for some 18,000 molecules, from superconducting materials to antibiotics. Visitors can scan the data, which were contributed by site users, for molecules sporting a specific combination of elements. The results appear as a standard "Crystallographic Information File" that includes atomic coordinates and the source of the measurements. A linked site furnishes predicted structures for more than 1500 compounds, such as boron-containing nanotubes (top image) and fluoroaluminate crystals.

www.crystallography.net

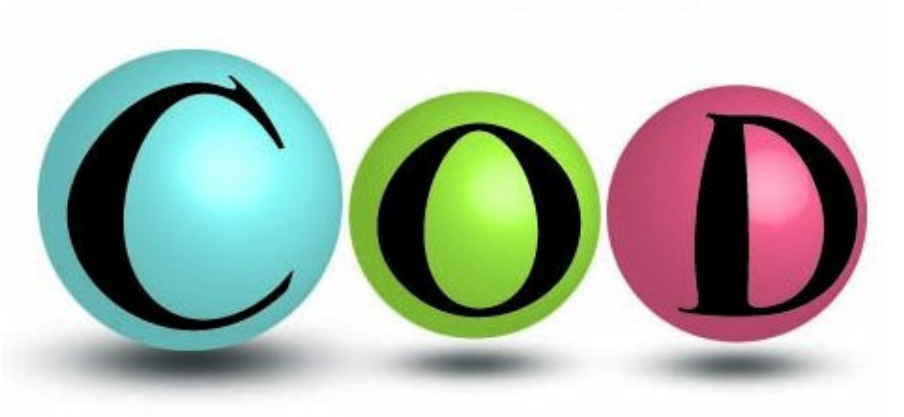
DATABASE

Dinosaur Name Game

Like the ancient beasts themselves, most of the names scientists have coined for dinosaurs over the last 2 centuries are defunct. At the new database TaxonSearch from paleontologist Paul Sereno of the University of Chicago, researchers can uncover which handles have survived and which have gone extinct as experts have refined taxonomies. Unlike other narrower references, the site focuses on taxonomic levels above the genus, and it will cover all archosaurs—the group that comprises dinosaurs and their kin—except for birds and crocodiles. Dig into the listings to find out who first named a group, its official definition, and its chronological range. For example, the name of the clade Ankylosauridae, to which the herbivore *Ankylosaurus* (above) belongs, dates back to 1908. And if a name has died out, you can learn why. Sereno has posted the first batch of 50 records and plans to add about 700 more within the next few weeks.

Send site suggestions to netwatch@aaas.org. Archive: www.sciencemag.org/netwatch

www.crystallography.net

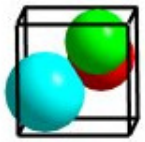


Crystallography Open Database

Upload data

or

Search the database



View the Petition for Open Data in Crystallography

Call to Volunteers

See also the **PCOD** : Predicted Crystallography Open Database

More on the COD project : **what's new**

Recent open access paper regarding COD development was published in Journal of Applied Crystallogra
versions are available.

COD Advisory Board thanks Crystal Impact GbR for their financial support of this paper pu

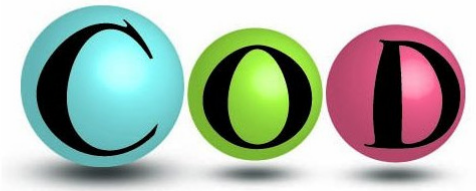
CIFs Donators - **Advice to potential CIF Donators**

