Crystallography Open Database: educational subsets and their usage in interdisciplinary college education at Portland State University

Peter Moeck[1], **Trevor J. Snyder**[2], **Werner Kaminsky**[3], all members of the International Advisory Board of the **C**rystallography **O**pen **D**atabase (COD), and all members of the **P**ortland **N**anoscience and **N**anotechnology **A**cademy (PNNA)

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[2] XEROX Wilsonville / Oregon
[3] Depart. Chemistry, University of Washington at Seattle

Funding: *NorthWest Academic Computing Consortium, National Science Foundation (most recent NEU: Nano-Science & Engineering: A STE Minor with General Education, EEC-1242197), Research Council of Lithuania, PANalytical, Crystal Impact* ***& our various home institutions***

Outline

1. Crystallography Open Database (COD) in its 11th year

2. Supporting efforts at Portland State University (PSU, in their 10th year)

3. Courses where basic crystallographic education is provided at PSU (mainly in disguise as nano-science and nano-tech)

4. 400/500 level course assignments (without solutions)

5. 3D printing from Crystallographic Information Files (CIF)

6. Summary and Outlook

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Crystallographic database

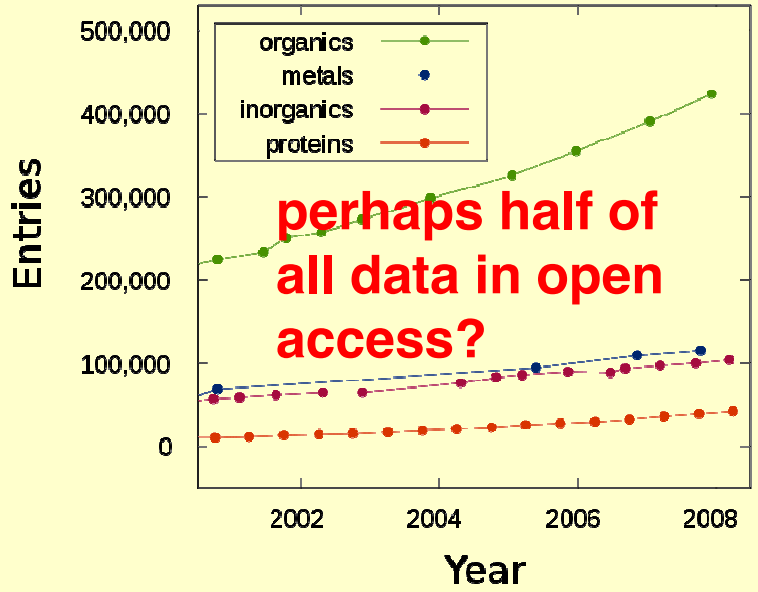
From Wikipedia, the free encyclopedia
(Redirected from Crystallographic databases)

A **crystallographic database** is a database specifically designed to store infor
having, in all three dimensions of space, a regularly repeating arrangement of at
morphology, and directionally dependent physical properties. A crystal structure

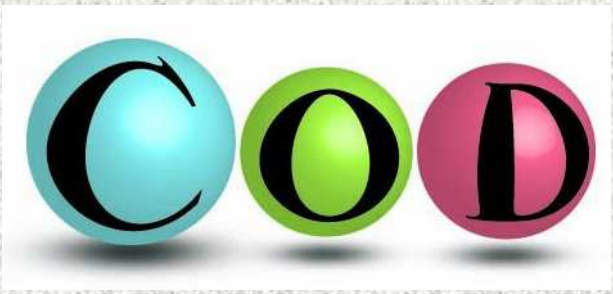
Crystal structures of crystalline material are typically determined from X-ray or ne
databases. They are routinely identified by comparing reflection intensities and l
powder-diffraction fingerprinting databases.

Crystal structures of nanometer sized crystalline samples can be determined via
diffraction data or structure factor amplitude and phase angle information from F
in crystal structure databases specializing in nanocrystals and can be identified b
entries in a lattice-fringe fingerprinting database.

Crystallographic databases can be categorized as crystallographic information f
biological macromolecules. They differ in access and usage rights and offer vary
visualization capabilities. They can be browser based or installed locally. Newer
Crystallographic Information File (CIF) as a universal data exchange format.



Crystallography Open Database



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http://www.crystallography.net

mirrors worldwide

http://cod.ibt.lt

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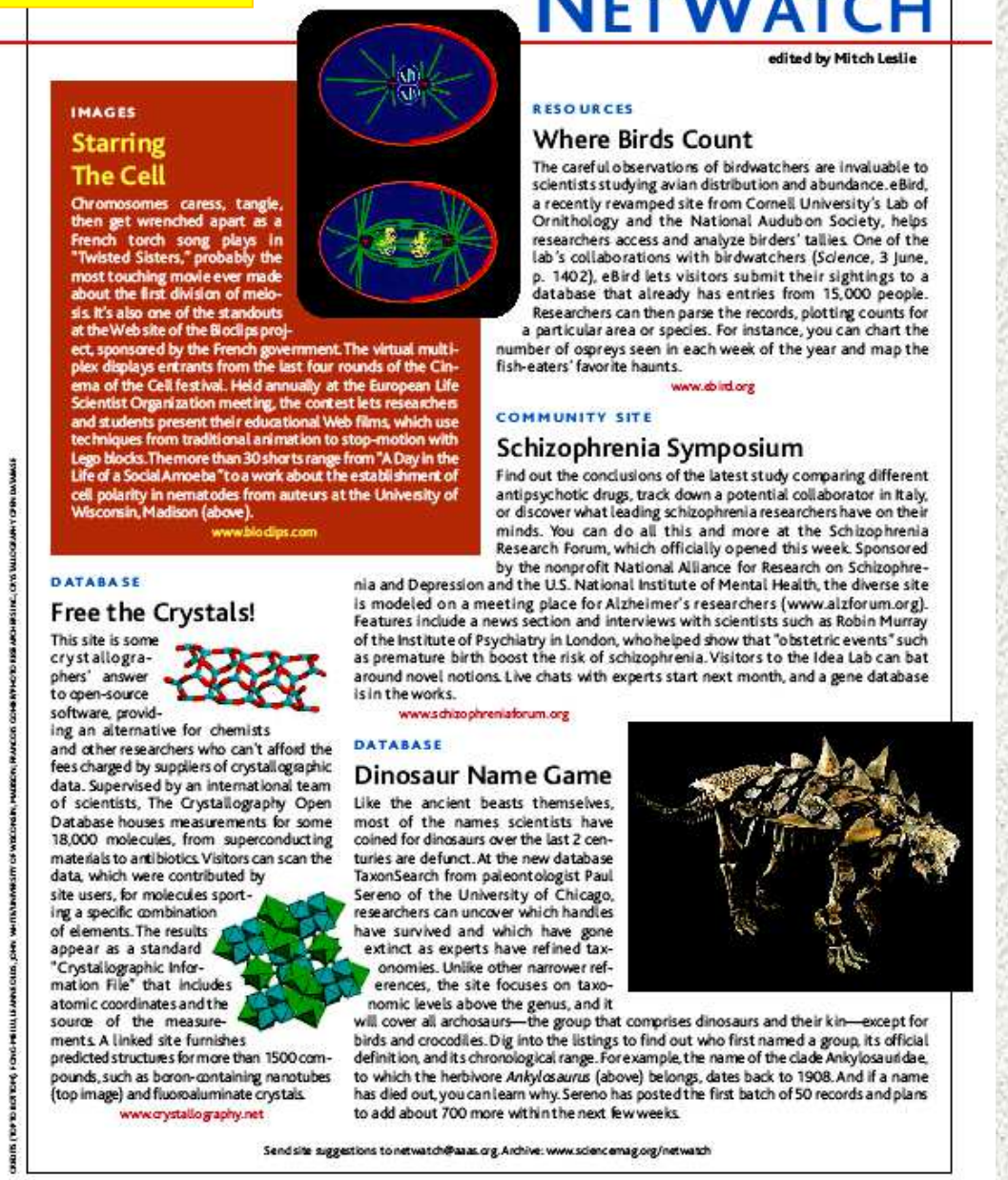
http://qiserver.ugr.es/cod

http://nanocrystallography.org

web portal: http://nanocrystallography.net

more than 240,000 entries



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

Crystallography Op ×

www.crystallography.net

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Open-access collection of crystal structures of organic, ino
metal-organic compounds and minerals, excluding biopol

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

COD Advisory Board thanks The Research Council of Lithuania for their financial
publication
"Crystallography Open Database (COD): an open-access collection of crystal
platform for world-wide collaboration",
Nucleic Acids Research. (2012) PDF version

We thank Crystal Impact GbR for their financial support of the publicati
"Crystallography Open Database - an open-access collection of crystal str
J. Appl. Crystallogr. (2009) PDF version

Currently there are **235786** entries in the COD.
Latest deposited structure: 7109374 on **2013-05-17** at **12:48:22 UT**

CIFs Donators

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_chemical_formula_sum              'As Ga O4'
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piezoelectric gallium arsenate, Ga As O4: temperature and pressure
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  'Armand, P'
  'Yot, P'
  'Cambon, O'
  'Goiffon, A'
  'McIntyre, G J'
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_cell_length_c                     11.3871(4)
_cell_angle_alpha                  90
_cell_angle_beta                   90
_cell_angle_gamma                  120
_cell_volume                       245.9
_cell_formula_units_Z              3
_symmetry_space_group_name_H-M     'P 31 2 1'
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_symmetry_cell_setting             trigonal
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  'y-x,-x,2/3+z'
  'y,x,-z'
  '-x,y-x,1/3-z'
  'x-y,-y,2/3-z'
loop
```

http://www.crystallography.net/result.php?id=20171%

Results

Result : There are 100 entries in the selection

You can download the COD numbers of the selection as a text file

You can download all files as a single ZIP archive

Searching COD ID like 20171%

COD ID: 2017100	
CIF file	Formula : - C5 H9 N O6 S -
HKL data	Comments : Minkov, Vasily S.; Boldyreva, Elena V. DL-Cysteinium semioxalate Acta Crystallographica Section C 65(5) (2009) o245-o247
Original IUCr paper	Space group :P -1 Cell volume: 443.62 Cell parameters:5.6664; 9.0149; 9.7749; 109.349; 102.282; 100.119;

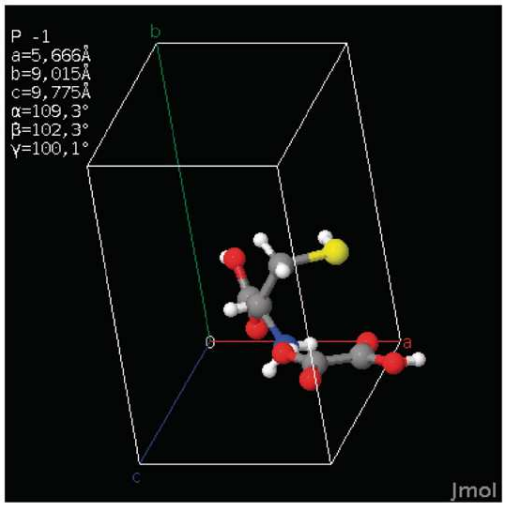
Gražulis S. et al. *Nucl. Acids Res.* 40 (2012) D420-D427, open access

Results | 2017100 - CIF informa...

Information card for 2017100

2017099 << **2017100** >> 2017101

Preview



CIF file

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HKL data file

Download 2017100.hkl

Original IUCr paper

Structure parameters

Common name	DL-cysteinium semioxalate
Chemical name	DL-Cysteinium semioxalate

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loop_
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_squared_calc
_refln_F_squared_meas
_refln_F_squared_sigma
_refln_observed_status
1 0 0 88.50 107.46 1.41 o
2 0 0 443.74 483.55 3.27 o
3 0 0 105.70 102.49 1.73 o
4 0 0 109.80 97.14 0.68 o
5 0 0 61.24 59.93 0.88 o
```


Acta Crystallographica Section C

Crystal Structure Communications

Volume 65, Part 5 (May 2009)

organic compounds

html | pdf | cif | 3d view | structure factors | cited in | similar papers | b

Acta Cryst. (2009). C**65**, o245-o247 [doi:10.1107

DL-Cysteinium semioxalate

V. S. Minkov and E. V. Boldyreva

Abstract: Two chiral counterparts (L- and D-cysteinium
are present in the structure of the title compound, C_3H_8
anion ratio. The carboxy group of the cysteinium cation
relative to the amino group. The crystal structure is built
cysteinium cations are connected to each other not direc
semioxalate anions linked to each other *via* O-H...O hydr
interesting feature of the crystal structure is the absenc
bonds.

Formula: $C_3H_8NO_2S^+ \cdot C_2HO_4^-$

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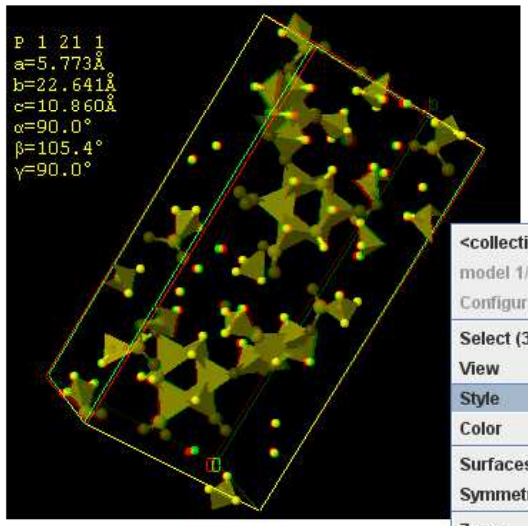
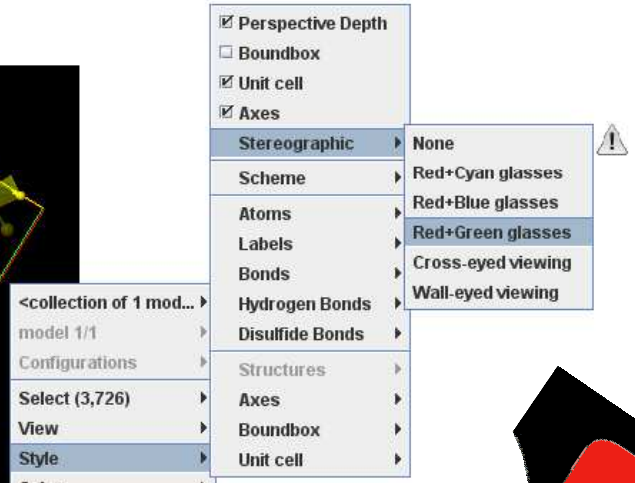
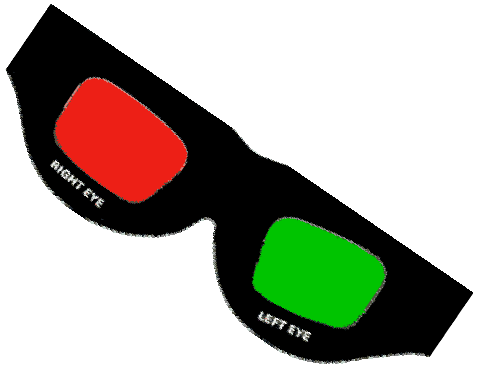
7109374 << **7150000** >> 7150001

Preview







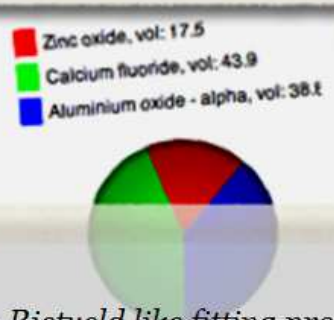
Coordinates 7150000.cif

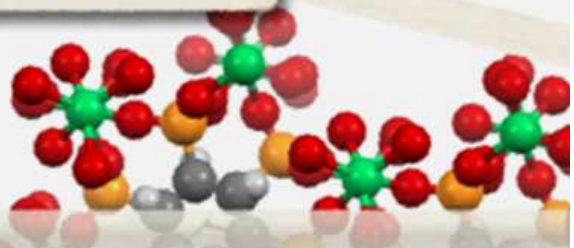
Structure parameters

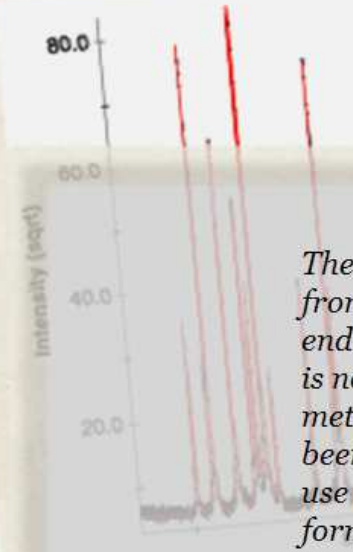
Formula	31 N O15 -
Calculated formula	31 N O15 -
Title of publication	elated to carba-pyranoses: synthesis of acetylated derivatives of 4-amino-2,4-dideoxy-3-O-(bet carba-pyranose from a D-glucose template.

Full Profile Search Match

by L. Lutterotti using COD







The "FPSM method" uses a Rietveld like fitting procedure to test all possible crystal structures from a Database, rank them and find the more probable in your diffraction pattern. In the end a Rietveld phase quantification is done with the phases identified. Be aware that if a phase is not present in the database (COD is used here), it cannot be found nor quantify; so this method is limited to only the phases for which a crystal structure has been determine and has been uploaded to the COD database. This page has been constructed to permit other people to use the method and test it on their data. To use it you need to upload a datafile in proper format. Use .prn, a double column format with no title line, first column contains the 2theta coordinates (d space for TOF), the second column the intensity (corrected for incident intensity for TOF). You need also to specify some additional instrument characteristics (wavelength, geometry etc.). If the selected instrumental broadening function much the one of your instrument, then a reasonable analysis of crystallite sizes and microstrain is reported.

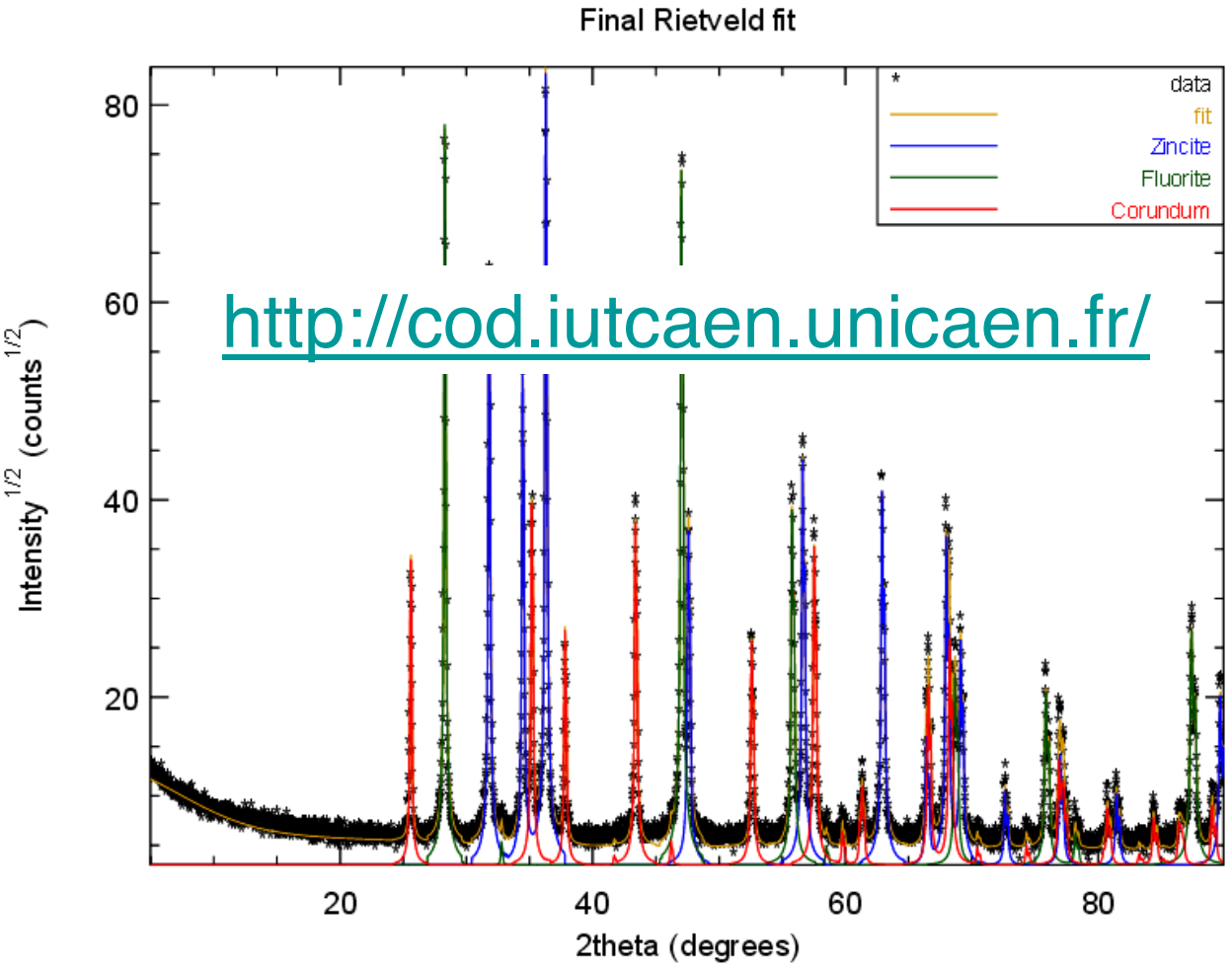
See paper: L. Lutterotti, H. Pilliere, C. Fontugne, P. Boullay, D. Chateigner (2013), submitted to J. Appl. Cryst.

