

# Final Report: NWACC 2007 Project: Nanocrystal structure and morphology visualizations

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## Summary of our Achievements

The project web site has been established at <http://nanocrystallography.research.pdx.edu/> and the NWACC logo is displayed prominently on all web pages that belong to this site, see bottom of Fig. 1. (Note that our site is rather popular as demonstrated by the more than 4,400 hits since January 1<sup>st</sup>, 2008.)

We provide at <http://nanocrystallography.research.pdx.edu/CIF-searchable/>, Fig. 1, free access to a subset of the open-access Crystallography Open Database (COD, see appendix) and our own three additional (and the COD complementing) Internet base crystallographic databases. Our databases at Portland State University (PSU) contain the records of approximately 25,000 structure determinations. Queries of all of these databases can be downloaded in the standard Crystallographic Information File (CIF) format [1] and displayed in a variety of modes (including anaglyph stereo) by java based applets.

The screenshot shows a web browser window with the URL <http://nanocrystallography.research.pdx.edu/search.py/index>. The page title is "Interactive Crystallography Databases". The left sidebar contains a navigation menu with links for Home, Interactive Databases (COD Subset, Nano-Crystallography Database, Crystal Morphology Database, Wiki Crystallography Database), Tools, Login, Crystallography Background (Paper, Geomolby), NWACC, and Links. The main content area displays four database options:

- COD Subset (20264)**: Search and view
- Nano-Crystallography Database (2)**: Search and view, Login/Register for upload
- Crystal Morphology Database (4)**: Search and view
- Wiki Crystallography Database (8934)**: Search and view, Upload data

Below these sections, a paragraph states: "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." Another paragraph notes: "The COD Subset available here is a mainly inorganic and educational subset of the Crystallography Open Database (COD) project. The data have been cleaned".

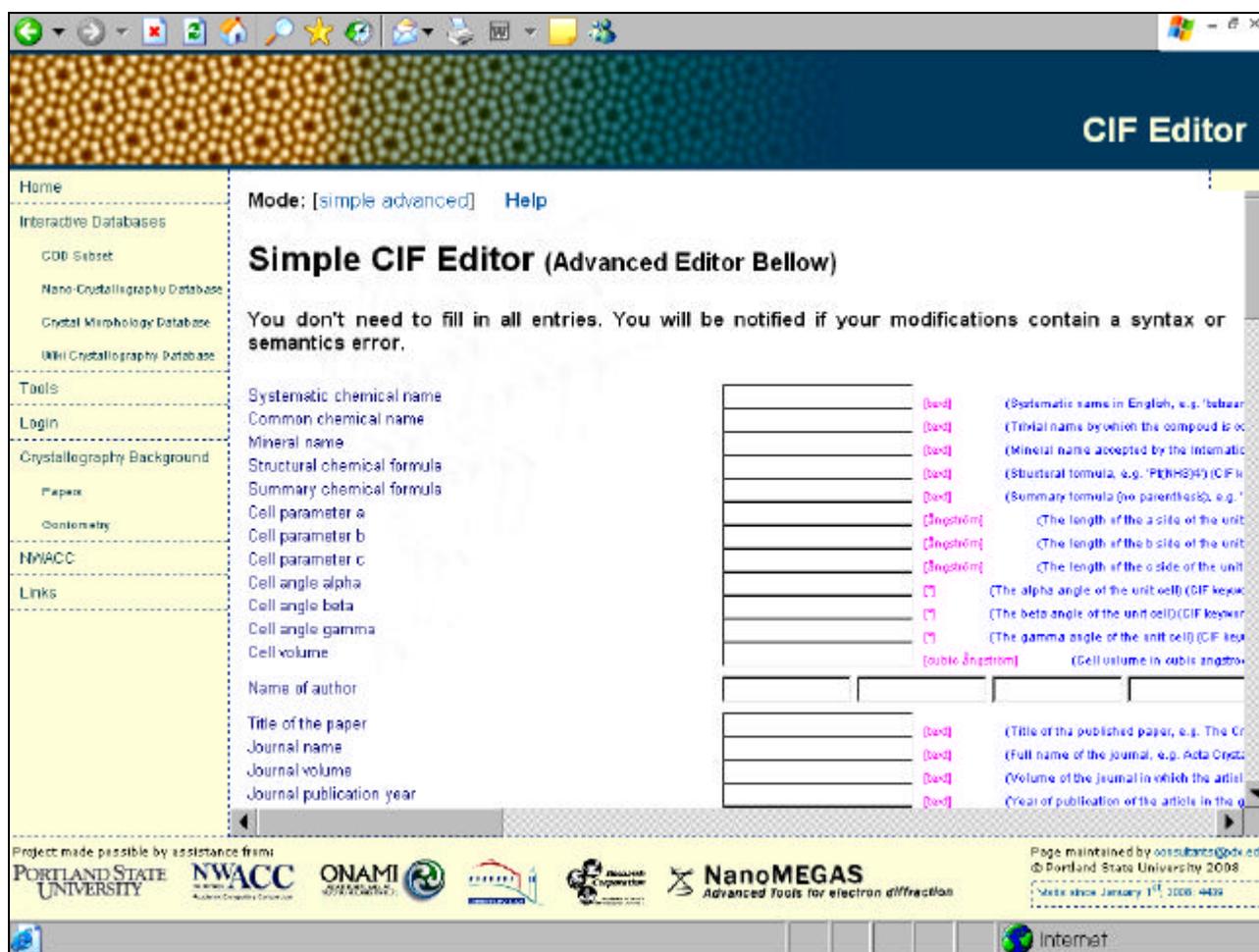
The footer includes logos for Portland State University, NWACC, ONAMI, and NanoMEGAS. It also contains the text: "Project made possible by assistance from: PORTLAND STATE UNIVERSITY, NWACC, ONAMI, and NanoMEGAS. Page maintained by [pmoeck@pdx.edu](mailto:pmoeck@pdx.edu) © Portland State University 2008. Hits since January 1<sup>st</sup> 2008: 4400".