Statistics of access generated by http-analyze and visitors programs

Currently there are **80946** entries in the COD

All data on this site have been placed in the public domain by the contributors

www.nanocrystallography.org



Crystallography Open Database

Upload data

or

Search the database

Sign the Petition for Open Data in Crystallography

Call to Volunteers

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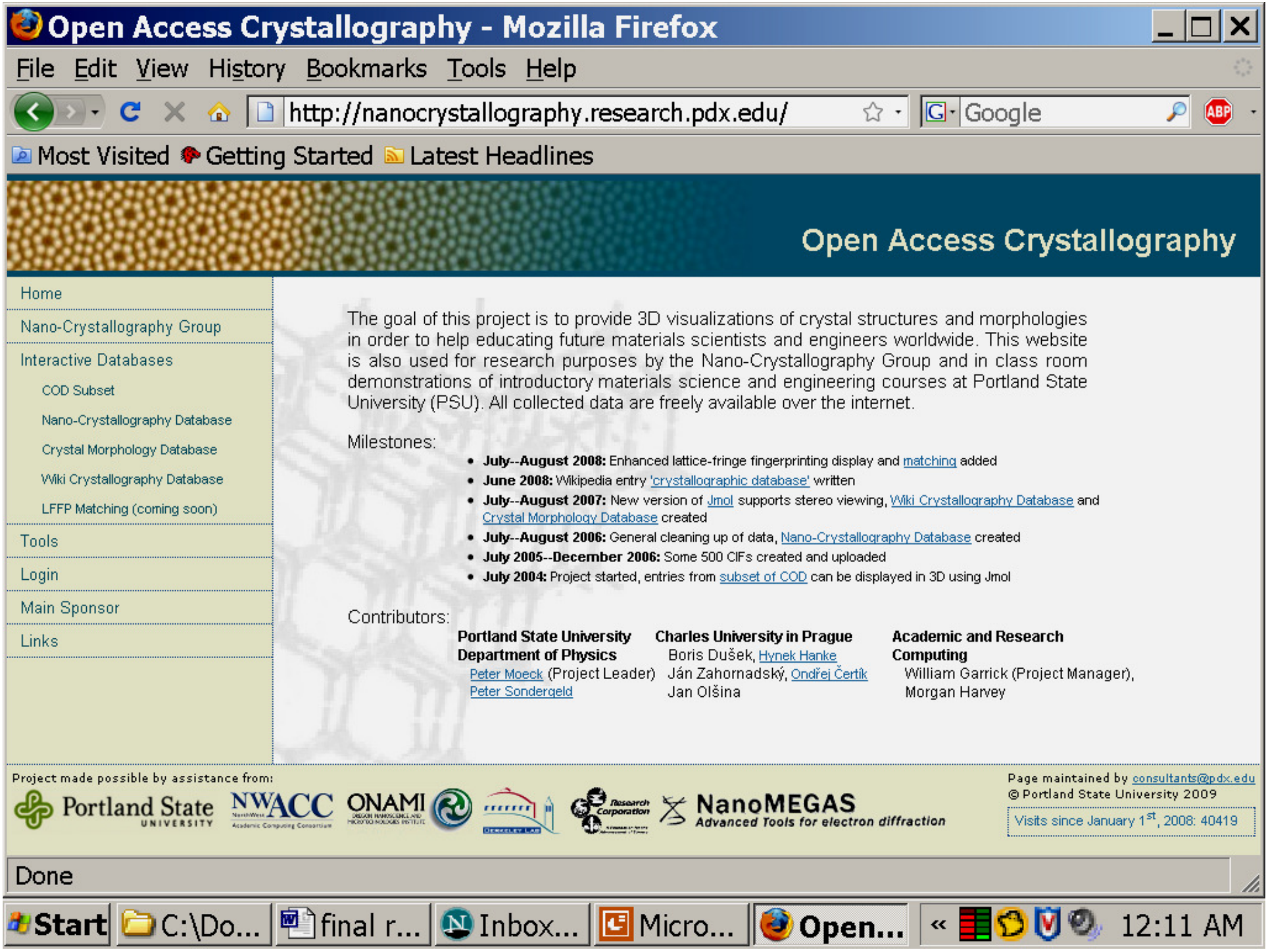
CIFs Donators - **Advice to potential CIF Donators**

Statistics of access generated by http-analyze and visitors programs

Updated daily: 80946 entries in the COD

All data on this site have been placed in the public domain by the contributors


Open Access Crystallography - Mozilla Firefox
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http://nanocrystallography.research.pdx.edu/
Google
Most Visited Getting Started Latest Headlines
Open Access Crystallography
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The goal of this project is to provide 3D visualizations of crystal structures and morphologies in order to help educating future materials scientists and engineers worldwide. This website is also used for research purposes by the Nano-Crystallography Group and in class room demonstrations of introductory materials science and engineering courses at Portland State University (PSU). All collected data are freely available over the internet.
Milestones:
July--August 2008: Enhanced lattice-fringe fingerprinting display and matching added
June 2008: Wikipedia entry 'crystallographic database' written
July--August 2007: New version of Jmol supports stereo viewing, Wiki Crystallography Database and Crystal Morphology Database created
July--August 2006: General cleaning up of data, Nano-Crystallography Database created
July 2005--December 2006: Some 500 CIFs created and uploaded
July 2004: Project started, entries from subset of COD can be displayed in 3D using Jmol
Contributors:
Portland State University
Department of Physics
Peter Moeck (Project Leader)
Peter Sondergeld
Charles University in Prague
Boris Dušek, Hynek Hanke
Ján Zahornadský, Ondřej Čertík
Jan Olšina
Academic and Research Computing
William Garrick (Project Manager),
Morgan Harvey
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Research Corporation
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Advanced Tools for electron diffraction
Page maintained by consultants@pdx.edu
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Visits since January 1st, 2008: 40419
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http://nanocrystallography.research.pdx.edu/search.py,