Diffraction pattern and sample composition

Found phases and quantification:

Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9004178	Zincite	20.5148	29.1683	1893.8	4.76139e-08
1000043	Fluorite	42.3438	33.7285	2154.45	0.00036731
9007498	Corundum	37.1414	37.1032	1941.94	0.000229095

Final Rietveld analysis, Rw: 0.154707, GofF: 1.90021



34.160	88
34.180	90
34.200	94
34.220	129
34.240	148
34.260	201
34.280	219
34.300	313
34.320	449
34.340	580
34.360	858
34.380	1102
34.400	1600
34.420	2152
34.440	2777
34.460	2830
34.480	2766
34.500	2381
34.520	2052
34.540	1697
34.560	1354
34.580	961
34.600	696
34.620	392
34.640	265
34.660	187
34.680	146

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Validation and Deposition Interface

Log in | Upload a file | Validate data | Deposit structures | Finish

Choose deposition type

-- choose one --

Depositor details

Your name:

Your COD password (if you do not have a COD account yet, please type a new password that you remember and we will create an account for you):

Your e-mail address (*it will not be disclosed to 3rd parties*):

Begin deposition

About this Validation Interface

This interface allows you to upload, validate and edit CIF files before submitting them for deposition.

Steps

The process of files deposition, after you have uploaded your data is pretty simple.
First step, after files have been uploaded, is validation. Our scripts perform some checks to see if all necessary data are present in the submitted file. Results are displayed to you next to your files.
If a file is correct, you can deposit it to COD. After the deposition, COD numbers for the newly deposited structures will be displayed.
If a file is not correct you can edit it file in your browser window and validate it once more.

File formats

Currently we accept two types of files:

- Plain CIF files;
- ZIP archives, which does contain CIF files.

Top of the page

Done | Internet | 100%

1. Crystallography Open Database (COD) in its 11th year

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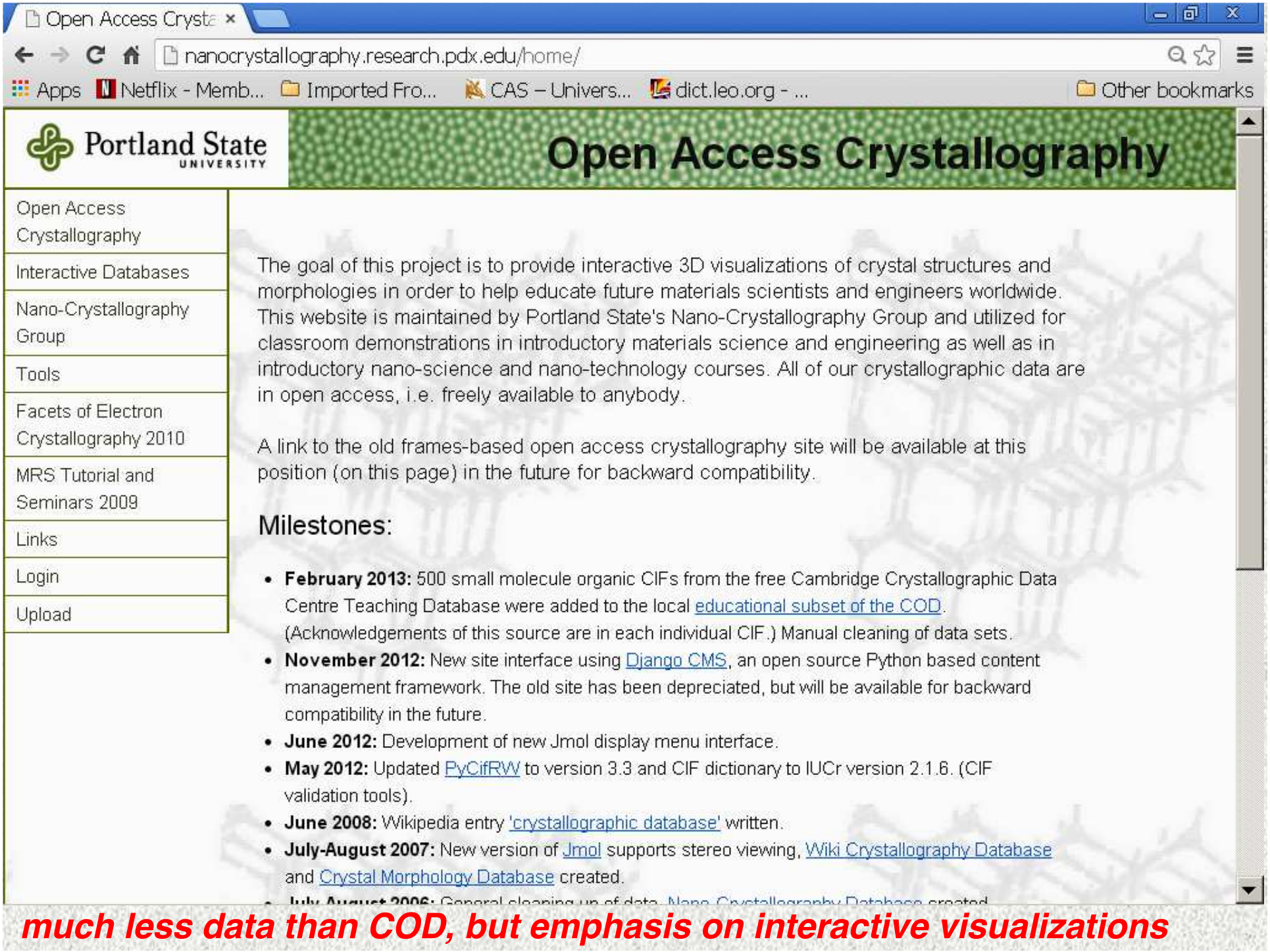

much less data than COD, but emphasis on interactive visualizations


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You have the recommended Java installed (Version 7 Update 45).
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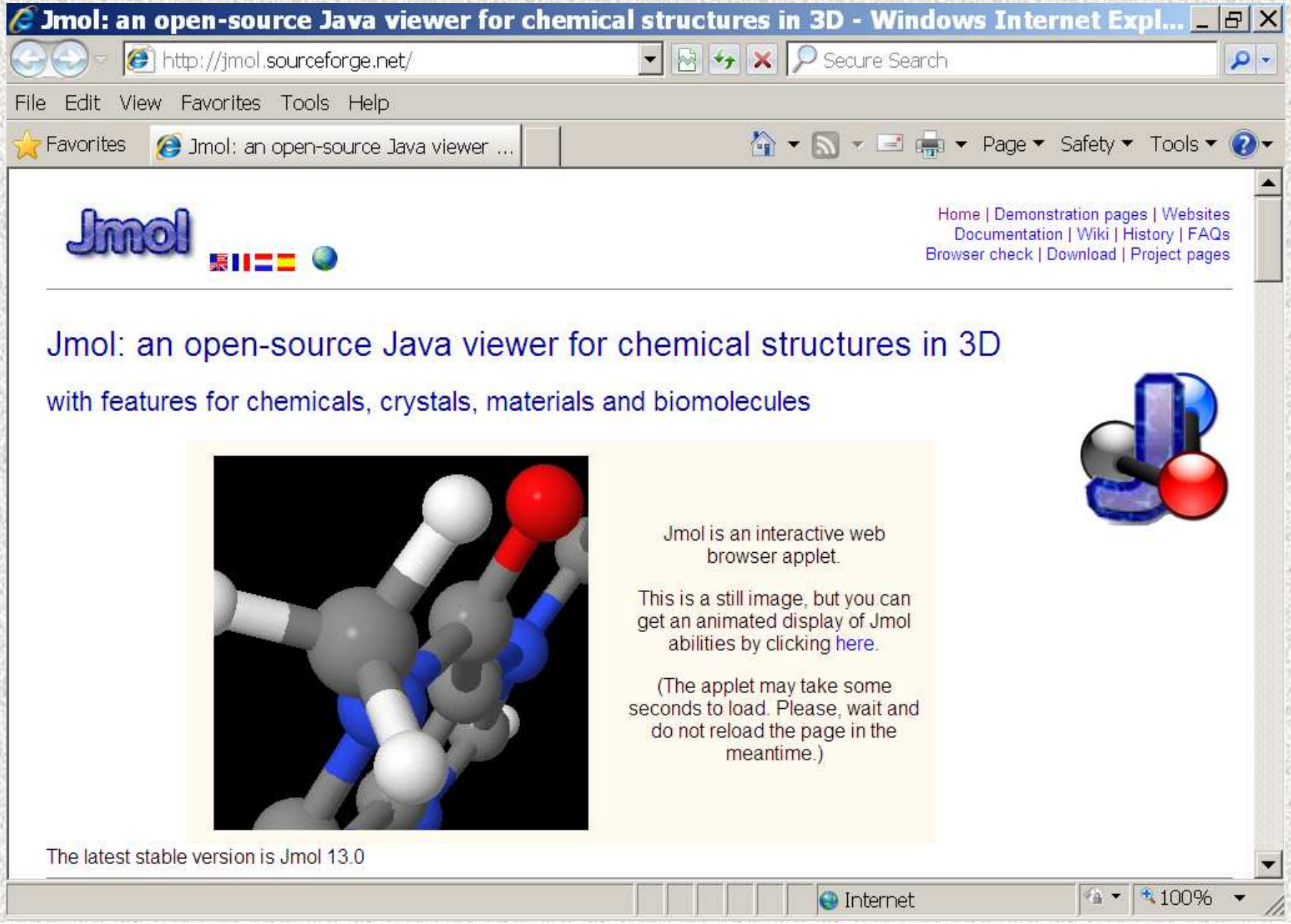
Feedback

Jmol: an open-source Java viewer for chemical structures in 3D.
http://www.jmol.org/



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jmol.sourceforge.net

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Security Warning

Do you want to run this application?

An unsigned application from the location below is requesting permission to run.

Location: http://jmol.sourceforge.net

Running unsigned applications like this will be blocked in a future release because it is potentially unsafe and a security risk.

More Information

Select the box below, then click run to start the application

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Run | Cancel

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Jmol: an open-source J

with features for chemicals,

This is the Jmol applet in action.

It is running a script written in the Jmol/RasMol/Chime scripting language.

It is *not* a movie, slide show, or animated image file ... Jmol is an interactive web browser applet.

The latest stable version is Jmol 13.0

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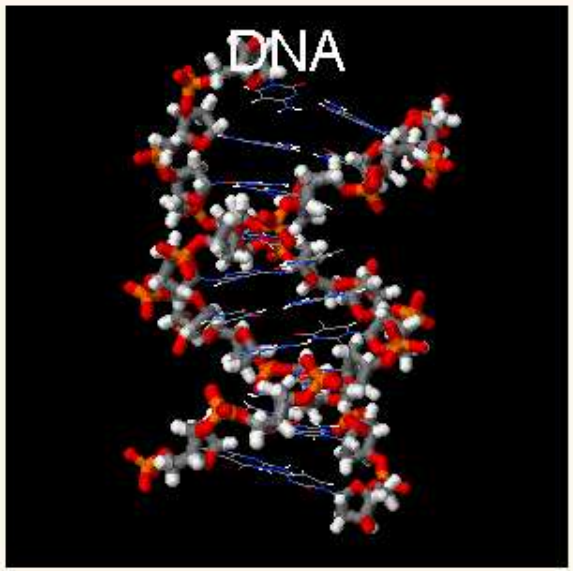
Jmol: an open-source Java viewer for chemical structures in 3D

with features for chemicals, crystals, materials and biomolecules



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Jmol: an open-source Java viewer for chemical structures in 3D - Mozilla Firefox

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Jmol: an open-source Java viewer for chemical structures in 3D

with features for chemicals, crystals, materials and biomolecules

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Check the warning message from your browser and/or enable Java applets in your web browser preferences, or install the Java Runtime Environment from www.java.com

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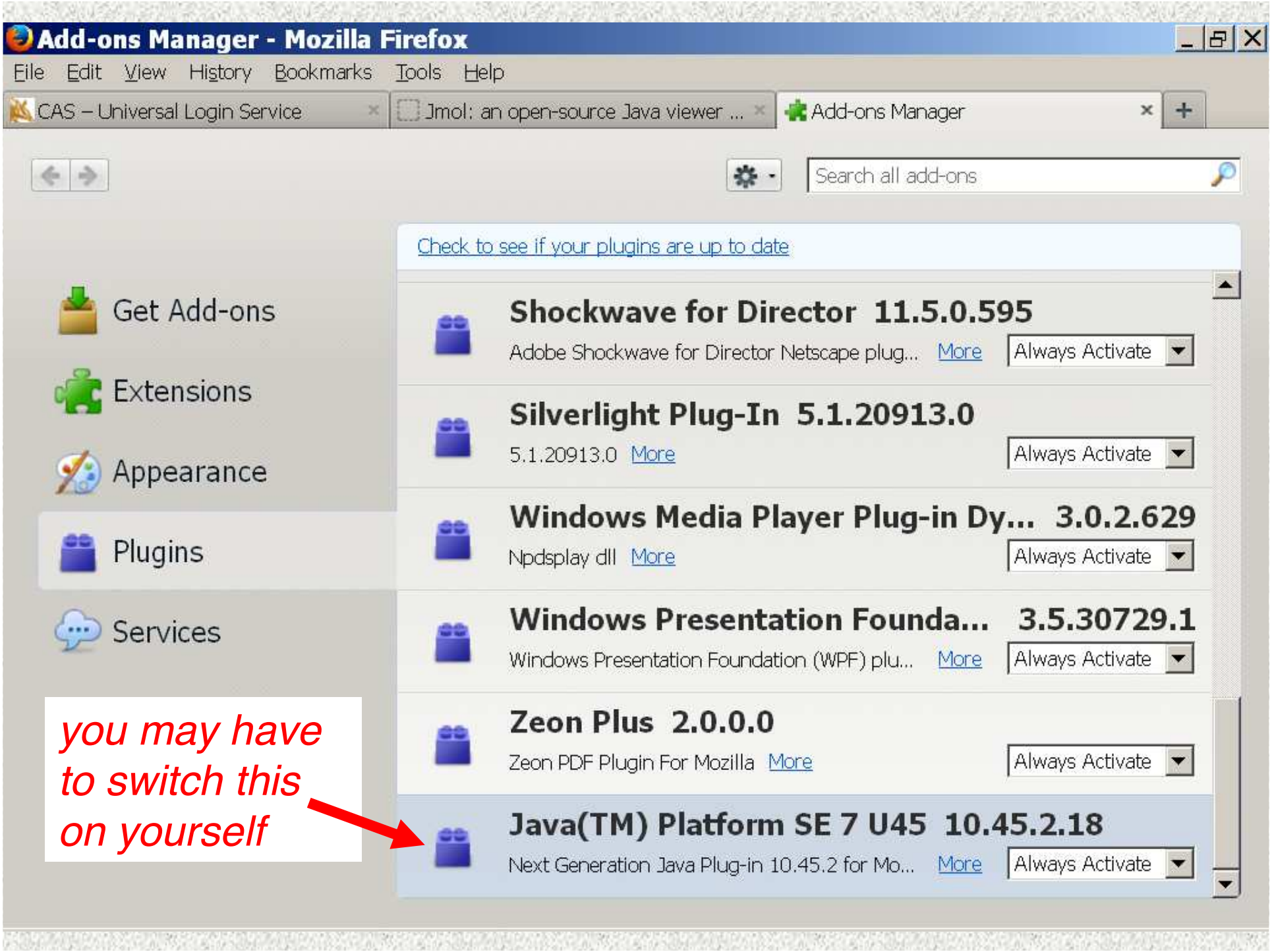
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CAS – Universal Login Service
Jmol: an open-source Java viewer ...
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Adobe Shockwave for Director Netscape plug... More
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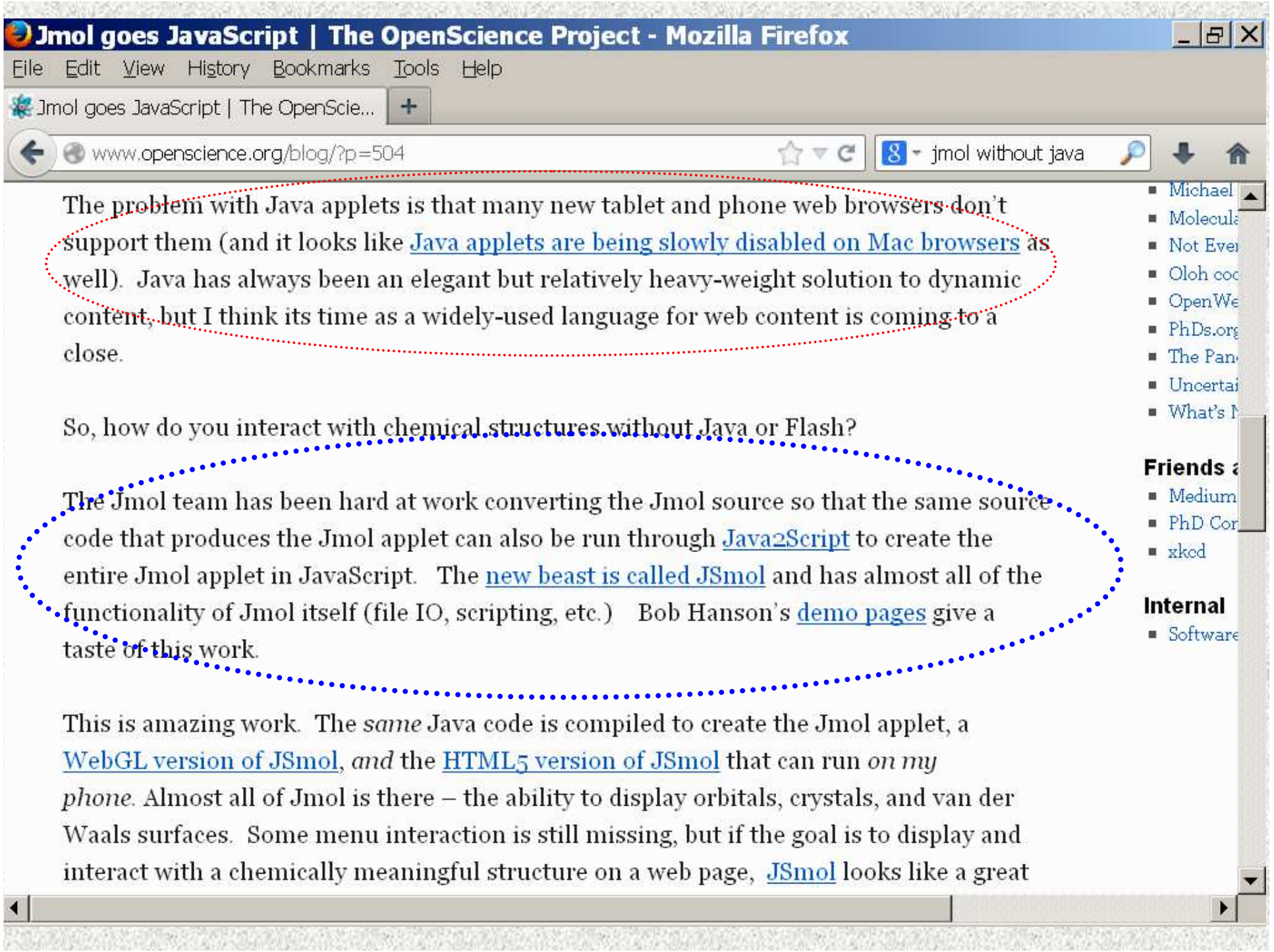
Silverlight Plug-In 5.1.20913.0
5.1.20913.0 More
Always Activate
Windows Media Player Plug-in Dy... 3.0.2.629
Npdsplay dll More
Always Activate
Windows Presentation Founda... 3.5.30729.1
Windows Presentation Foundation (WPF) plu... More
Always Activate
Zeon Plus 2.0.0.0
Zeon PDF Plugin For Mozilla More
Always Activate
Java(TM) Platform SE 7 U45 10.45.2.18
Next Generation Java Plug-in 10.45.2 for Mo... More
Always Activate
you may have to switch this on yourself