**Figure 1.** Screen shot from the page that gives access to PSU's four open-access crystallographic databases, (<http://nanocrystallography.research.pdx.edu/CIF-searchable/>). Note that as of April 13, 2008, the different web pages that constitute the whole website were accessed over 4,400 times.

We have been identified by World Science News ([www.world-science.net](http://www.world-science.net)) as a high-traffic scientific-data dissemination site and were kindly asked to provide a link to their open-access science news services. Reciprocally we (the Nanocrystallography Group, Portland State University, Ore.) are acknowledged as a supporter of their site (at <http://www.world-science.net/x01>).

Our databases are a mainly inorganic and educational subset of the COD, a dedicated “Nano-Crystallography Database” (NCD), a dedicated “Crystal Morphology Database” (CMD), and the “world’s first” open-access crystallography database “Wicki-CD” in the “wikipedia format”. The latter of these databases has been filled initially with approximately 9,000 minerals. Mineral data have been uploaded to our “Wicki CD” because there are many people interested in mineralogy and many active mineral collectors worldwide. We do hope that some of these people will contribute at least some of their knowledge to the world’s first website where everything about an inorganic crystal that is stable in the natural environment can be collected, searched, and openly accessed.

This is possible because our databases utilize the so-called “CIF format”. The CIF (for Crystallographic Information File) format and the associated CIF dictionaries [1] are the outcome of major efforts by the International Union of Crystallography (IUCr, which is a non-profit organization that represents the common interests of the world’s crystallographers and is also the main publisher of crystallographic reference books and journals). CIF is in essence a kind of “language” in which everything about a crystal can be communicated between human beings (who also read English), between human beings and computers, and between computers alone. In order to facilitate the upload of data by people who are not familiar with the CIF language, we provided both a simple and an advanced CIF Editor/Upload Protocol, Fig. 2.