Interactive Cryst... | Inbox :: Inbox (3)

Interactive Crystallography Databases

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  - Nano-Crystallography Database
  - Crystal Morphology Database
  - Wiki Crystallography Database
  - LFFP Matching (coming soon)
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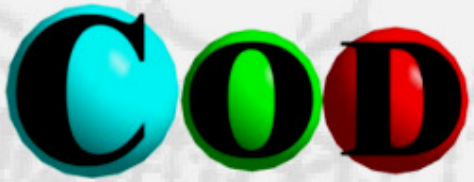

COD Subset
Search and view

Nano-Crystallography Database
Search and view Login/Register for upload

Crystal Morphology Database
Search and view

Wiki Crystallography Database
Search and view Upload data

Several crystallography databases are offered for browsing, each of which having a slightly different purpose. You can search the databases, display the contained CIFs, view 3D models of the crystal structure and morphology or compute and display their lattice fringe fingerprint plots.

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Visits since January 1st, 2008: 40371

Search

Search by these properties:

Text	magnetite
With these elements	
Without these elements	
Minimum and Maximum volume	
Strict number of elements	
Symmetry cell setting	
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c (min, max)	
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gamma (min, max)	

Database: (•) cod ( ) ncd ( ) cmd ( ) wcd

Search | Reset | (Help...) | (Back)

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Search Result

Found 59 results

(Search again) (Interactive Databases) (Help...)

Formula: Fe_3O_4
Source: Bragg, W H Nature (London) The Structure of Magnetite and the Spinels Nature (London) 95 (1915) 561 561
Space group: F d -3 m S
Cell volume: 575.93
Cell parameters: a = 8.3200Å, b = 8.3200Å, c = 8.3200Å; α = 90.000°, β = 90.000°, γ = 90.000°
User comments: None

CIF	3D Model	Lattice-Fringe Fingerprint	Edit
View	View (old)	Kinematic	Comment
Download	View Structure (new window)	Dynamic	Deletion Mark

Formula: Fe_3O_4
Source: Magnetite Wechsler B A Lindsley D H Prewitt C T Crystal structure and cation distribution in titanomagnetites (Fe3-xTixO4) MT100-1350 American Mineralogist 69 (1984) 754 770
Space group: F d 3 m
Cell volume: 591.82
Cell parameters: a = 8.3958Å, b = 8.3958Å, c = 8.3958Å; α = 90.000°, β = 90.000°, γ = 90.000°
User comments: None

CIF	3D Model	Lattice-Fringe Fingerprint	Edit
View	View (old)	Kinematic	Comment
Download	View Structure (new window)	Dynamic	Deletion Mark