Jmol goes JavaScript | The OpenScience Project - Mozilla Firefox
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Jmol goes JavaScript | The OpenScie...
www.openscience.org/blog/?p=504
jmol without java
The problem with Java applets is that many new tablet and phone web browsers don't support them (and it looks like Java applets are being slowly disabled on Mac browsers as well). Java has always been an elegant but relatively heavy-weight solution to dynamic content, but I think its time as a widely-used language for web content is coming to a close.
So, how do you interact with chemical structures without Java or Flash?
The Jmol team has been hard at work converting the Jmol source so that the same source code that produces the Jmol applet can also be run through Java2Script to create the entire Jmol applet in JavaScript. The new beast is called JSmol and has almost all of the functionality of Jmol itself (file IO, scripting, etc.) Bob Hanson's demo pages give a taste of this work.
This is amazing work. The same Java code is compiled to create the Jmol applet, a WebGL version of JSmol, and the HTML5 version of JSmol that can run on my phone. Almost all of Jmol is there – the ability to display orbitals, crystals, and van der Waals surfaces. Some menu interaction is still missing, but if the goal is to display and interact with a chemically meaningful structure on a web page, JSmol looks like a great
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Interactive Databases - Windows Internet Explorer

http://nanocrystallography.research.pdx.edu/databases/

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- Open Access Crystallography
- Interactive Databases
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  - EDU-COD
  - Crystal Morphology Database
  - Nano-Crystallography Database
  - Wiki Crystallography Database
- Nano-Crystallography Group
- Tools
- Facets of Electron Crystallography 2010
- MRS Tutorial and Seminars 2009
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- Upload

Crystallography Open Database [Mirror, modified search interface and Jmol displays] Search and view

Wiki Crystallography Database Search and view

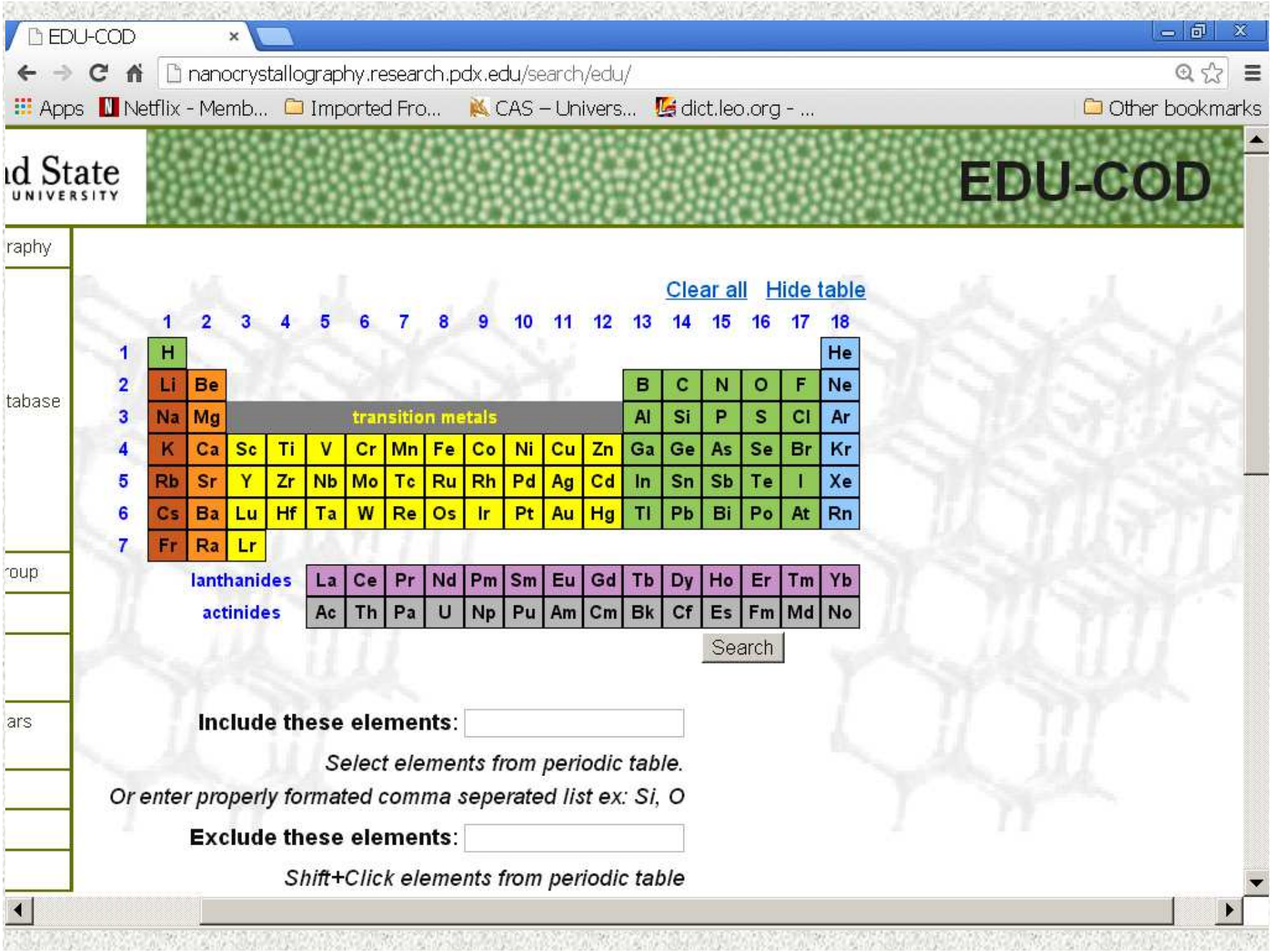
Educational subset of COD Search and view

Nano-Crystallography Database Search and view

Crystal Morphology Database Search and view

Several crystallography databases are offered for browsing. You can search the databases, download and display the contained Crystallographic Information Files (CIFs), view 3D models of the encoded crystal structures and morphologies.

We also provide the North American mirror of the Crystallography Open Database (COD). This is the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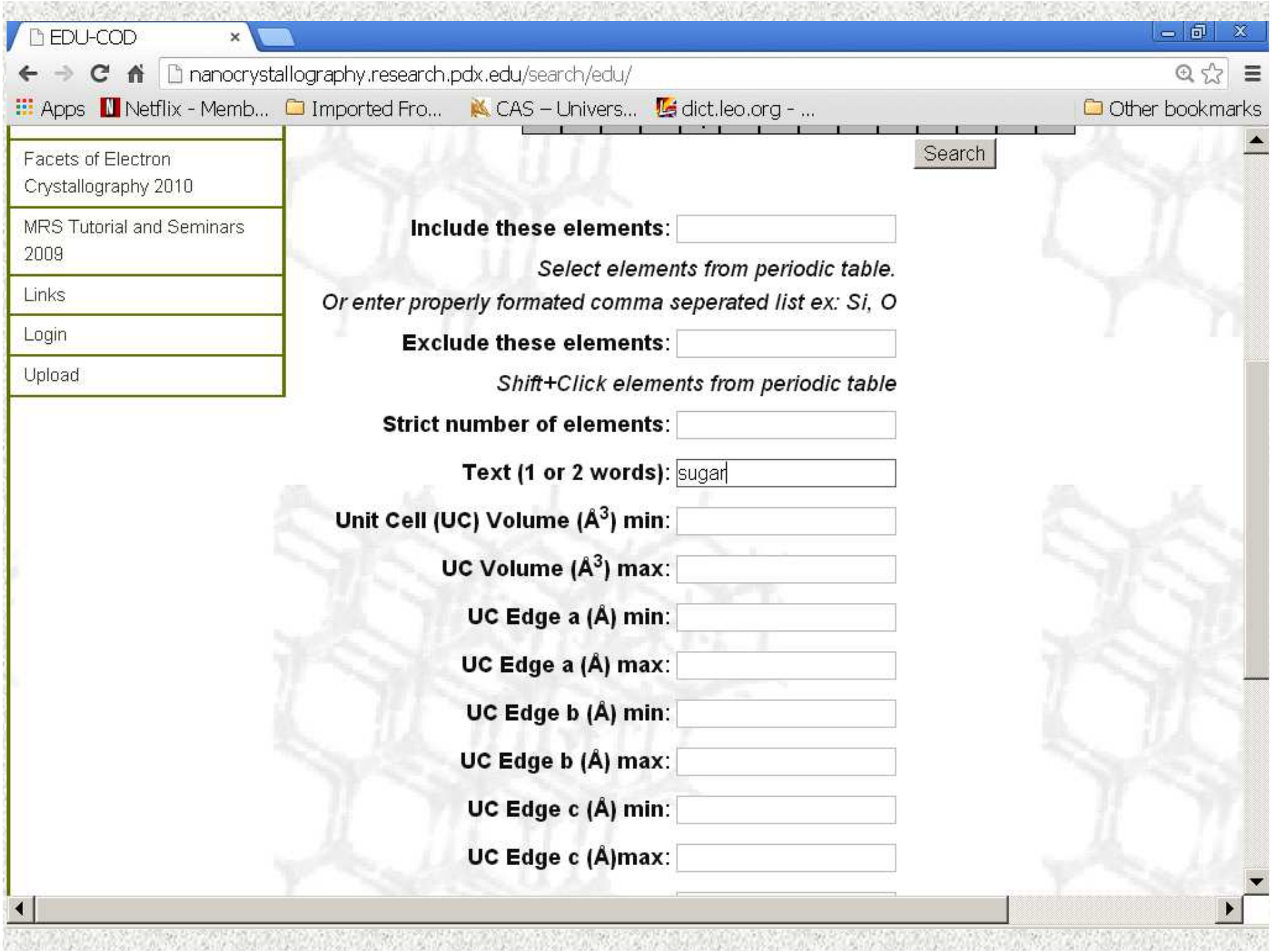
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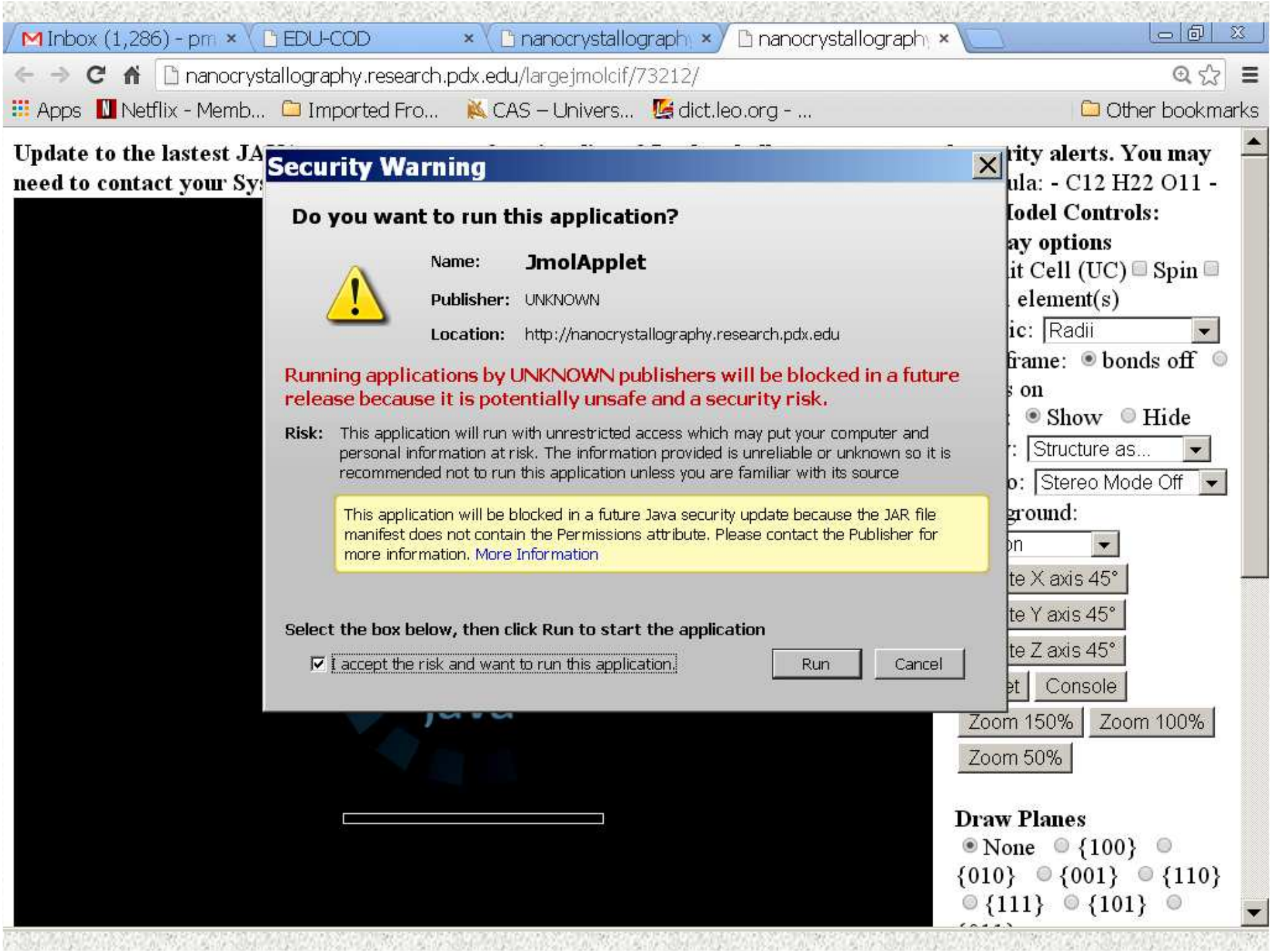
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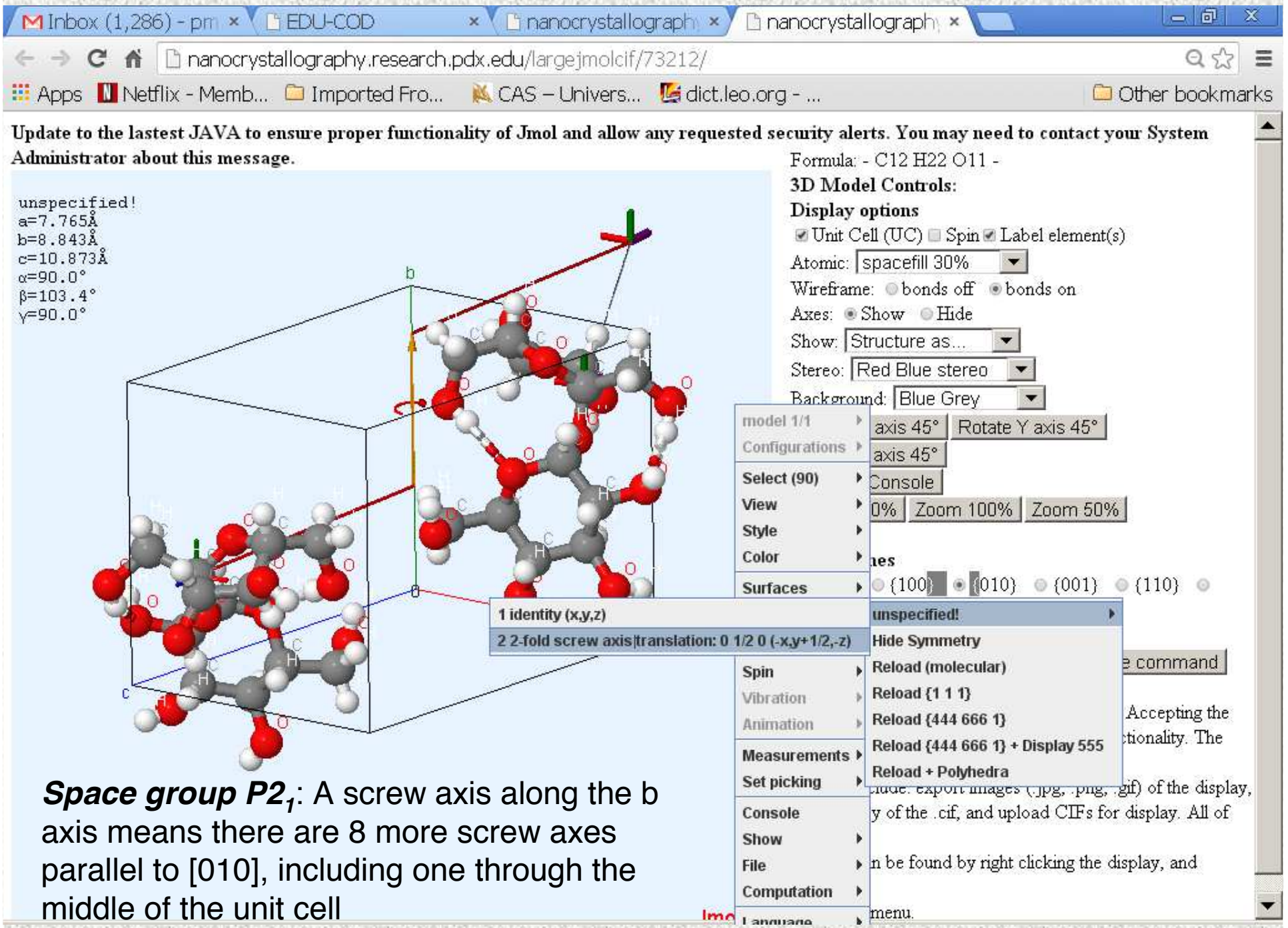
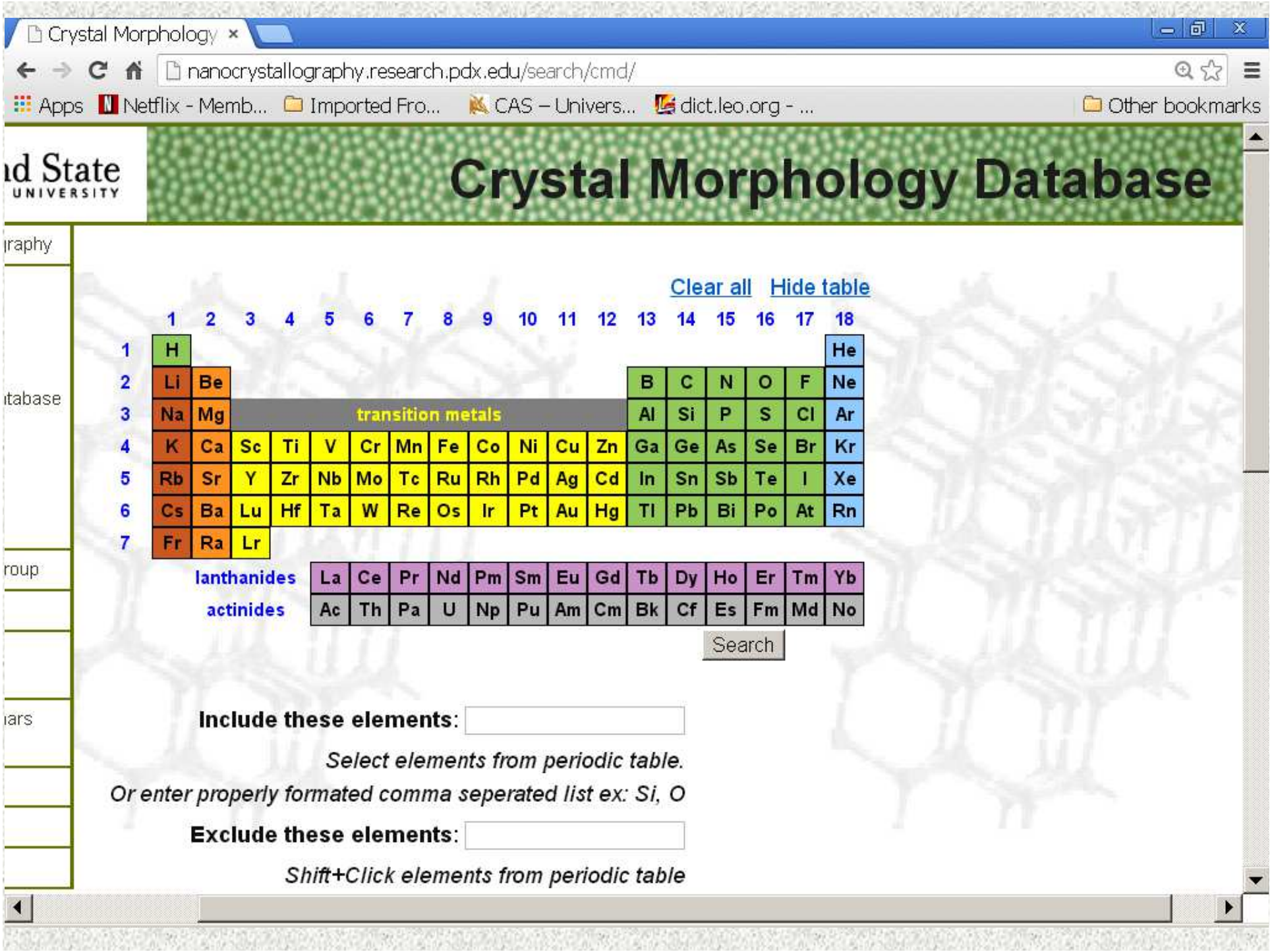
Security Warning
Do you want to run this application?
Name: JmolApplet
Publisher: UNKNOWN
Location: http://nanocrystallography.research.pdx.edu
Running applications by UNKNOWN publishers will be blocked in a future release because it is potentially unsafe and a security risk.
Risk: This application will run with unrestricted access which may put your computer and personal information at risk. The information provided is unreliable or unknown so it is recommended not to run this application unless you are familiar with its source
This application will be blocked in a future Java security update because the JAR file manifest does not contain the Permissions attribute. Please contact the Publisher for more information. More Information
Select the box below, then click Run to start the application
I accept the risk and want to run this application.
Run
Cancel