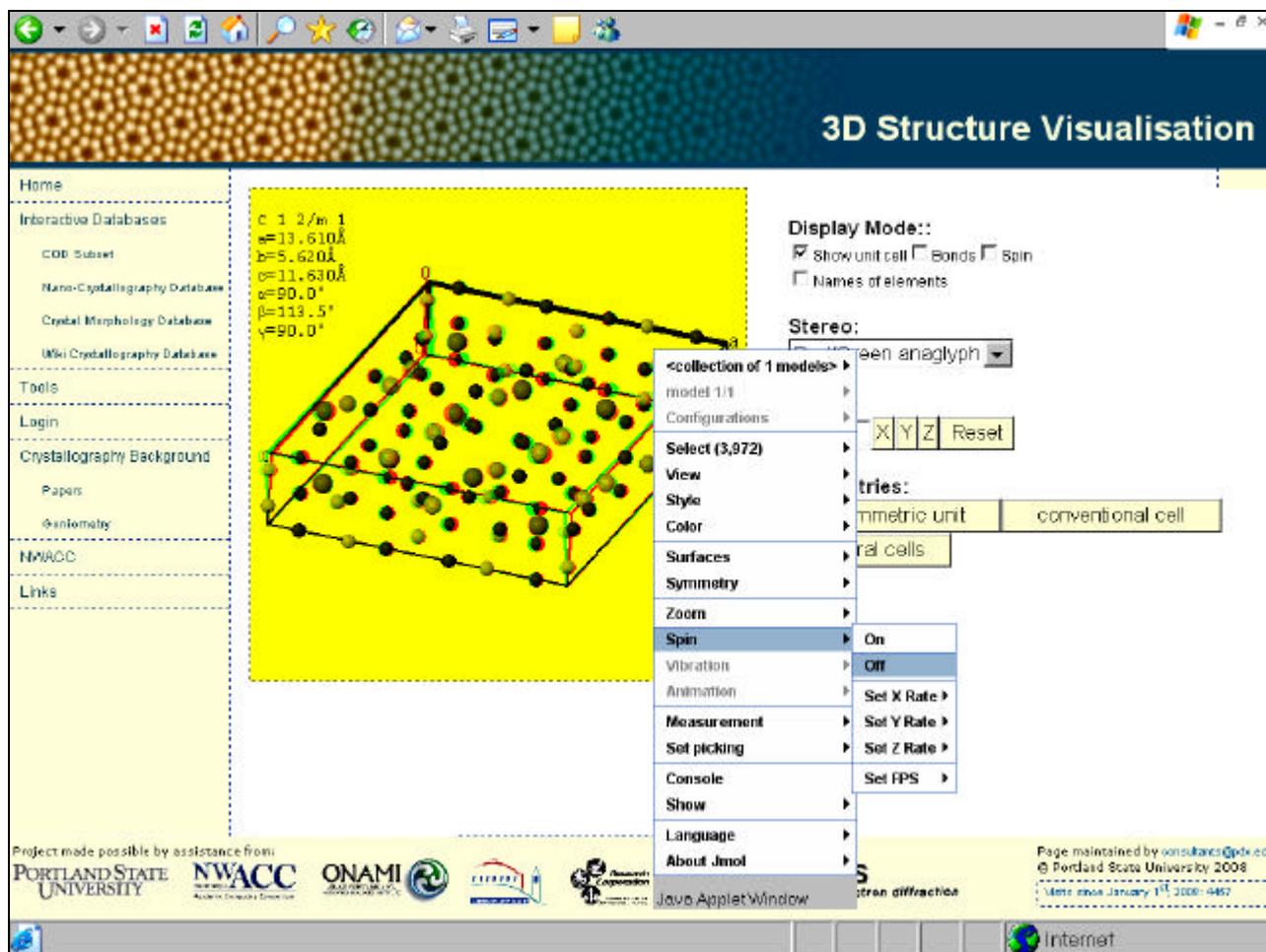


**Figure 2:** Screenshot of our simple CIF editor. This editor allows for the creation of CIF entries for our databases (including the Wiki-Crystallography Database) by the “crystal and minerals loving” general public.

Our Nano-Crystallography Database (NCD), on the other hand, is a research database with registered users from the community of nanocrystallographers. While access is free to the general public, the uploading of data requires registration. We also improved significantly the displays of the crystal structures for all of our databases (by providing capabilities for 3D anaglyph, Fig. 3) stereo displays, Fig. 4.