Formula: $Fe_{2.75}O_4Ti_{0.25}$

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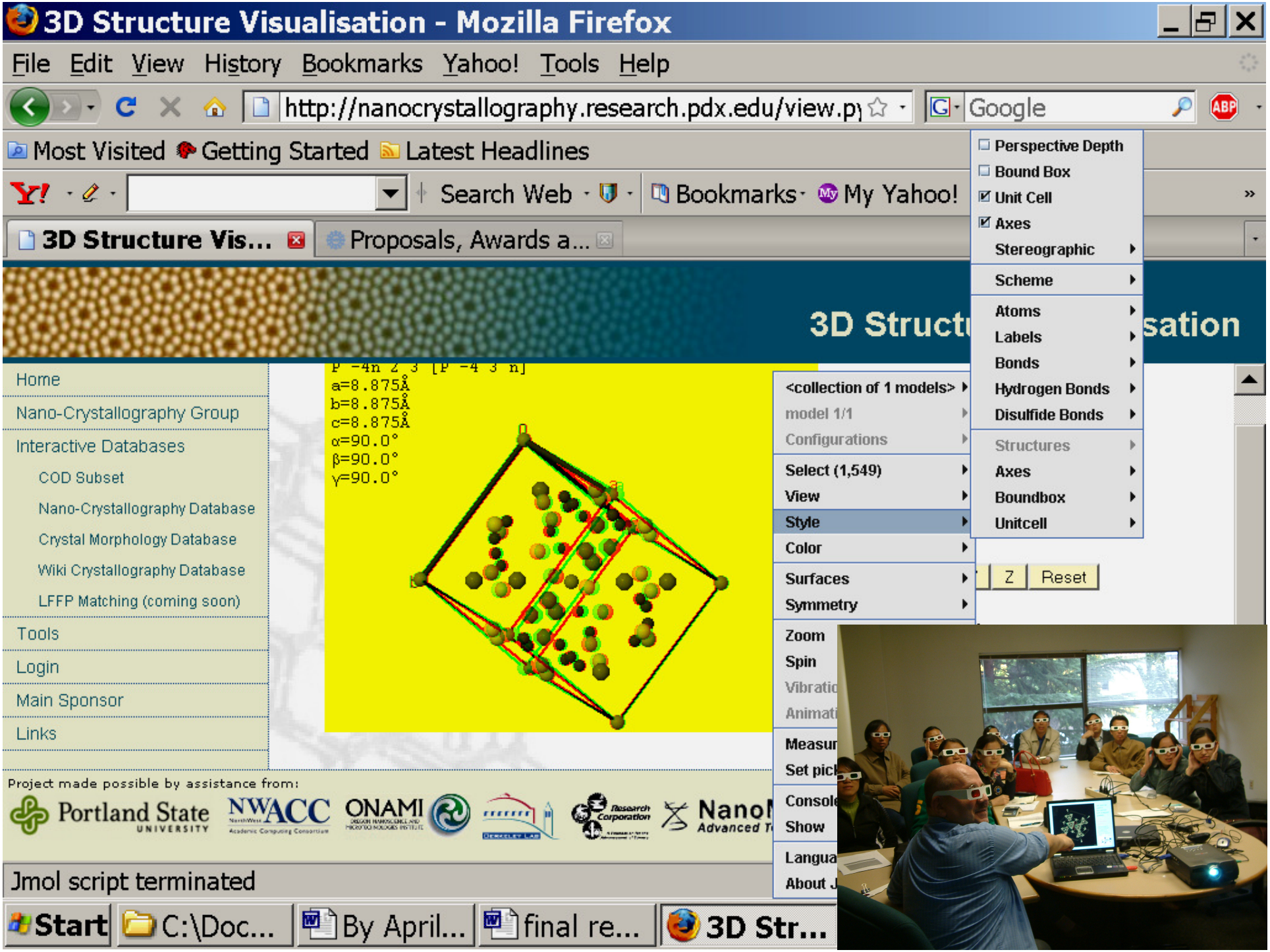
3D Structure Visualisation - Mozilla Firefox
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http://nanocrystallography.research.pdx.edu/view.p
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NWACC
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3D Morphology Visualisation - Mozilla Firefox

File Edit View History Bookmarks Yahoo! Tools Help

http://nanocrystallography.research.pdx.edu/view.p

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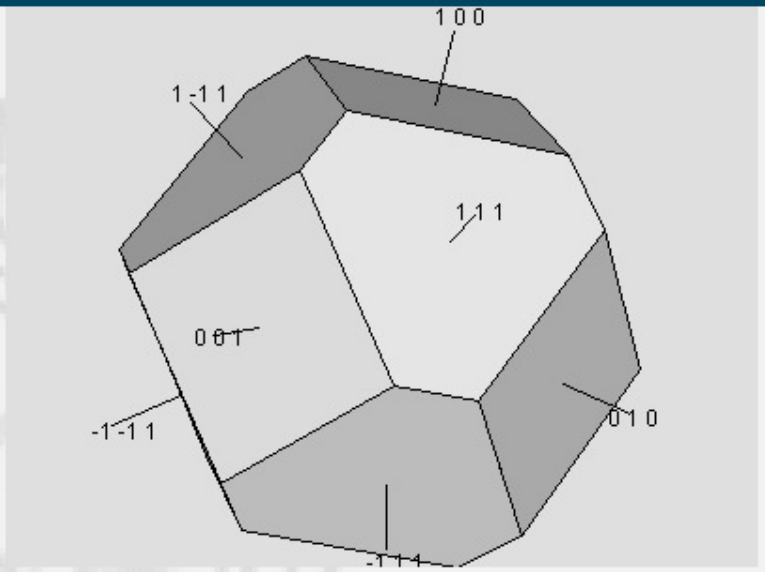

The area on the left displays crystal morphology as given in the CIF. By holding your left mouse button and moving the mouse cursor, you can turn the crystal around. Your right mouse button will let you access a popup menu with other capabilities, like crystal faces modification, color settings and others.