Space group $P2_1$: A screw axis along the b axis means there are 8 more screw axes parallel to [010], including one through the middle of the unit cell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6 Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
7 Fr Ra Lr
lanthanides La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
actinides Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No
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Or enter properly formated comma seperated list ex: Si, O
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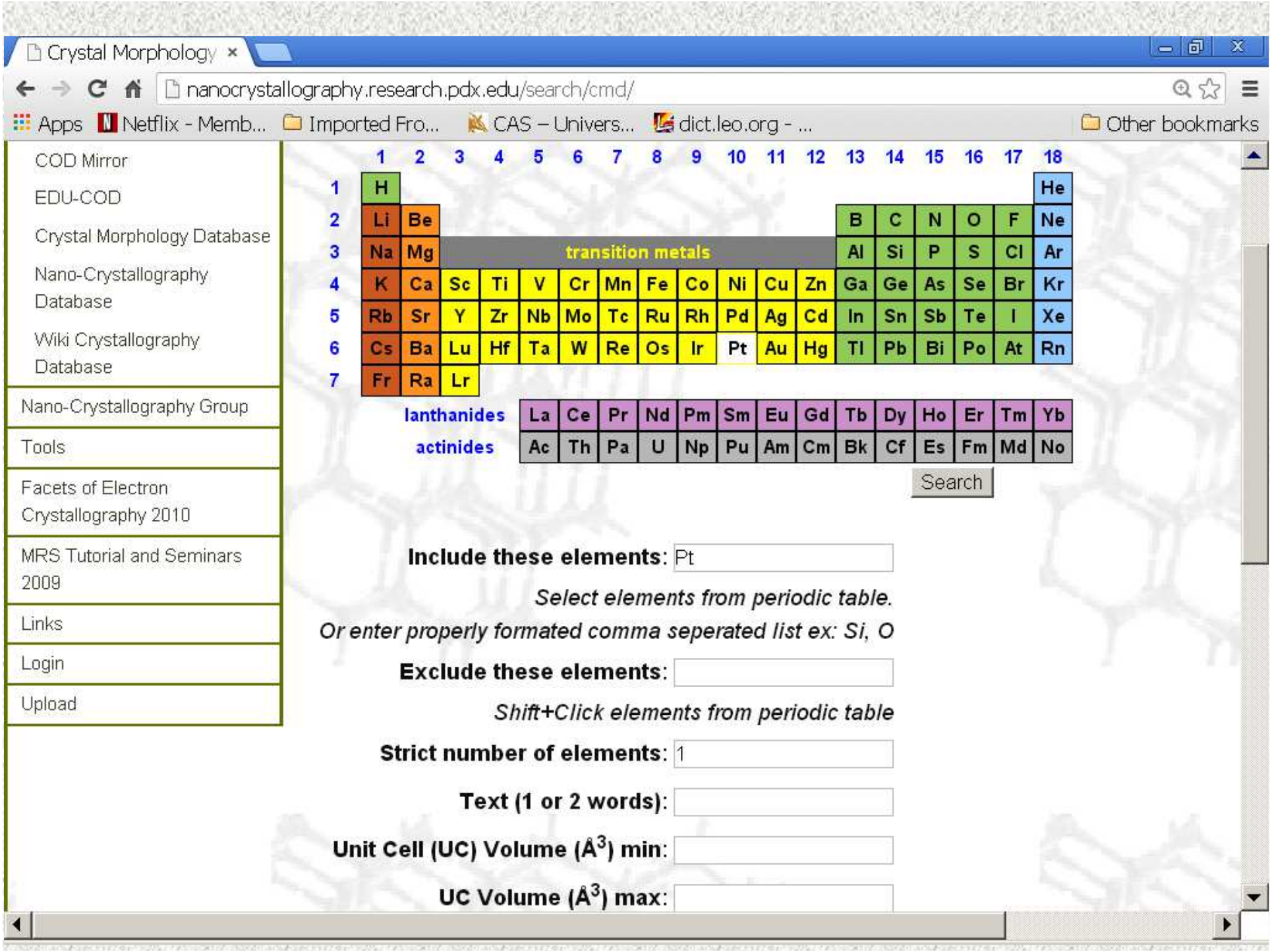
Shift+Click elements from periodic table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Li Be B C N O F Ne
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Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
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actinides Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No
Search
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Select elements from periodic table.
Or enter properly formated comma seperated list ex: Si, O
Exclude these elements:
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Crystal Morphology ×

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Crystal Morphology Database

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- Interactive Databases
  - COD Mirror
  - EDU-COD
  - Crystal Morphology Database
  - Nano-Crystallography Database
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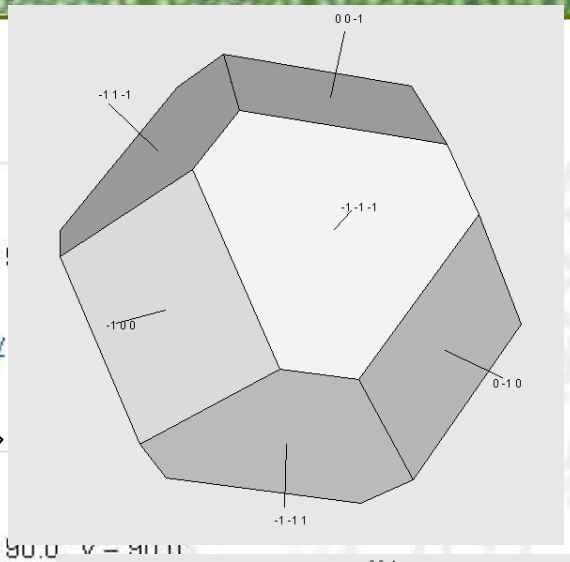
There are 4 results.

Formula:- Pt -
Cell Parameters: *a* = 3.923Å *b* = 3.923Å *c* = 3.923Å *α* = 90.0° *β* =
Cell Volume = 60.37Å^3
View CIF | View Structure in Jmol V12 | View Structure in Jmol (large window) | View Morphology



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Cell Volume = 60.37Å^3
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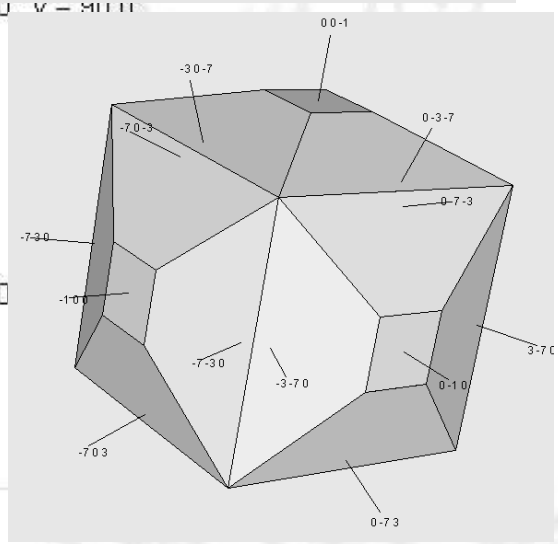

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Cell Parameters: *a* = 3.923Å *b* = 3.923Å *c* = 3.923Å *α* = 90.0° *β* = 90.0
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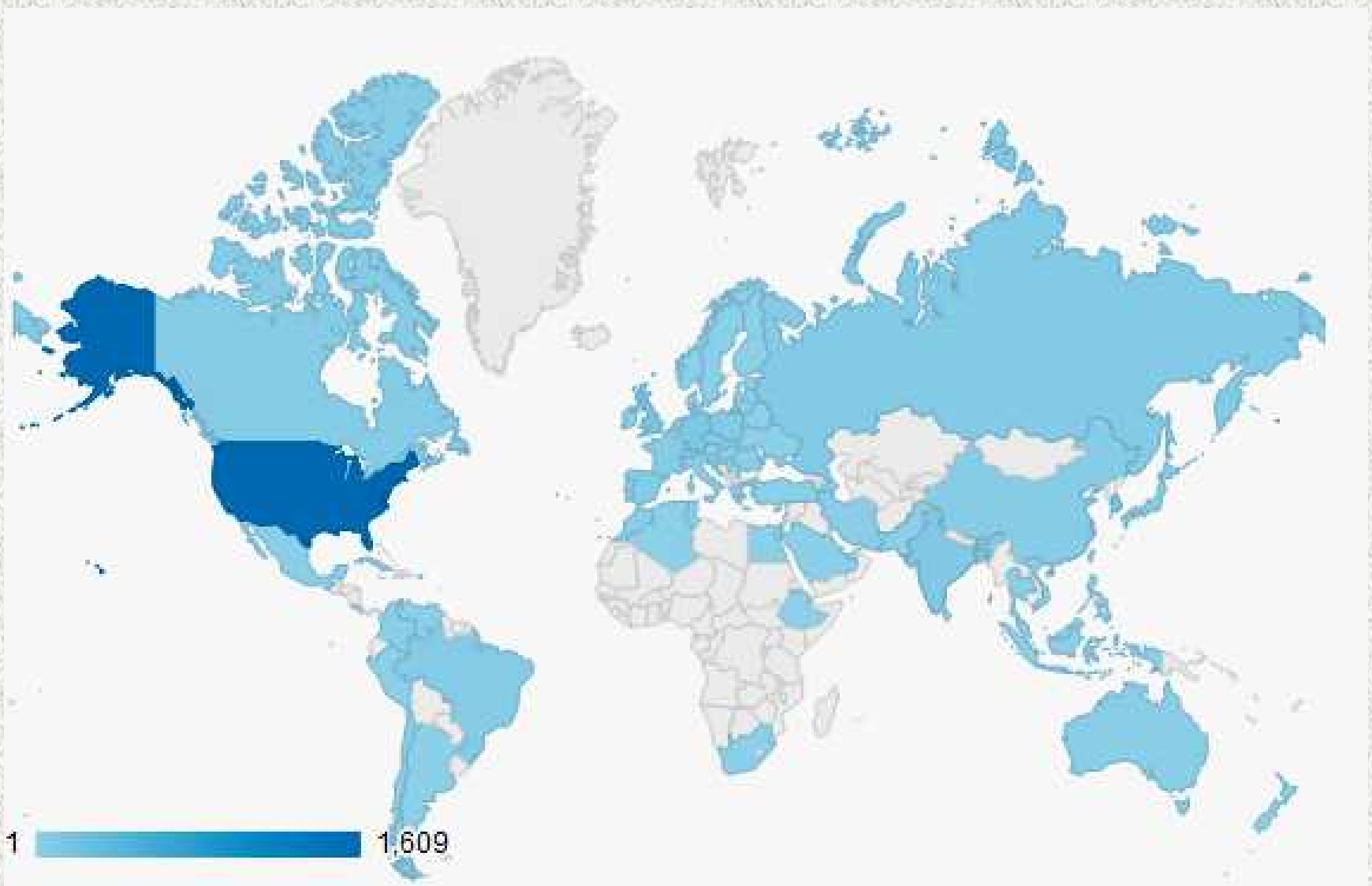
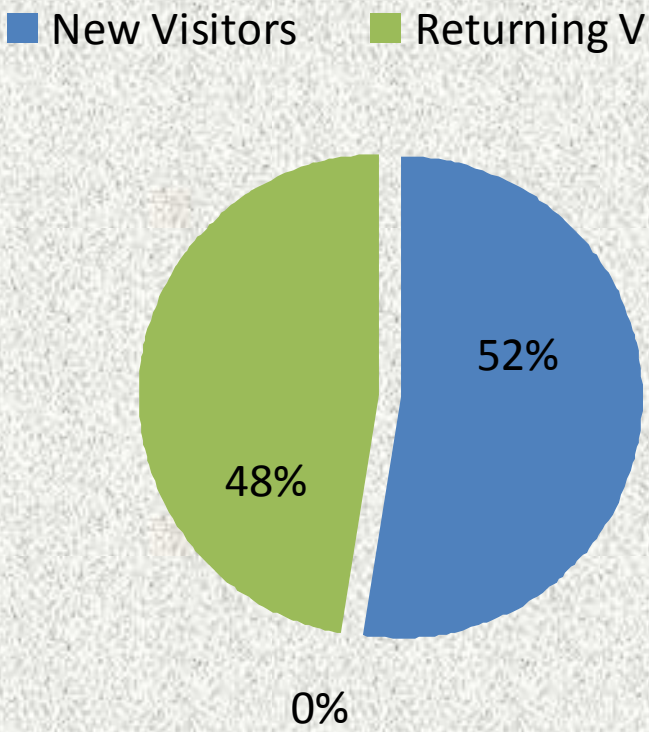


Results of the first year of counting access to nanocrystallography.research.pdx.edu, rewritten for tablet computers, end of July 2013

	Country / Territory	Visits ↓	Visits
		2,723 % of Total: 100.00% (2,723)	2,723 % of Total: 100.00% (2,723)
1.	United States	1,384	50.83%
2.	South Korea	186	6.83%
3.	Germany	113	4.15%
4.	United Kingdom	89	3.27%
5.	India	85	3.12%
6.	Russia	76	2.79%
7.	Poland	69	2.53%
8.	Canada	63	2.31%
9.	Brazil	50	1.84%
10.	Spain	44	1.62%

Results of the first year of counting access to nanocrystallography.research.pdx.edu, rewritten for tablet computers, end of July 2013



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Open Access Crystallography Resource Portal
all good open access crystallography resources, e.g. CIFs, space group drawings, history, …
IYCr2014
International Year of Crystallography: 100 years of modern crystallography http://www.iucr.org/iycr.
Welcome to the Open Access Crystallography Resource Portal
COD
Crystallography Open Database: Contains more then 240,000 small molecules and small to medium unit cell crystal structures (including minerals but excluding biopolymers). Main sites www.crystallography.net (in France) and cod.ibt.lt (in Lithuania). Less frequently updated mirrors cod.ensicaen.fr (in France), qiserver.ugr.es/cod (in Spain), nanocrystallography.org and nanocrystallography.research.pdx.edu/search/codmirror/ (in North America).
http://nanocrystallography.net
EΔU COD
C M D {1 1 1}
Portland State University's Nano-Crystallography Group: nanocrystallography.research.pdx.edu hosts small educational open access databases of common crystal structures (e.g. EDU-COD and

1. Crystallography Open Database (COD) in its 11th year

2. Supporting efforts at Portland State University (PSU, in their 10th year)

***3. Courses where basic crystallographic education is provided at PSU** (mainly in disguise as nano-science and nano-tech)*

4. 400/500 level course assignments (without solutions)

5. 3D printing from Crystallographic Information Files (CIF)

6. Summary and Outlook

www.pdx.edu/pnna/courses

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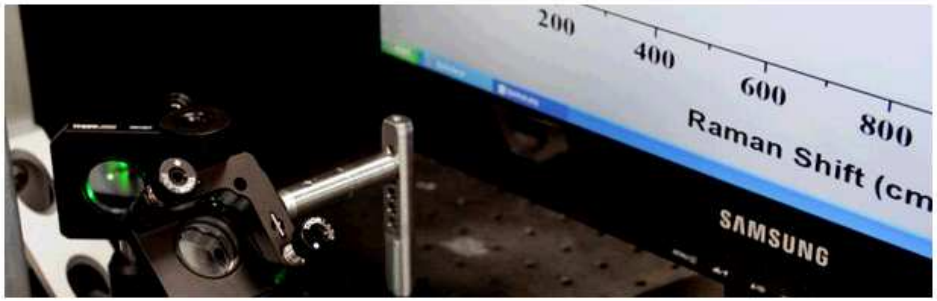

Currently PNNA members are offering the following courses related to nanoscience and nanotechnology.

PH 382 "Introduction to Nanoscience and Nanotechnology"

An introductory upper division (science) course that will serve all interested science, engineering, social science, and humanities students. The learning objectives are: (1) Appreciation of how science and technology at the nanometer length scale differ from traditional science and technology at larger length scales; (2) Appreciation of the convergence of all natural sciences at the nanometer length scale; (3) Appreciation that this convergence offers unprecedented opportunities of nanoengineering resulting in nanotechnologies; and (4) Appreciation of the effects of nanoscience and nanotechnology on society and students' future personal life.

BI 372 "Nanotechnology, Society and Sustainability"

Nanotechnology has broad implications and applications, ranging from environmental remediation and/or contamination to social justice and equity applications in developing countries, to biomedical treatments and interventions, to intellectual property dilemmas. Students will gain familiarity with nanotechnology within these contexts, and develop skills in analyzing and balancing risks and benefits grounded in a sound understanding of the science behind nanotechnology applications.

ECE 317 "Nanotechnology: Modeling & Simulations"

Introduction to basic electrical concepts, nanotechnology, and the principles of modeling and simulation. Modeling and simulation are used to examine environmental and health hazards and the applications of nanotechnology in environmental and biomedical sensing and in current and future nanoelectronic technologies.