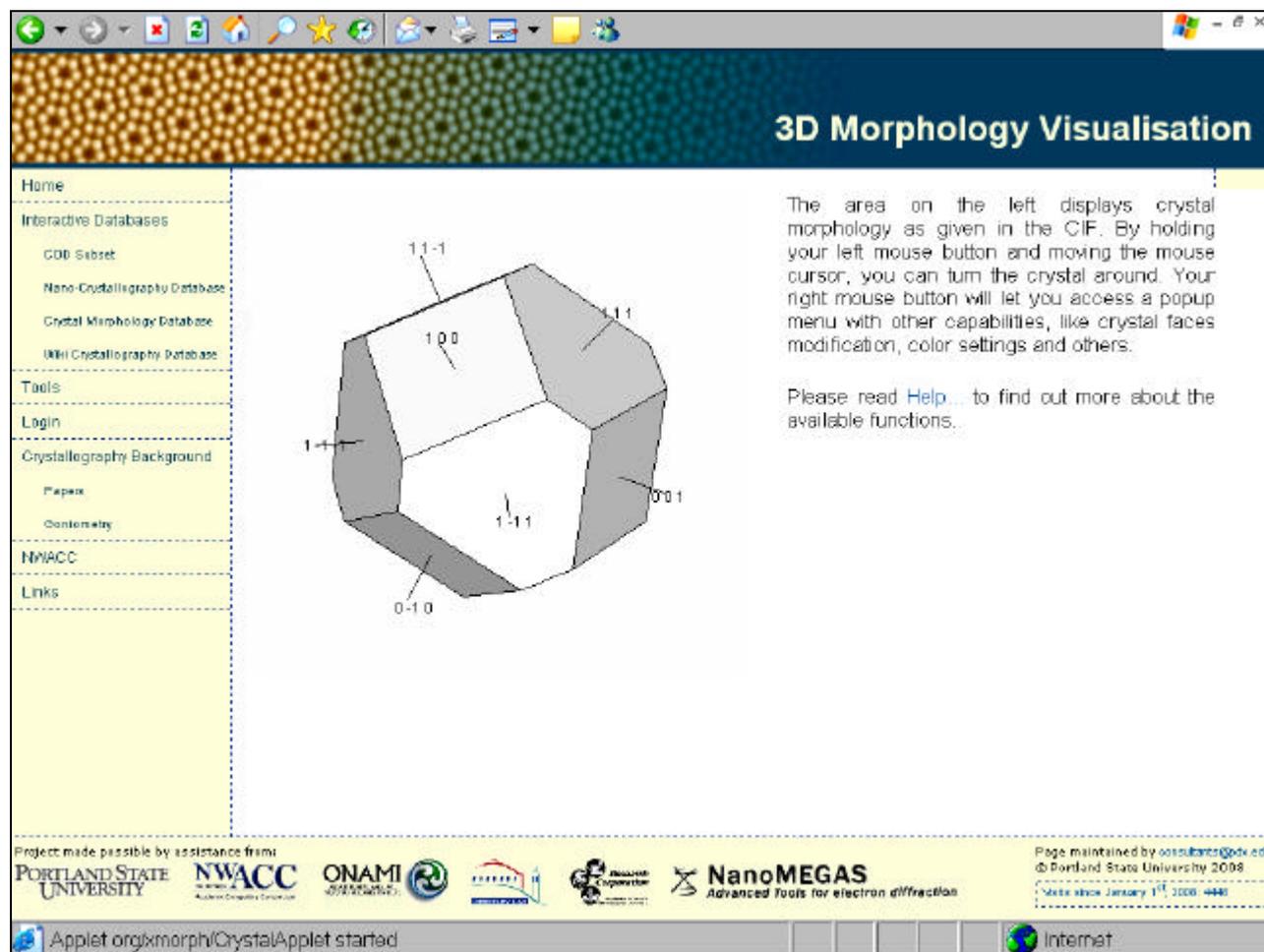


**Figure 3:** The PI of this proposal demonstrating a crystal structure (in the large extra-window format) from our open-access databases to a group of visiting physics professors and instructors from the People's Republic of China where we all wear anaglyph glasses.



**Figure 4.** Visualization (in one of the anaglyph three-dimensional display modes) of a crystal structure from our open access database (at the atomic level). The opened Java Applet demonstrates the versatility of our new display mode.

Our Crystal Morphology Database (CMD) has a strong educational component and is topical because there is a renewed interest in the knowledge of crystal morphology that is driven by the demonstration that not only the size of a nanocrystal matters with respect to its properties, but also its morphology. (Catalytic properties of nanocrystals have, for example, recently been shown to be controlled by crystal morphology, ref. [2]!). Early mineralogists and crystallographers did develop a comprehensive and systematic crystal morphology description on the basis of the spatial arrangement of symmetry elements about 100 years ago. The same framework can now be reused and expanded for nanocrystals, but needs to be popularized within the community of researchers and educators that deal with nanocrystals. Figure 5 shows our crystal morphology display program in action.



**Figure 5.** Screenshot of our new, interactive 3D Crystal Morphology Visualization program. The highly unusual, artificially created morphology of a platinum nanocrystal is displayed. Note that this nanocrystal morphology has for platinum nanocrystals been associated with a 400 % increased catalytic activity (for the same nanoparticle size), ref. [2].