Please read Help... to find out more about the available functions.

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Visits since January 1st, 2008: 35161

Done

Start C:\Doc... By April... final re... 3D Mo... 11:51 AM

Lattice Fringe-Fingerprint Matching

Narrow match search by these properties:

With these elements	Al	Si	O	H				
Without these elements								
Minimum and Maximum volume	500	650						
Strict number of elements	4							
Symmetry cell setting	monoclinic							
a (min, max) [A]	4.9	5.1						
b (min, max) [A]	6.5	6.6						
c (min, max) [A]	5.1	5.2						
alpha (min, max) [deg]								
beta (min, max) [deg]	115	117						
gamma (min, max) [deg]								
Smallest reciprocal vector [nm^{-1}]								
2nd smallest reciprocal vector in the pair [nm^{-1}]								
Their angle [deg]								

Input your LFFP in specified format here.

Database: (•) cod ( ) ncd ( ) cmd ( ) wcd

Match Reset (Help...) (Back)

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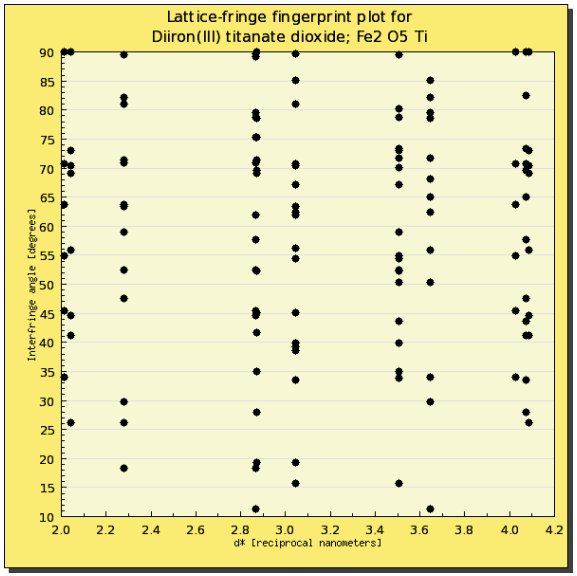
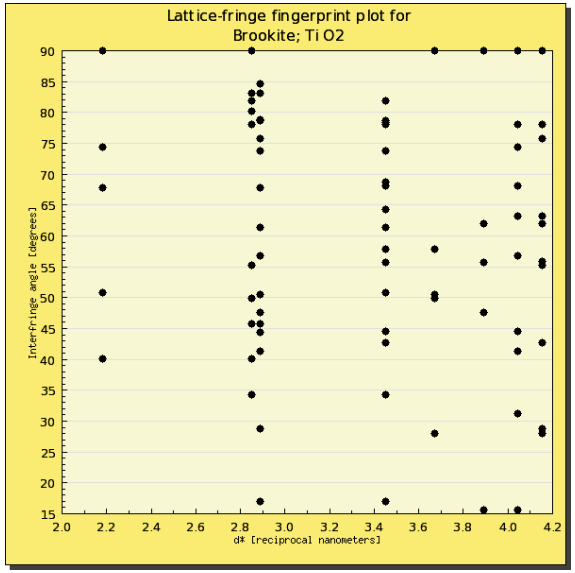
0.24 nm point resolution **pseudo-brookite** **brookite**