CH 445/545, ECE 410, and PH 410/510 "Fabrication and Characterization of Nanomaterials"

is a hands on training course on standard as well as emergent fabrication and characterization techniques. In the 02 credit version students are exposed to the process of designing and fabricating of patterns on silicon

currently, there is a total of 7 courses offered, three of then at the 300 level

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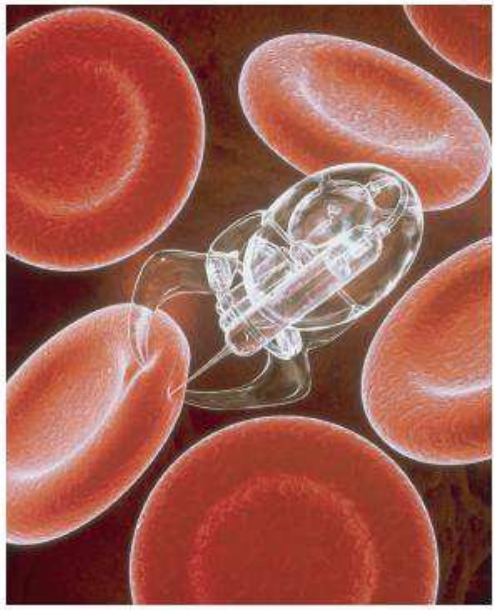
PH 382, part of a new 4 course sequence on the basis of recent NSF funding

Three lecture course sequence, one laboratory course under development, supporting information on poster by Morris, Weasel and Moeck

Introduction to Nanoscience and Nanotechnology for STEM and non STEM students as part of Portland State's general education program, called University Studies – Science Cluster

My approach:

that is nonsense



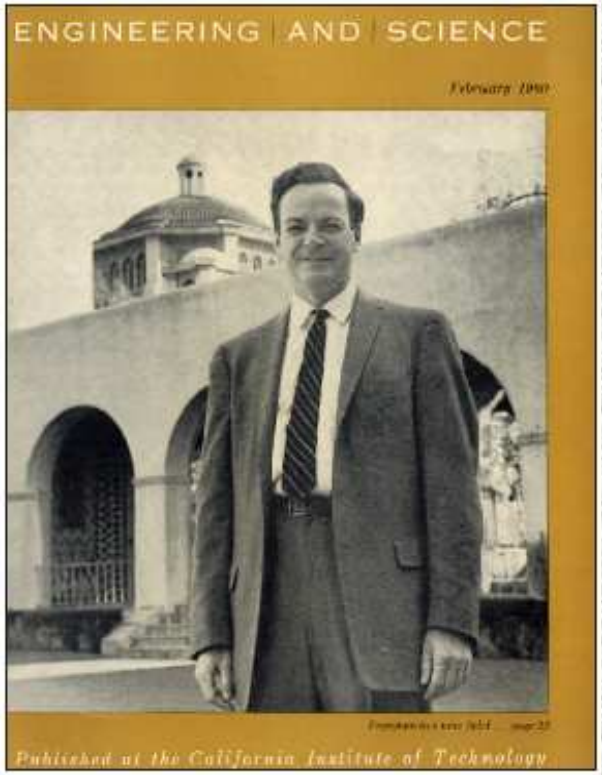
why? Because this guy worked it out more than 100 years ago!

"… there is no such thing as nanotechnology. Nanotechnology is now the buzzword and an umbrella term to designate nothing less than the state-of-the-art in science and technology in what is the normal progression and evolution of the relationship of humankind with its habitat and environment."

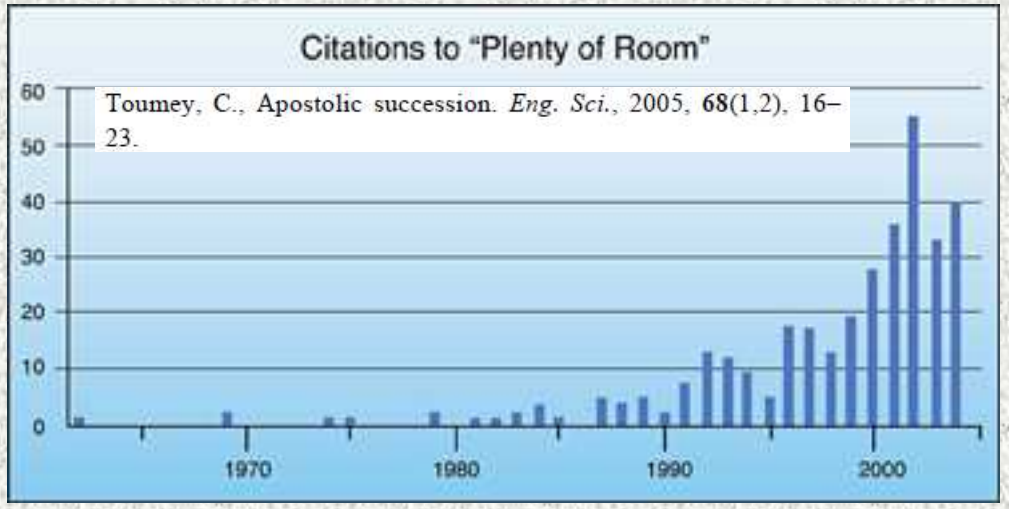
D. Jost, "Nanotechnology for Policymakers, An Introduction from the Physical Science Perspective", *nccr trade regulations*, Swiss national center of competence in research, working paper no. 2009/21, May 2009; http://phase1.nccr-trade.org/images/stories/publications/IP9/ed.Nanotechnology Introduction v9 march2009.pdf

whole course has the message "do consider taking more science and engineering classes, it's both interesting and useful at the same time"

There's plenty …



Eng. Sci. **23**(5) 22-36, 1960



"I am not inventing antigravity, which is possible someday only if the laws are not what we think. I am telling you what could be possible if the laws are what we think; ***we are not doing it simply because we haven't gotten around to it****."*

"… ***"it is an unwritten rule on Nature Nanotechnology that Richard Feynman's famous 1959 lecture 'There's Plenty of room at the Bottom' should not be referred to at the start of articles unless absolutely necessary,"*** wrote editor in chief Peter Rodgers in the December 2009 isue …
Not that Rodgers has anything against the talk, he went on to say—he'd simply like to see a little variety in his opening lines. (He forbids references to Moore's law for the same reason.) …"

DS (might be Sara DiPalma, copy editor of ***Engineering and Science*** Volume LXXIII, Number 1, WINTER 2010)
http://calteches.library.caltech.edu/705/1/ES73.1.2010.pdf

from 1905/1906 onwards Nanoscience becomes quantitative, published February 8, 1906

ANNALEN
DER
PHYSIK.

BEGRÜNDET UND FORTGEFÜHRET DURCH
F. A. C. GREN, L. W. GILBERT, J. C. POGGENDORFF, G. UND E. WIEDEMANN.

VIERTE FOLGE.

BAND 19.

DER GANZEN REIHE 324. BAND.

KURATORIUM:
F. KOHLRAUSCH, M. PLANCK, G. QUINCKE,
W. C. RONTGEN, E. WARBURG.

UNTER MITWIRKUNG
DER DEUTSCHEN PHYSIKALISCHEN GESELLSCHAFT
UND INSBESONDERE VON
M. PLANCK

HERAUSGEGEBEN VON
PAUL DRUDE.

MIT FÜNF FIGURENTAFELN.

LEIPZIG, 1906.
VERLAG VON JOHANN AMBROSIUS BARTH.

3. ***Eine neue Bestimmung der Molekül-dimensionen; von A. Einstein.***

Die ältesten Bestimmungen der wahren Größe der Moleküle hat die kinetische Theorie der Gase ermöglicht, während die an Flüssigkeiten beobachteten physikalischen Phänomene bis jetzt zur Bestimmung der Molekülgrößen nicht gedient haben. Es liegt dies ohne Zweifel an den bisher unüberwindlichen Schwierigkeiten, welche der Entwickelung einer ins einzelne gehenden molekularkinetischen Theorie der Flüssigkeiten entgegenstehen. In dieser Arbeit soll nun gezeigt werden, daß man die Größe der Moleküle des gelösten Stoffs in einer nicht dissoziierten verdünnten Lösung aus der inneren Reibung der Lösung und des reinen Lösungsmittels und aus der Diffusion des gelösten Stoffes im Lösungsmittel ermitteln kann, wenn das Volumen eines Moleküls des gelösten Stoffs groß ist gegen das Volumen eines Moleküls des Lösungsmittels. Ein derartiges gelöstes Molekül wird sich nämlich bezüglich seiner Beweglichkeit im Lösungsmittel und bezüglich seiner Beeinflussung der inneren Reibung des letzteren annähernd wie ein im Lösungsmittel suspendierter fester Körper verhalten, und es wird erlaubt sein, auf die Bewegung des Lösungsmittels in unmittelbarer Nähe eines Moleküls die hydrodynamischen Gleichungen anzuwenden, in welchen die Flüssigkeit als homogen betrachtet, eine molekulare Struktur derselben also nicht berücksichtigt wird. Als Form der festen Körper, welche die gelösten Moleküle darstellen sollen, wählen wir die Kugelform.

§ 1. **Über die Beeinflussung der Bewegung einer Flüssigkeit durch eine sehr kleine in derselben suspendierte Kugel.**

Es liege eine inkompressible homogene Flüssigkeit mit dem Reibungskoeffizienten k der Betrachtung zugrunde, deren Geschwindigkeitskomponenten u, v, w als Funktionen der Koordinaten x, y, z und der Zeit gegeben seien. Von einem beliebigen Punkt x_0, y_0, z_0 aus denken wir uns die Funktionen u, v, w als Funktionen von $x-x_0$, $y-y_0$, $z-z_0$ nach

Wir wollen die Rechnung für wässerige Zuckerlösung durchführen. Nach den oben mitgeteilten Angaben über die innere Reibung der Zuckerlösung folgt zunächst für 20° C.:

$$NP^3 = 200.$$

Nach Versuchen von Graham (berechnet von Stefan) ist der Diffusionskoeffizient von Zucker in Wasser bei 9,5° C. 0,384, wenn der Tag als Zeiteinheit gewählt wird. Die Zähigkeit des Wassers bei 9,5° ist 0,0135. Wir wollen diese Daten in unsere Formel für den Diffusionskoeffizienten einsetzen, trotzdem sie an 10 proz. Lösungen gewonnen sind und eine genaue Gültigkeit unserer Formel bei so hohen Konzentrationen nicht zu erwarten ist. Wir erhalten

$$NP = 2{,}08 \cdot 10^{16}.$$

Aus den für NP^3 und NP gefundenen Werten folgt, wenn wir die Verschiedenheit von P bei 9,5° und 20° vernachlässigen,

$$P = 9{,}9 \cdot 10^{-8}\ \text{cm},$$
$$N = 2{,}1 \cdot 10^{23}.$$

Der für N gefundene Wert stimmt der Größenordnung nach mit den durch andere Methoden gefundenen Werten für diese Größe befriedigend überein.

Bern, den 30. April 1905.

(Eingegangen 19. August 1905.)

A. Einstein, “Eine neue Bestimmung der Moleküldimensionen”, *Annalen der Physik*, vol. **19**, pp. 289-306, 1906

11. ***Berichtigung zu meiner Arbeit: „Eine neue Bestimmung der Molekül-dimensionen“*** [1]***;***
von A. Einstein.

Vor einigen Wochen teilte mir Hr. Bacelin, der auf Veranlassung von Hrn. Perrin eine Experimentaluntersuchung über die Viskosität von Suspensionen ausführte, brieflich mit, daß der Viskositätskoeffizient von Suspensionen nach seinen Resultaten erheblich größer sei, als der in § 2 meiner Arbeit entwickelten Formel entspricht. Ich ersuchte deshalb Hrn. Hopf, meine Rechnungen nachzuprüfen, und er fand in der Tat einen Rechenfehler, der das Resultat erheblich fälscht. Diesen Fehler will ich im folgenden berichtigen.

Legt man die berichtigte Formel zugrunde, so erhält man für das Volumen von 1 g in Wasser gelöstem Zucker statt des in § 3 angegebenen Wertes 2,45 cm³ den Wert 0,98, also einen vom Volumen 0,61 von 1 g festem Zucker erheblich weniger abweichenden Wert. Endlich erhält man aus der inneren Reibung und Diffusion von verdünnten Zuckerlösungen statt des im Anhange jener Arbeit angegebenen Wertes $N = 4{,}15 \cdot 10^{23}$ für die Anzahl der Moleküle im Grammolekül den Wert $6{,}56 \cdot 10^{23}$.

Zürich, Januar 1911.

(Eingegangen 21. Januar 1911.)

ibid vol. **34**, pp. 591-592, 1911

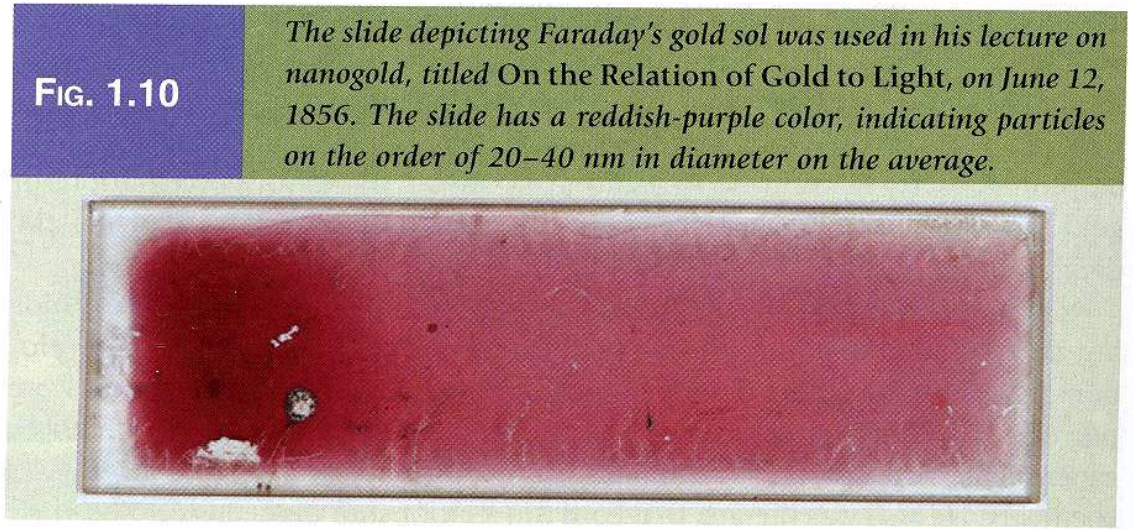


FIG. 1.10 *The slide depicting Faraday's gold sol was used in his lecture on nanogold, titled* On the Relation of Gold to Light, *on June 12, 1856. The slide has a reddish-purple color, indicating particles on the order of 20–40 nm in diameter on the average.*

Source: Image reprinted with permission from the Whipple Museum of the History of Science, Cambridge University.

Michael Faraday, Experimental relations of gold (and other metals) to light; the Bakerian lecture, *Phil. Trans. Royal Soc. London*, vol. 147, pp. 145-181, **1857**

Faraday's conjecture on size dependency of a physical property

"… a mere variation in the size of the particles gave rise to a variety of resultant colours …"

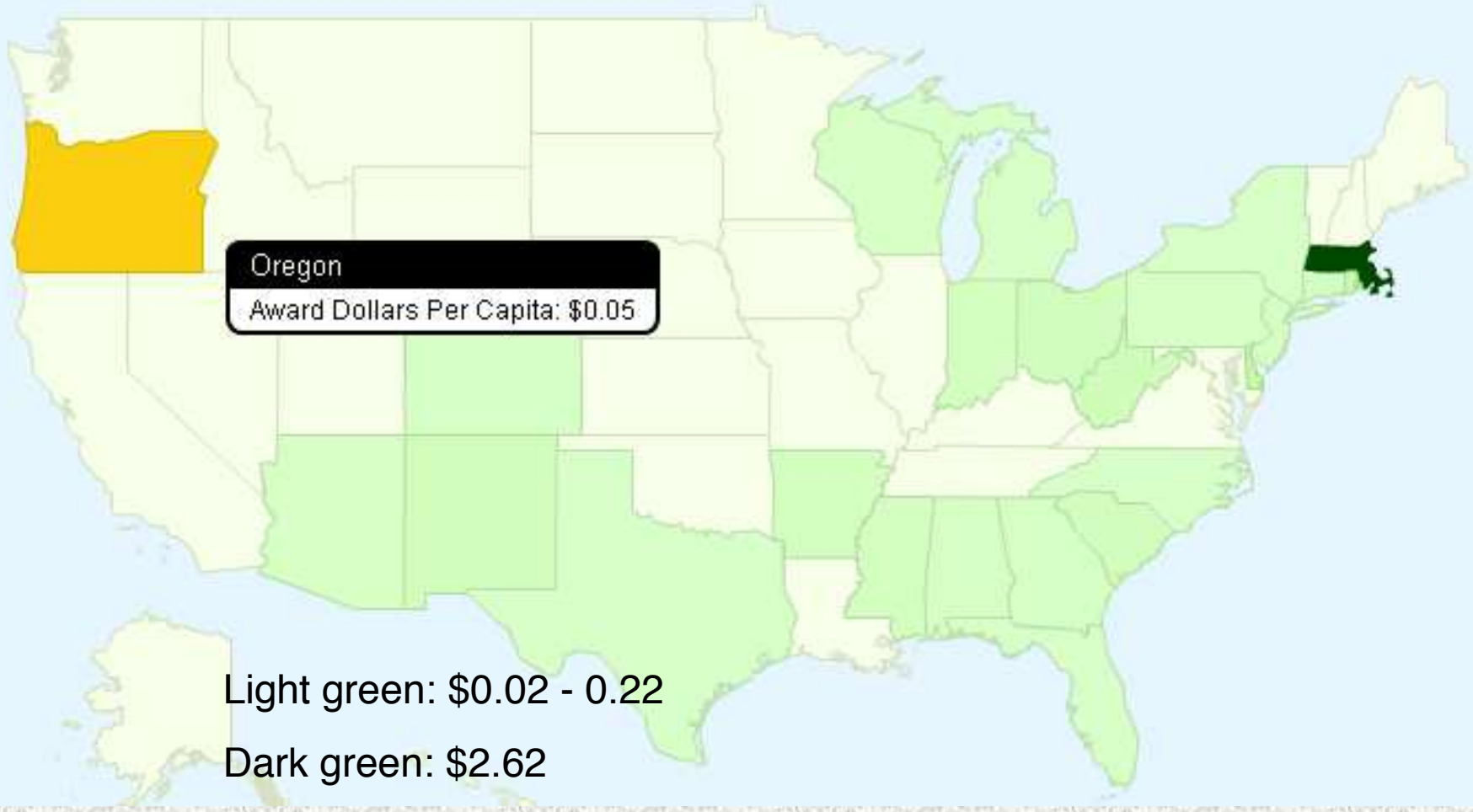
So qualitative nanoscience is some 150 years old !