## Closing financial statement

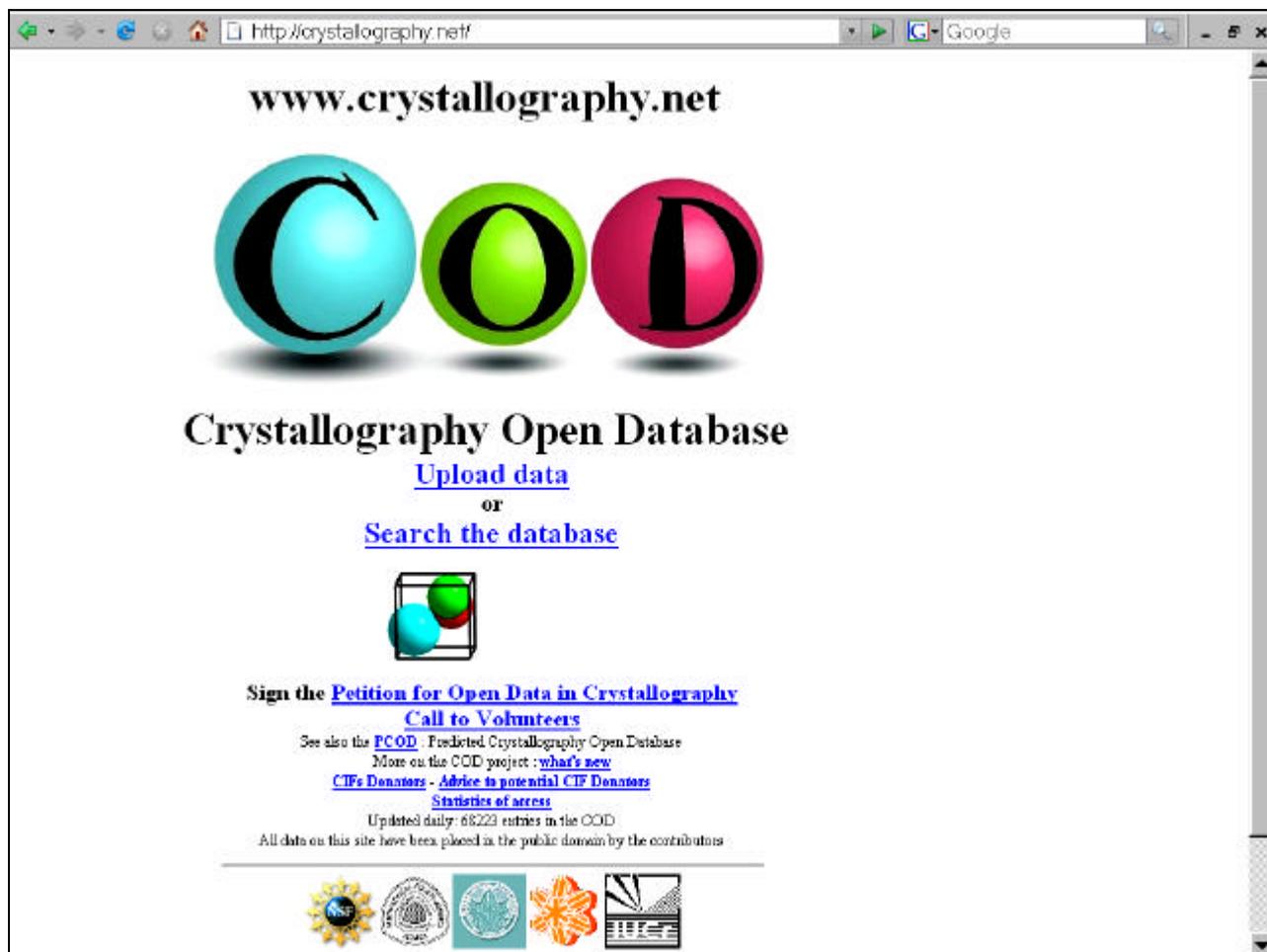
All funds have been expended according to the guidelines defined by the NWACC.

## References

[1] International Tables for Crystallography, Volume G, Definition and exchange of crystallographic data, S. Hall and B. McMahon, eds., Springer, Dordrecht, 2005

[2] N. Tian, Z.-Y. Zhou, S.-G. Sun, Y. Ding, Z. L. Wang: *Synthesis of Tetrahedral Platinum Nanocrystals with High-Index Facets and High Electro-Oxidation Activity*, *Science* **316** (2007) 732-735

## Appendix



Screen shot from the access page to the Crystallography Open Database (COD). Note that there are more than 68,000 entries as of April 13, 2008 in the COD and that the PI of this project is a member of the International Advisory Board of this database. Portland State University is scheduled to become the third mirror in the world (and first in the Americas) for this website.