modern
analytical TEM

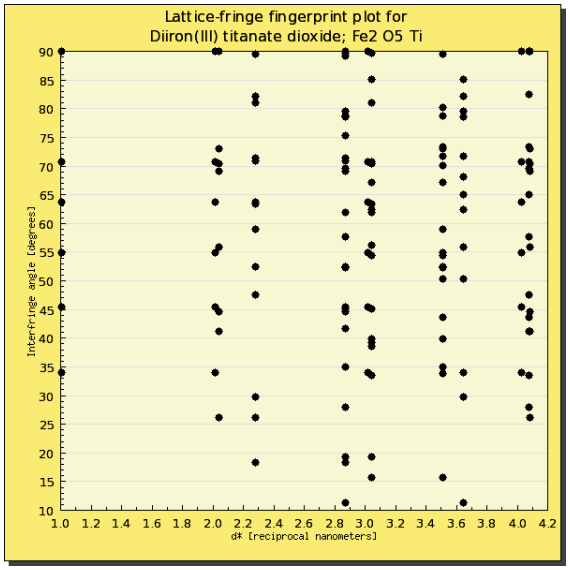
kinematic

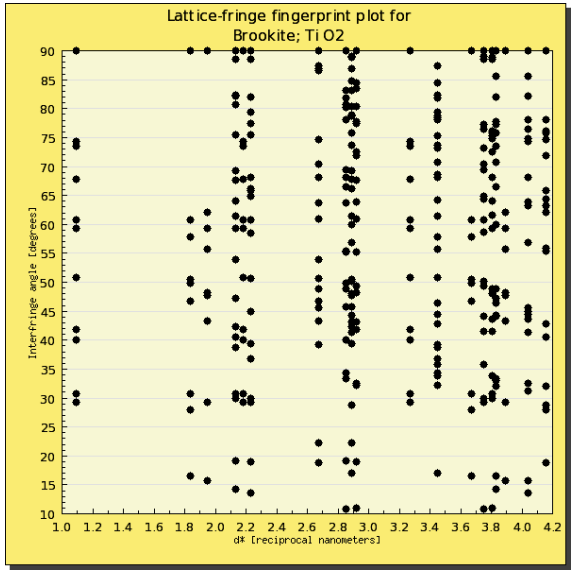




dynamic

taking account of double and multiple diffraction within one nanocrystal





downloadable from our web site as *.png or Bitmap after search and calculations

The Wiki Crystallography Database and its initial set-up with selected mineral data from the Crystallography Open Database recognizes the fact that there is a wealth of crystallographic / mineralogical knowledge distributed in non-digital form all over the world. As the computational infrastructure for such a project is very modest and a “common language” exists in the form of the Crystallographic Information File (CIF) of the International Union of Crystallography (IUCr) we – the people of the world with interests in crystals and minerals – laymen and scientists alike could together create this world’s open-access digital depository for such data.
Please do participate and enjoy the following little anecdote by Sir William Lawrence Bragg:

I said to the proprietor of a shop in Ballater, on Deeside, “That’s a fine group of smoky quartz in your window.” He replied “That’s no smoky quartz, that’s topaz. It’s a crystal. You can tell crystals by the angles between their faces. If you’re interested, I’ll lend you a book on the subject.” On return to base I looked up a book on mineralogy which said ”Smoky quartz, also known as Cairngorm, is called Topaz in Scotland.”

This is from *A Random Walk in Science: The high standard of education in Scotland*, published by IOP, as quoted in J. R. Helliwell, *X-ray crystal structure analysis in Manchester: from W. L. Bragg to the present day*, Z. Kristallogr. 217 (2002) 385-389.

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Mode: [simple advanced] Help

Simple CIF Editor

You don't need to fill in all entries. You will be notified if your modifications contain a syntax or semantics error.

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Common chemical name		[text] (Trivial name by which the
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Journal volume		[text] (Volume of the journal in
Journal publication year		[text] (Year of publication of the
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Journal last page of article		[text] (The number of the journa
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Number of formula units in cell [number] (Number of formula ur

Atom symbol
Oxidation number

Site label
Atom or site symbol
Wyckoff symbol
Site multiplicity
X fractional coordinate
Y fractional coordinate
Z fractional coordinate
Isotropic atomic displacement (U)
Isotropic atomic displacement (B)

Crystal description [text] (A description of the qualit
Crystal identification [text] (Crystal morphology, e.g. '
Crystal color [text] (Experimental crystal colo
Crystal color lustre [one of ['metallic', 'dull', 'clear']]

Crystal face h index
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Update Reset

Advanced CIF Editor

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Besides some man-made joy and misery, ***"Life is a partial, continuous, progressive, multiform and conditionally interactive self-realization of the potentialities of atomic electron states."*** (J. D. Bernal)

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