Leading eventually to improved silver based photography, colloids, sols and gels, polymers **(collectively soft materials), catalysts, … are all nanoengineered products**

☑ Show award dollars per capita

NSF must have liked some of our ideas, now we are on the map, …

Nanotechnology Undergraduate Education (NUE) in Engineering, Active Awards



Light green: $0.02 - 0.22

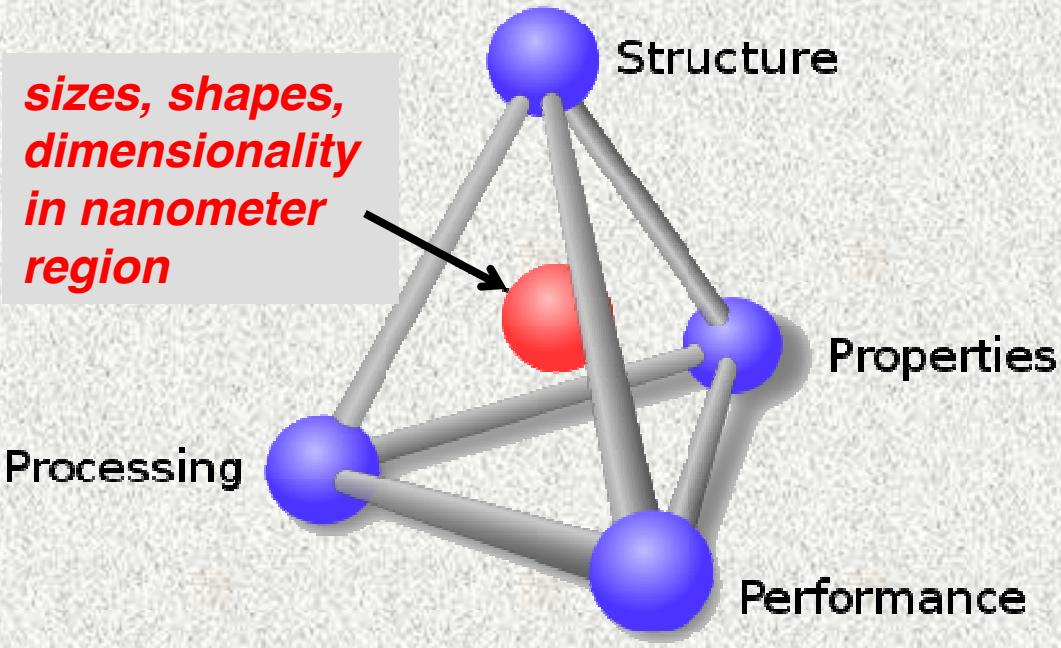
Dark green: $2.62

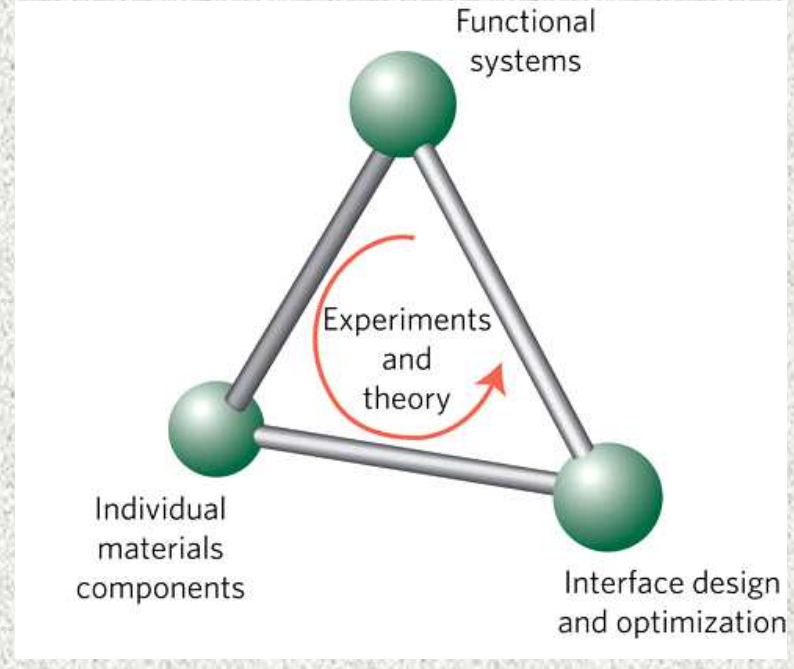
PH 481/581, Introduction to Nano-materials science and engineering, running since 2006

Arthur von Hippel's **1956** vision for the then emerging field of materials science and engineering

"… instead of taking prefabricated materials and trying to devise engineering applications consistent with their macroscopic properties, one builds materials from their atoms and molecules for the purpose at hand."

A. R. von Hippel, "Molecular Engineering", *Science*, vol. 123 (issue 3191), pp. 315-317, 1956; MIT *Techn. Rep.* 101, October 1955; *Molecular Science and Molecular Engineering*, Technology Press of MIT Press and Wiley & Sons, New York, 1959.





modified ***Materials Science and -Engineering Tetrahedron****, linking interconnected key concepts as well as interactions between Materials Scientists and -Engineers*

"... system materials engineering emphasizes the study of the interactions between individual composites of a system, and how these interactions give rise to the function and performance of the final system."

http://www.nature.com/nmat/journal/v11/n7/fig_tab/nmat3367_F2.html, *P. Yang, J-M. Tarascon, Nature Materials 11 (2012) 560-563*

Nanoscience and Nanotechnology: Evolving Definitions and Growing Footprint on the Scientific Landscape

*Michael L. Grieneisen and Minghua Zhang** DOI: 10.1002/smll.201100387

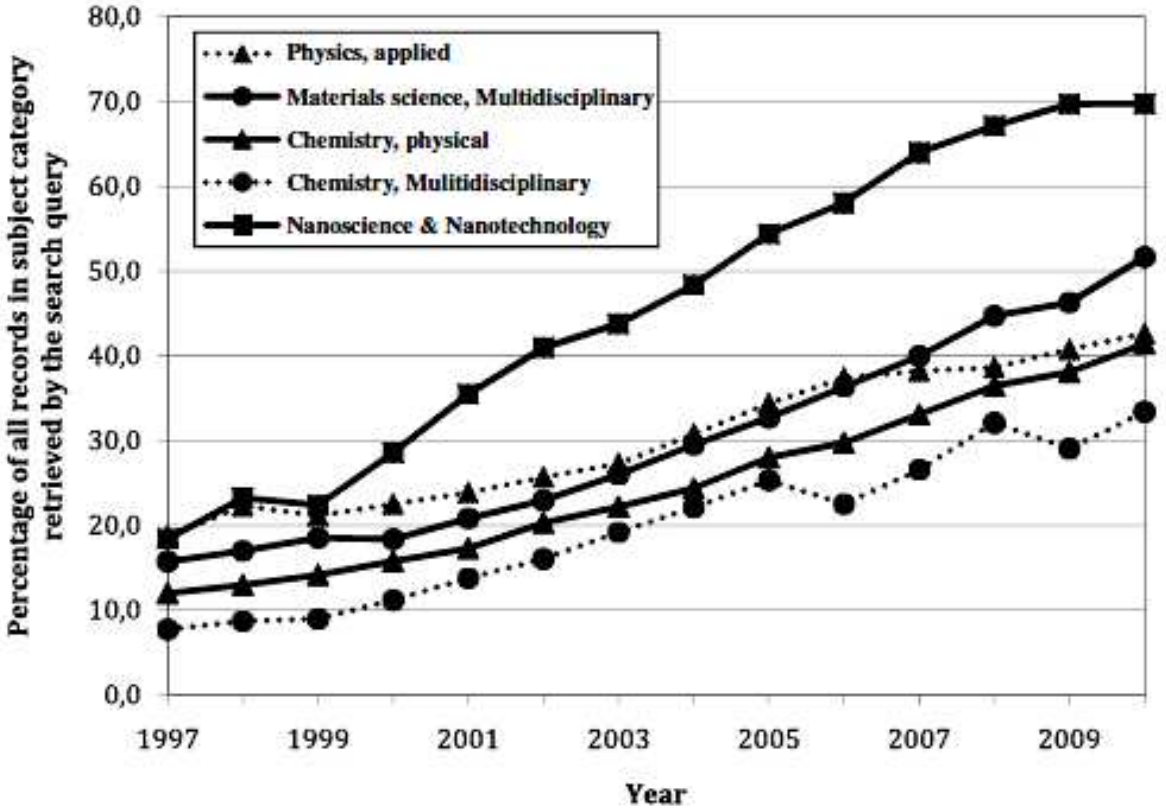
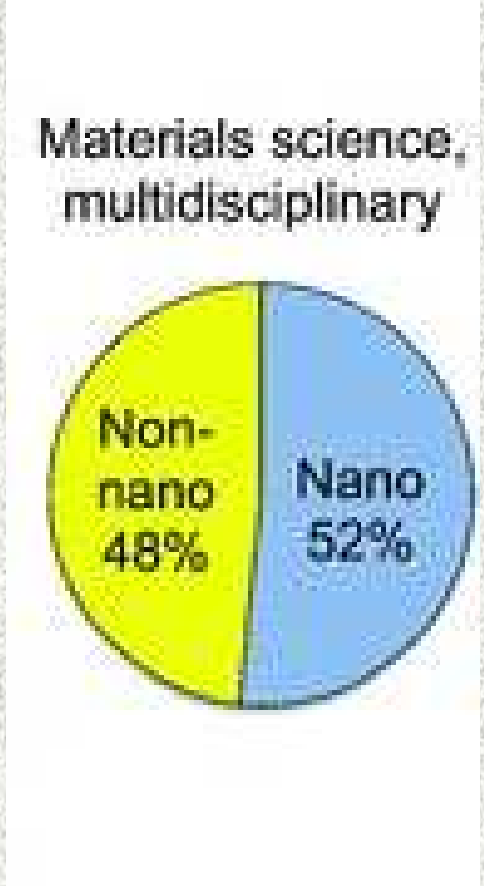
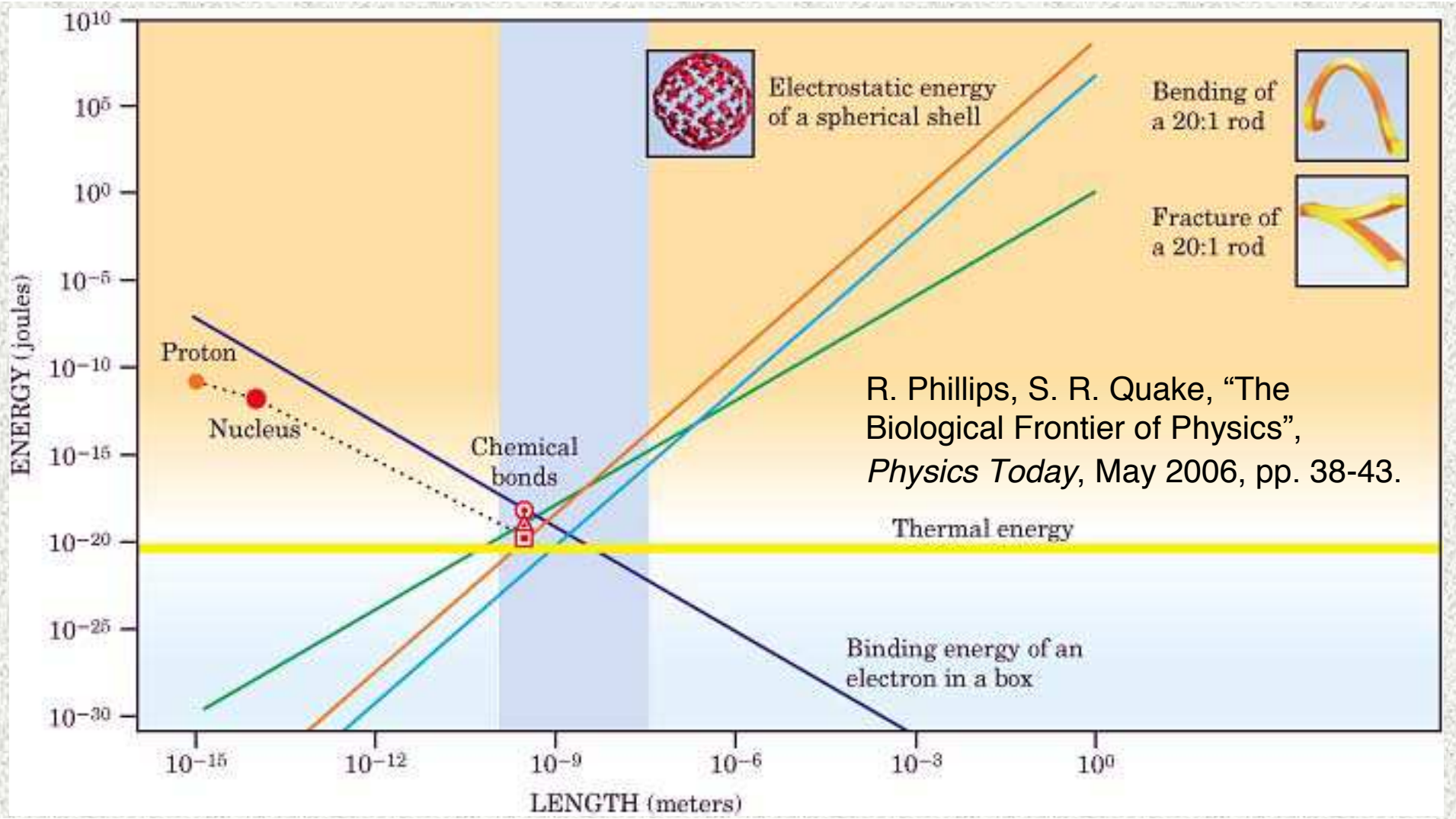


Figure 2. Percentage of all records in 5 top Web of Science subject categories which were retrieved by the search query in Table 1. These subject categories had the highest number of records retrieved by the search query for PY 2009. Because these are percentages, data for the partial year of 2010 are included. The footprint of nanoscience and nanotechnology within these fields has grown dramatically in just the past 13 years.





The confluence of energy scales is illustrated in this graph, which shows how thermal, chemical, mechanical, and electrostatic energies associated with an object scale with size. As the characteristic object size approaches that at which molecular machines operate (shaded), all the energies converge. The horizontal line shows the thermal energy scale kT which, of course, does not depend on an object's size. We estimate binding energy (purple) by considering an electron in a box; for comparison, the graph shows measured binding energies for hydrogen bonds (square), phosphate groups in ATP (triangle), and covalent bonds (circle), along with characteristic energies for nuclear and subatomic particles. In estimating the bending energy (blue), we took an elastic rod with an aspect ratio of 20:1 bent into a semicircular arc, and to compute the fracture energy (green) we estimated the energy in chemical bonds in a longitudinal cross section of the rod. The electrostatic energy (orange) was obtained for a spherical protein with singly charged amino acids of specified size distributed on the surface.

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http://web.pdx.edu/~pmoeck/nanoMSE.htm

Coursework read the "Crystal Structure Visualizations in three dimensions with support from the open access nanocrystallography database" J. Mater. Educ. 28(1), 87-95 (2006) by P. Moeck et al. *and answer the following questions on its basis, your actual working with open access databases, and from what you have learned in class.*

1. *What does the acronym CIF for?*
2. *How many entries are currently in the COD? (Check out their website for an actual number.)*
3. *What are the lattice parameters of NaCl?*
4. *How many formulae units are in the conventional unit cell ?*
5. *How many atoms are in the conventional unit cell?*
6. *Provide a screenshot of the conventional NaCl unit cell along the [100] direction.*
7. *Provide a screeshot of NaCl unit cell along the [110] direction.*
8. *Provide a screenshot of the conventional NaCl cell along the [111] direction.*
9. *What are the positions of the Na and Cl atom in the so called asymmetric unit?*
10. *Provide a screenshot of the conventional cell of FeO along the [111] direction, what are the similarities and differences to the conventional cell of NaCl?*

Joint assignment over a couple of weeks for both graduates and undergrads

For example first homework assignment:

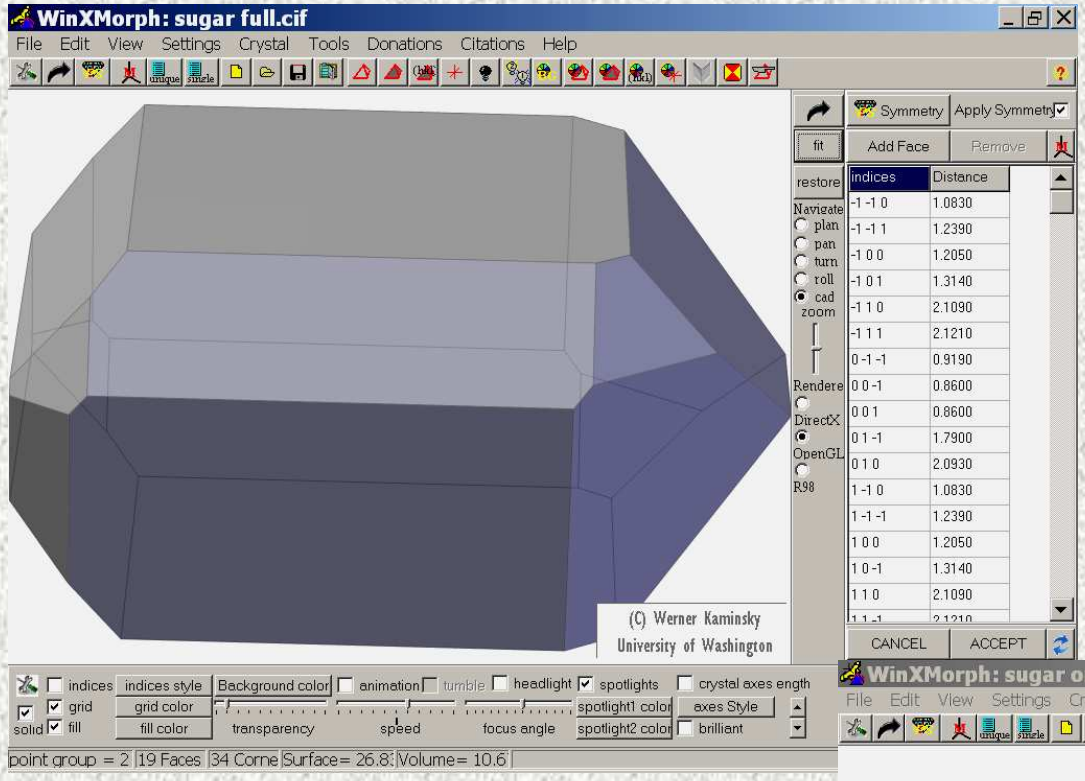
http://web.pdx.edu/~pmoeck/pdf/biotech%20future.pdf Freeman Dyson, Our Biotech Future, The New York Review of Books, http://www.nybooks.com/articles/archives/2007/jul/19/our-biotech-future/

for both graduates and undergraduates, in addition for graduates:

http://web.pdx.edu/~pmoeck/pdf/biology%20next%20revolution.pdf Nigel Goldenfeld and Carl Woese, Biology's next revolution, http://arxiv.org/abs/q-bio/0702015

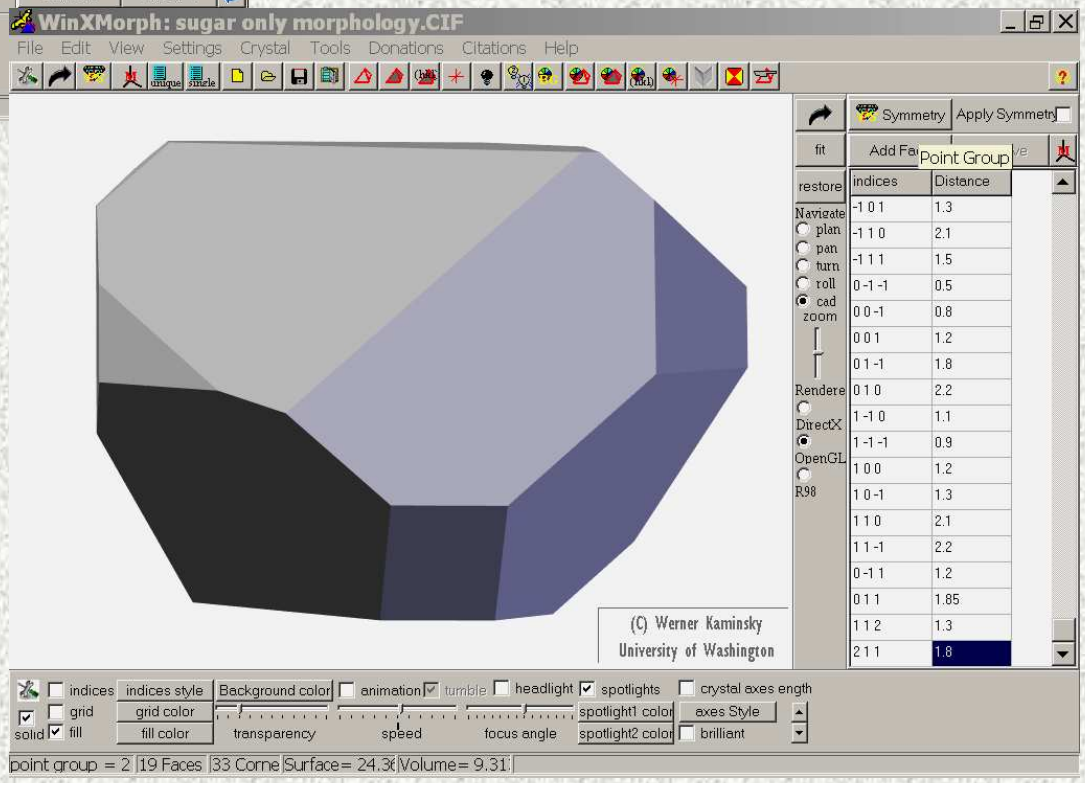
"Since much of nano-materials science and engineering necessarily involves communications within teams of nano-scientist and nano-engineers, one major objective of this course is to prepare you for working in interdisciplinary teams.

So you will have to read a couple of papers and write an ***informative opinion piece*** *about it, that piece is supposed to communicate something, so you have to absorb the information first, then to think about the needs of the people you are going to address, what they need to know, (skip what they already know), why they need to know what you are going to communicate to them, .. This should be well thought through and typically no longer than a page."*



allows for interactive discussions of: *crystal forms, tracht and habit, exomorphosis, relation between habit and structure, free surface energy, Gibbs-Curie law, equilibrium polyhedron, Wulff law, …*

students can check out how changing the "distance" in the program (which is proportional to a face's growth velocity), changes the relative size of a face and how that leads to variations in the habit,…



also used in this class,

Prof. Werner Kaminsky's ***WinXMorph***:
http://cad4.cpac.washington.edu/WinXMorphHome/WinXMorph.htm

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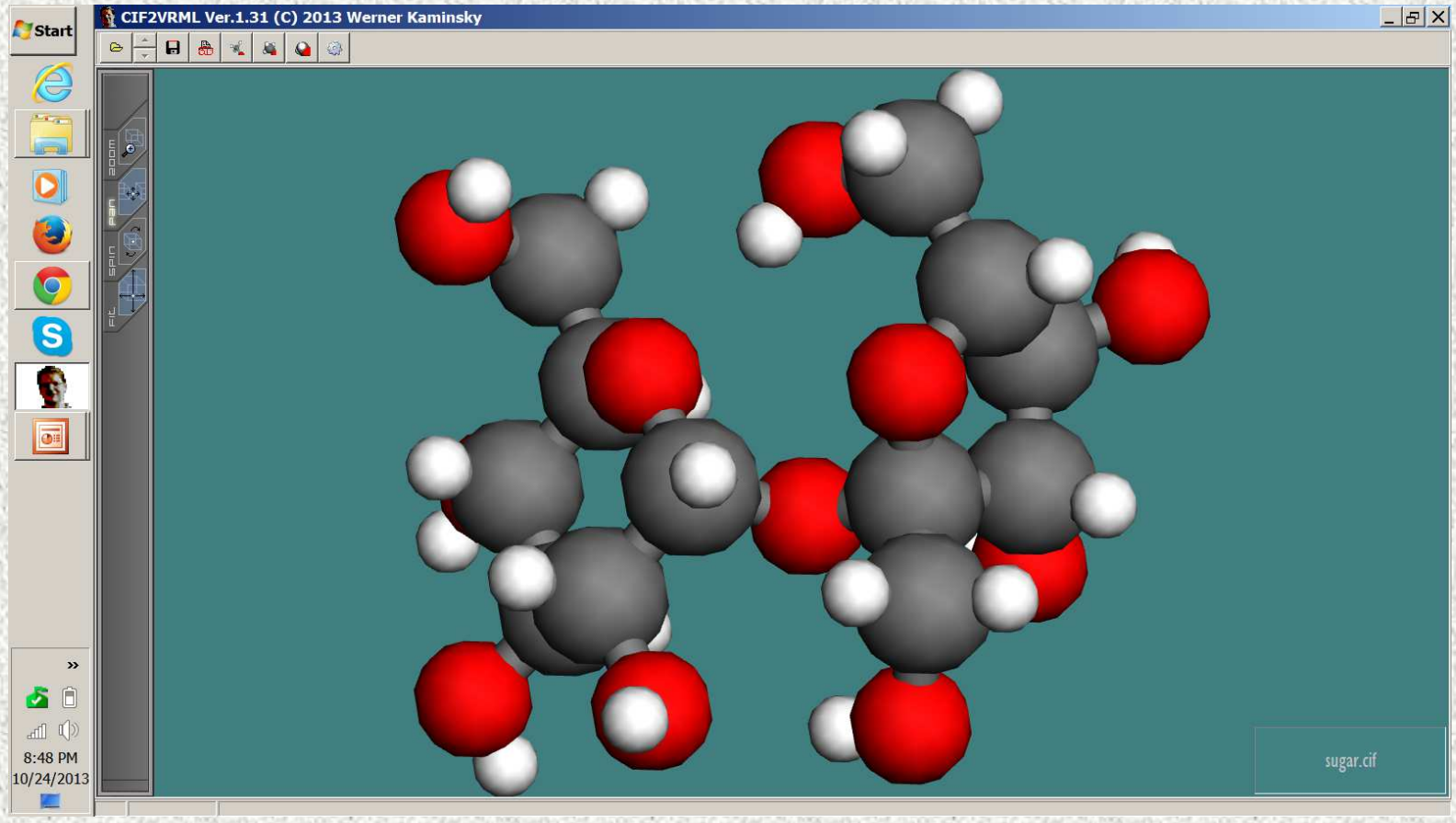
Virtual reality is great …



Prof. Werner Kaminsky's **CIF2VRML**:

http://128.95.152.162/Cif2VRMLHome/Cif2VRML.htm

scientist also like to build 3D models because …

Left: Reconstruction of the double helix model of deoxyribose nucleic acid containing some of the original metal plates; **Right:** used by Francis Crick and James Dewey Watson in 1953, (Source: Science Museum, http://www.sciencemuseum.org.uk/images/i045/10313925.aspx)

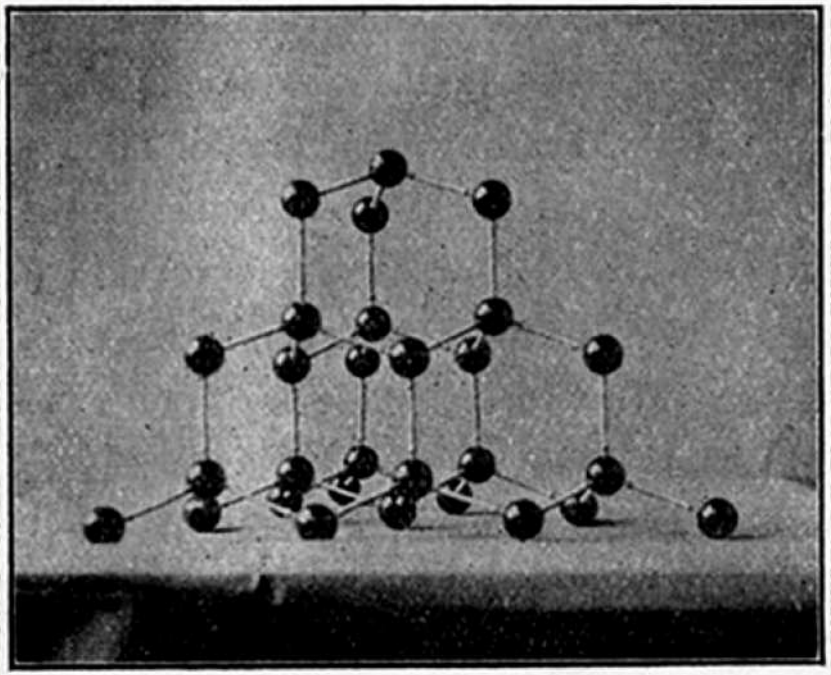
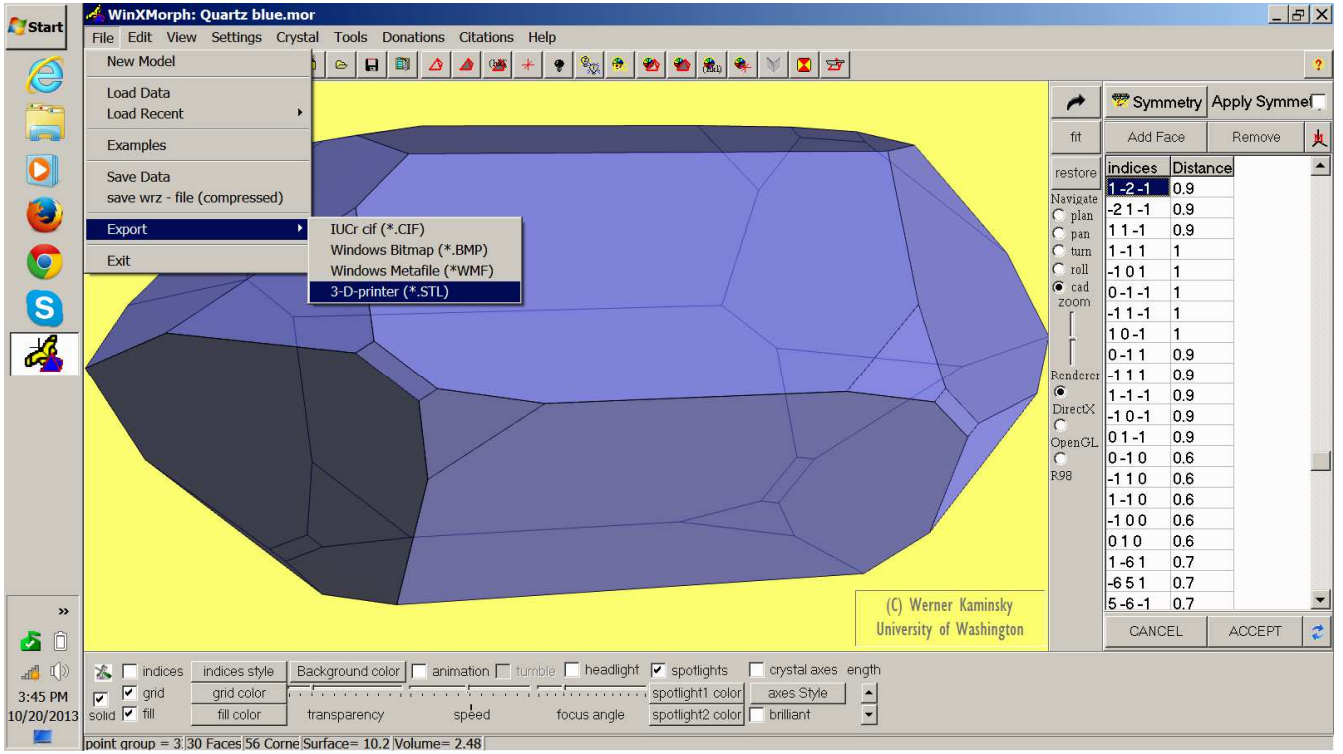


FIG. 7.—View perpendicular to a (111) axis.

Left: Hard sphere model of the diamond structure (space filling ≈ 34 %) by W. H. Bragg, Museum of the Royal Institution, London, photo by André Authier. (Source: http://blog.oup.com/2013/08/100th-anniversary-first-crystal-structure-determinations-bragg/#sthash.50BE8wiT.6mYKaBKB.dpuf.) **Right:** Ball and stick model of the diamond structure. (Source: FIG. 7 in W. H. Bragg and W. L. Bragg, The structure of diamond, *Proc. R. Soc. Lond. A* **89**, 277; published September 22, 1913.)

Wooden crystal morphology models of past centuries. (Source: Google Image search).



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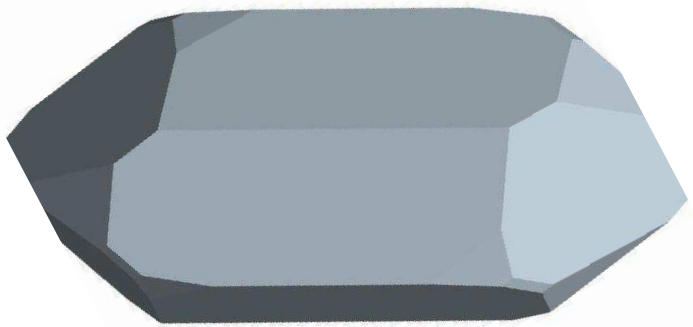
http://cad4.cpac.washington.edu/WinXMorphHome/WinXMorph.htm



3D printed model of α-quartz as printed out by **Dr. Trevor Snyder** (at XEROX Wilsonville, ($5 but prices will come down further) also supporting **poster Moeck, Snyder, and Kaminsky**

$300,000 - $"500 k"

- Process begins with 3D CAD data in STL file format
- STL data is "sliced" with software
- Dual heated nozzles trace each cross section, depositing thermoplastic material
- When a cross-section is complete, the build platform is slightly lowered and the process continues
- Completed parts are removed and support material is cleaned off

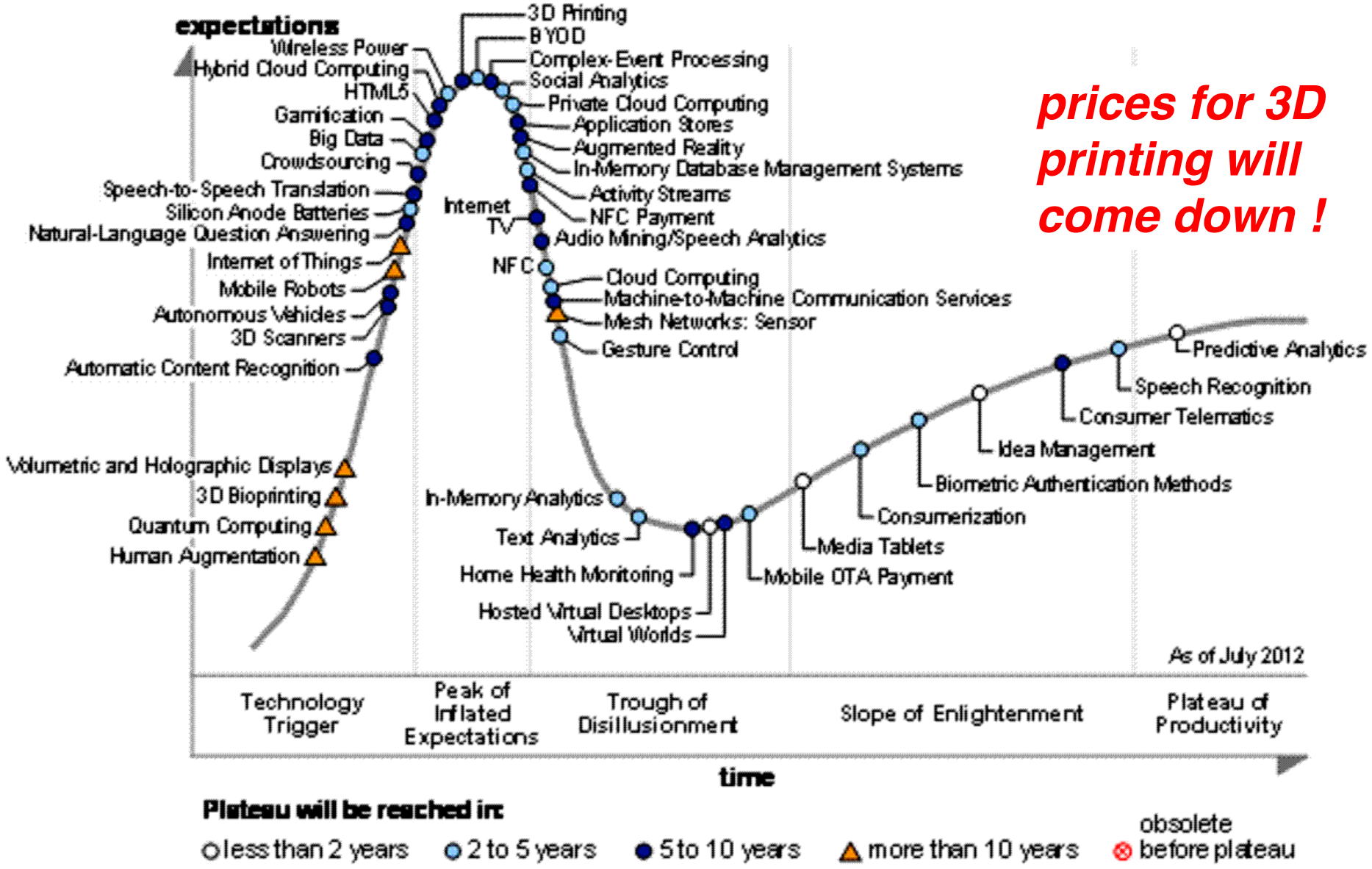
$500 - $1,000

https://www.youtube.com/watch?v=n9SGAS52ZCA

https://www.youtube.com/watch?v=ddtJVww8Zvw

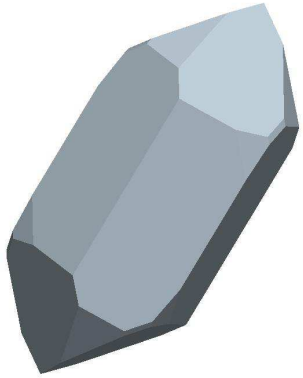
https://www.youtube.com/watch?v=yTh0rzCXefQ

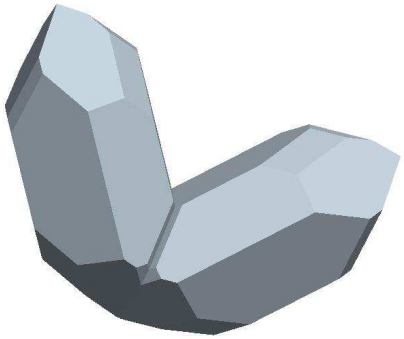
Figure 1. Hype Cycle for Emerging Technologies, 2012



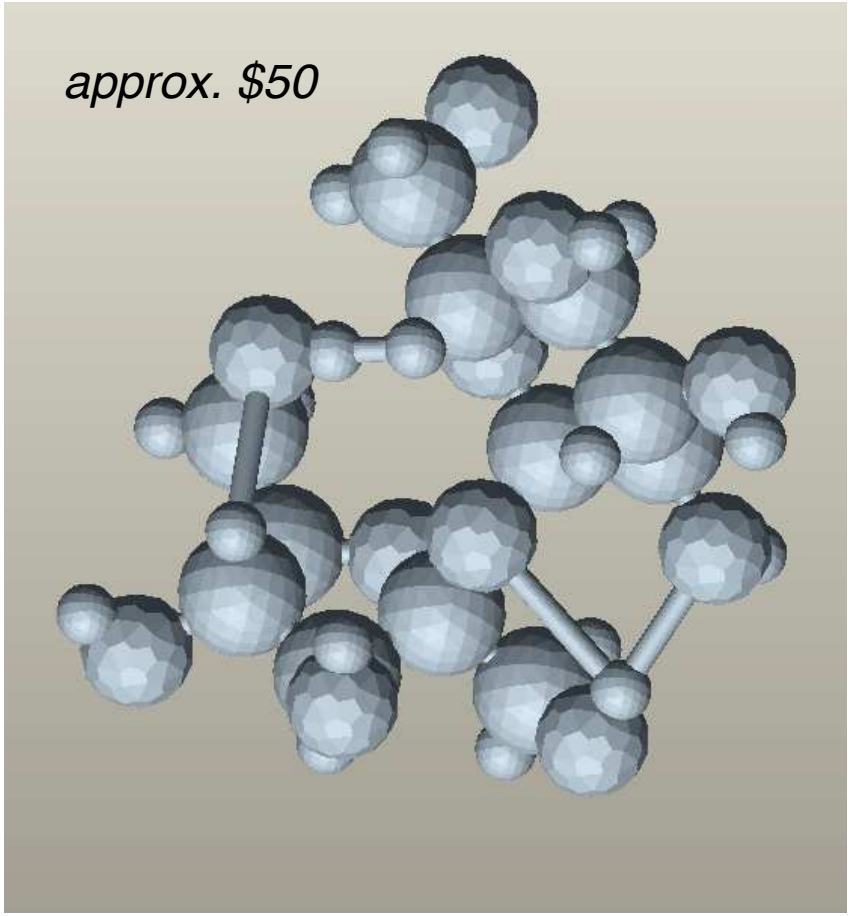
prices for 3D printing will come down !

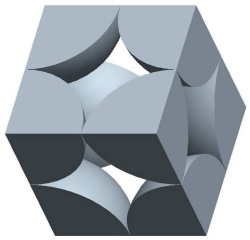
Source: Gartner (August 2012)

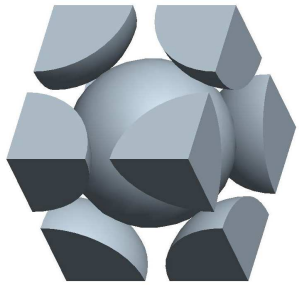




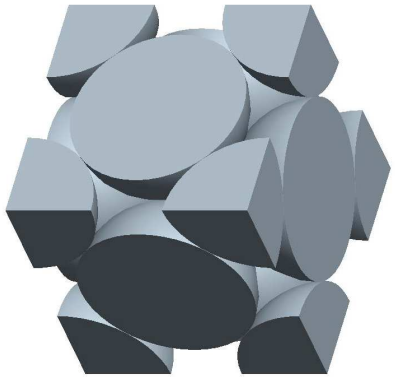
approx. $0.2 when printed on a $500 to $1,000 hobby machine (prints only build material)

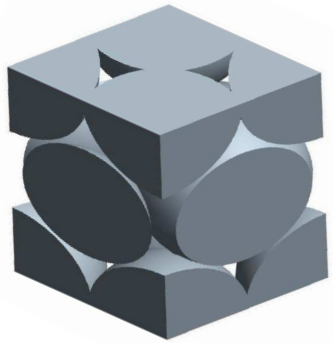






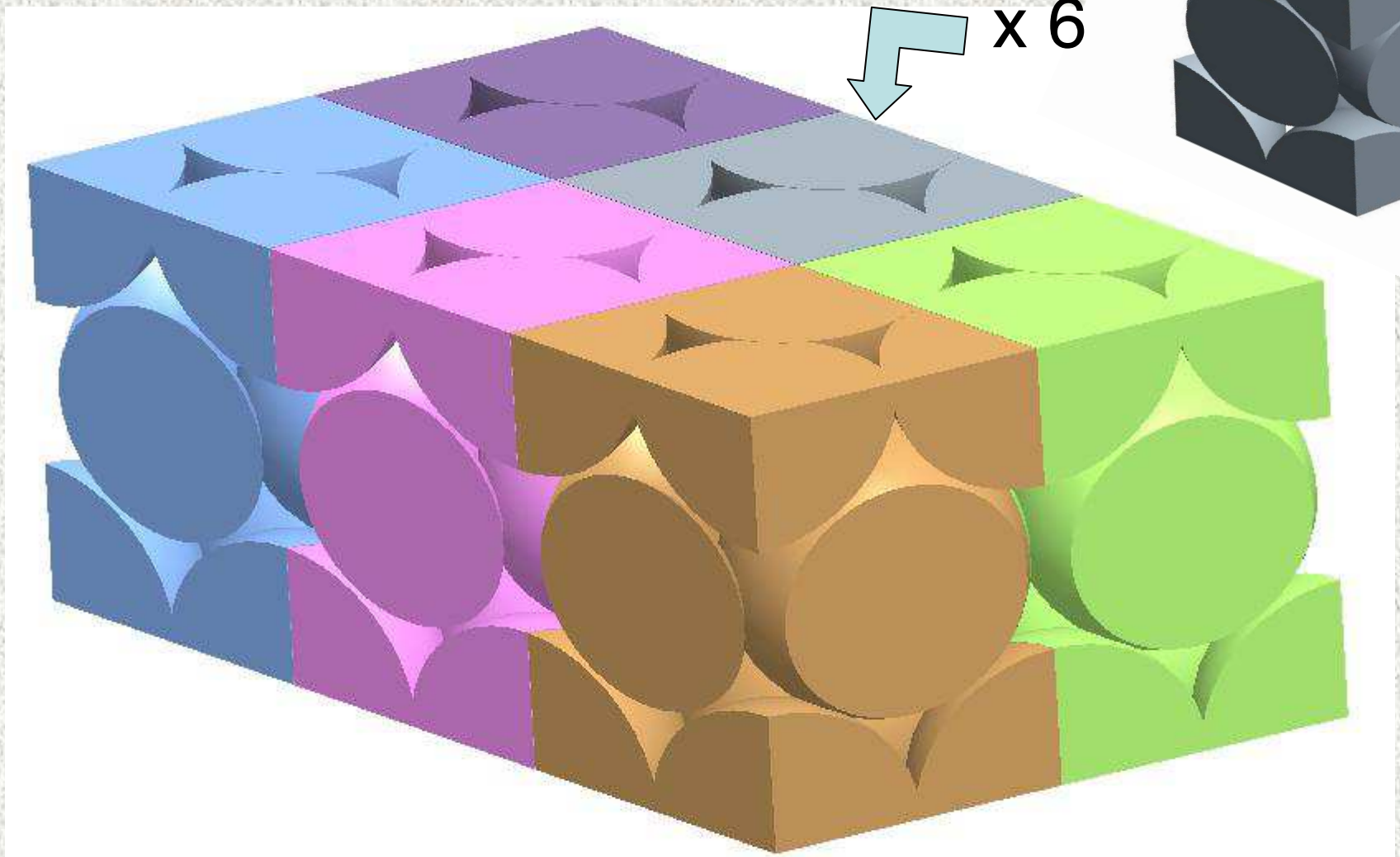
approx. $20 as both build and support material is needed (two nozzle machine)



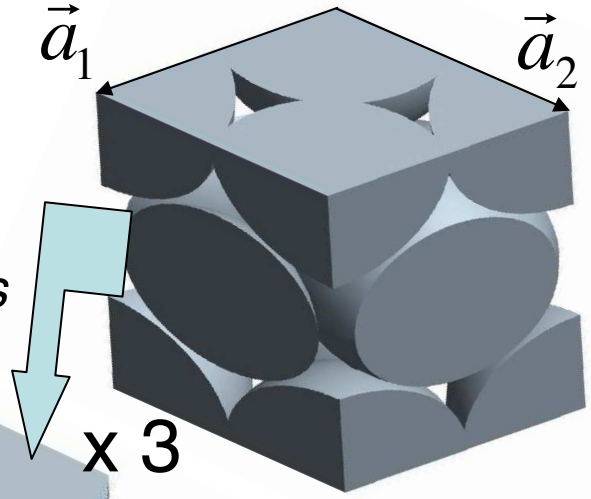


prices will come down further

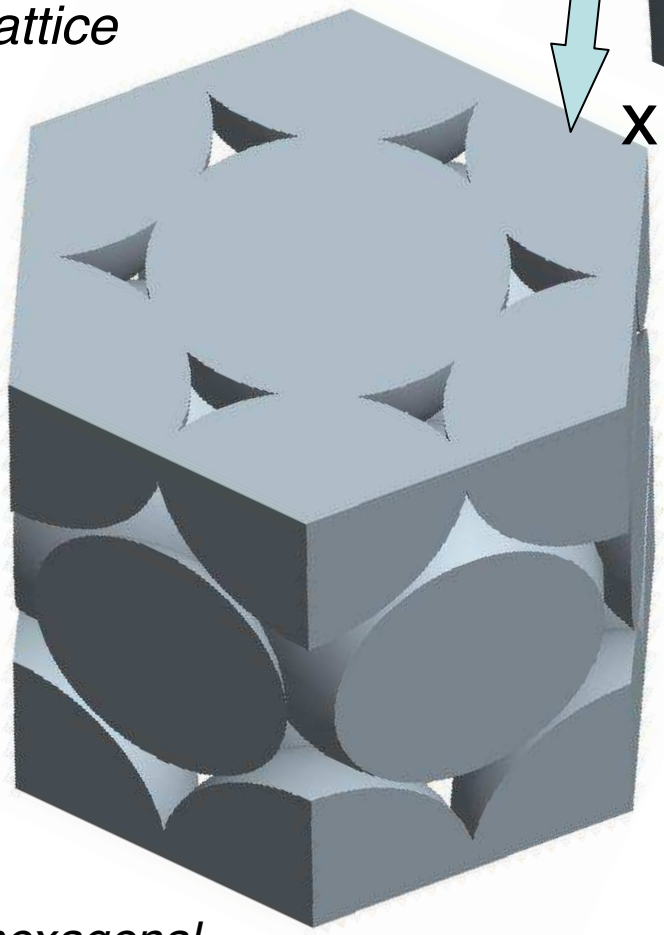
demonstrating to the students that this is actually the hexagonal unit cell



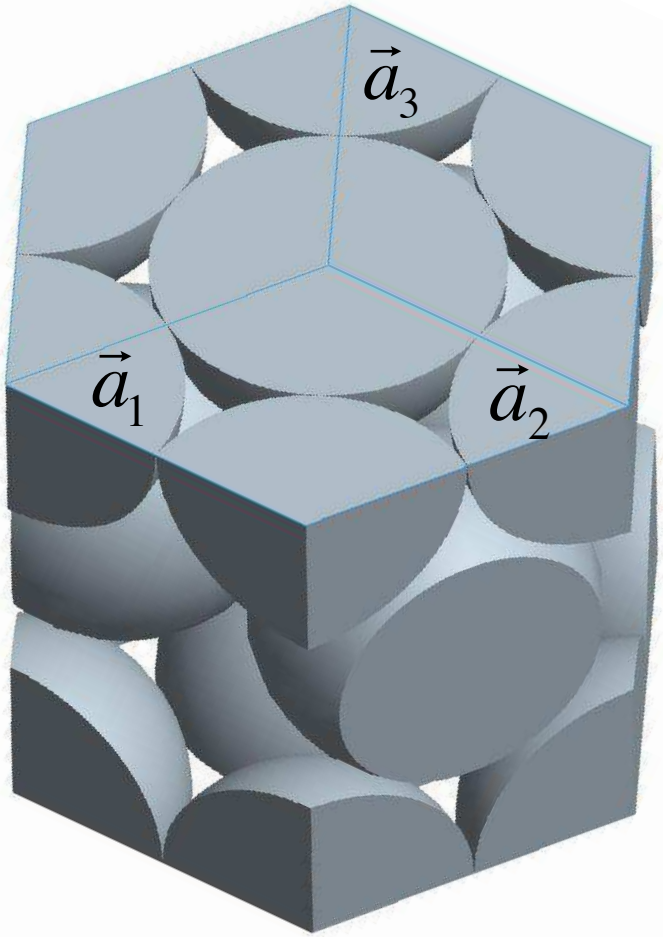
demonstrating to the students that the hexagonal prism is not the unit cell and that there is no such Bravais lattice



also useful for explaining the 4 index lattice direction and Miller plane indices for hexagonal crystals

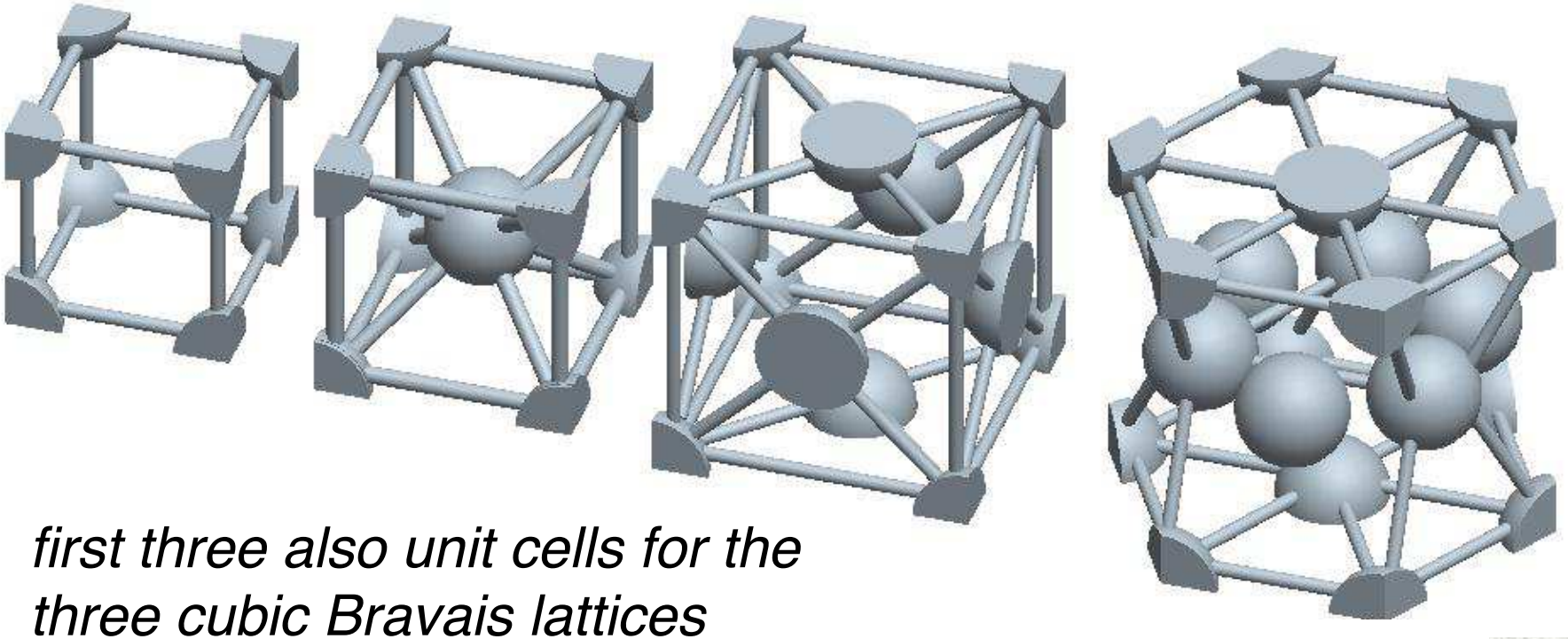


taking out a few sphere caps allows for better assessment of the intersites

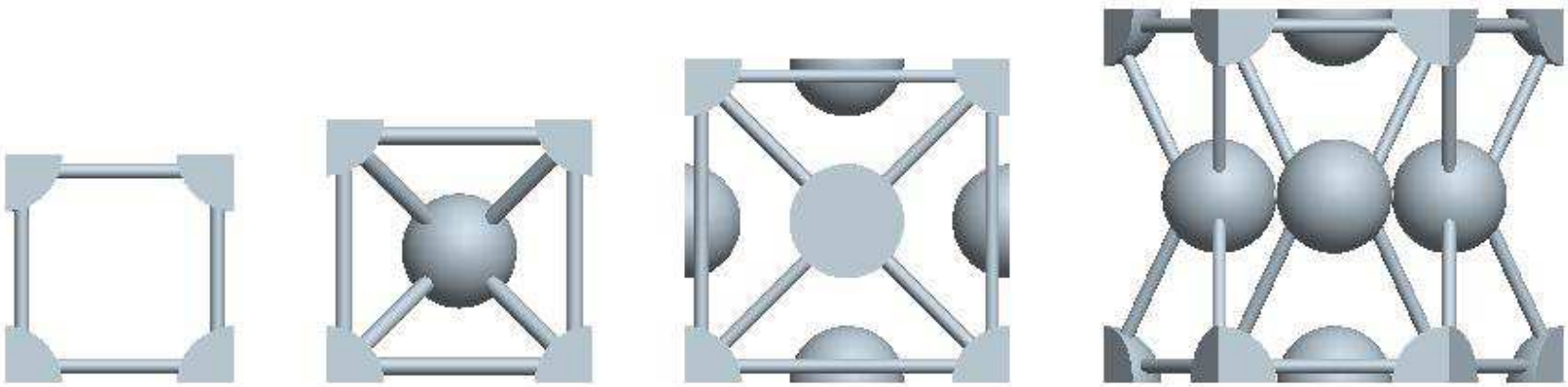


hexagonal lattice $[1000] \equiv [1\bar{1}00] \equiv [0100] \equiv [\bar{1}000] \equiv [0010] \equiv [0\bar{1}00]$ *but not for structure with basis*

set of "reduced sphere size" models for better assessment of the intersites



first three also unit cells for the three cubic Bravais lattices



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open access crystallographic databases, combined some 350,000 – 400,000 entries in CIF format

open access crystallography resource portal, nanocrystallography.net

COD in it's 11th year, more than 240,000 CIFs

EDU-COD and CMD in their 10th year, approx. 1,000 CIFs

used in teaching nano-materials science and -engineering at the 400/500 level for 8 years

will be used in new 300 level course as well, starting in the spring of 2014

free programs for conversion of CIF (molecule structure, crystal morphology) to STL by Prof. Werner Kaminsky
http://cad4.cpac.washington.edu/

3D printing will further come down in prizes, good for hand on models in class

plans for Bicrystallography Open Database

Interactive Databases - Windows Internet Explorer

http://nanocrystallography.research.pdx.edu/databases/

Google

Favorites | Inbox (1,142) - p... | Interactive Data... | Page | Safety | Tools

Portland State UNIVERSITY

Interactive Databases

- Open Access Crystallography
- Interactive Databases
  - COD Mirror
  - EDU-COD
  - Crystal Morphology Database
  - Nano-Crystallography Database
  - Wiki Crystallography Database
- Nano-Crystallography Group
- Tools
- Facets of Electron Crystallography 2010
- MRS Tutorial and Seminars 2009
- Links
- Login
- Upload

Crystallography Open Database [Mirror, modified search interface and Jmol displays] Search and view

Wiki Crystallography Database Search and view

Educational subset of COD Search and view

Nano-Crystallography Database Search and view

Crystal Morphology Database Search and view

Bicrystallography Open Database

searchable collection of CIFs for all kinds of simulations and visualizations of grain boundaries

to be derived from user inputs and freely modifiable at the atomic level

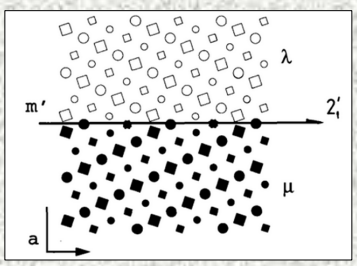
Several crystallography databases are offered for browsing. You can search the databases, downl and display the contained Crystallographic Information Files (CIFs), view 3D models of the encode crystal structures and morphologies.

We also provide the North American mirror of the Crystallography Open Database (COD). This is the

Bicrystallography Open Database

"… disclose generic relations between different interfaces, specify crystallographically equivalent variants of an interface and classify line defects in interfaces. The symmetry of a bicrystal imposes constraints on tensor properties of the bicrystal interface, provides classification of the interfacial vibrational modes, discloses possible interfacial transitions etc."

V. Janovec, Th. Hahn and H. Klapper, Twinning and domain structures, International Tables for Crystallography (2006), Vol. D, ch. 3.2, pp. 377-392.



No textbook, only a few original papers and book chapters

diamond, Σ = 5 (310)/[001] 36.9° tilt boundary, viewed down [001], **black white (two color) layer group *p2$_1$'am'***

R. C. Pond and J. P. Hirth, in Ehrenreich, H., *Solid State Physics: Advances in Research and Applications*, Volume 47, 1994, pp. 287-365

CeO_2 Σ = 5 (310)/[001] 36.9° tilt boundary dichromatic complex has 3 atoms per lattice point of dichromatic pattern I4/mm'm'

two color layer group ***c2'mc'*** - *a genuine back-white group, polar physical properties can exist*

p2'mm' - *polar physical properties cannot exist*

p2$_1$'mn' - *polar physical properties can exist*

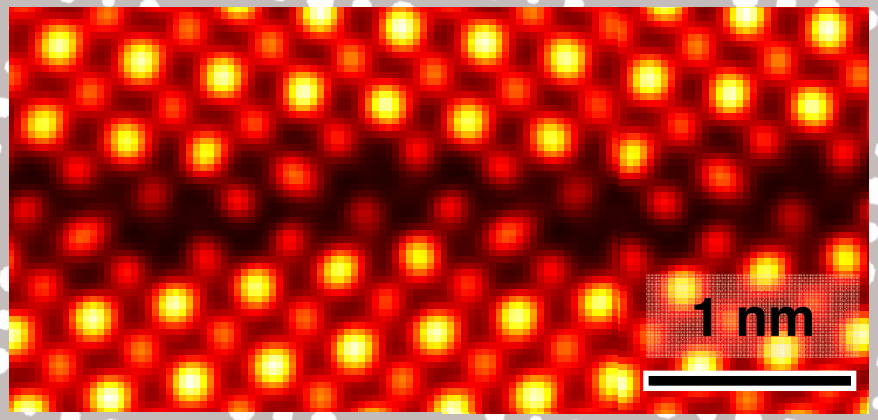
two color layer group ***c2'mm'*** – *a gray group, polar physical properties cannot exist*

CeO_2 Σ = 5 (120)/[001] 53.1° tilt boundary viewed down [001]

another "idea whose time has come"

primitive cubic lattice, 5 atoms per lattice point of dichromatic pattern
P4/mm'm', zero rigid body shift and expansion for simplicity

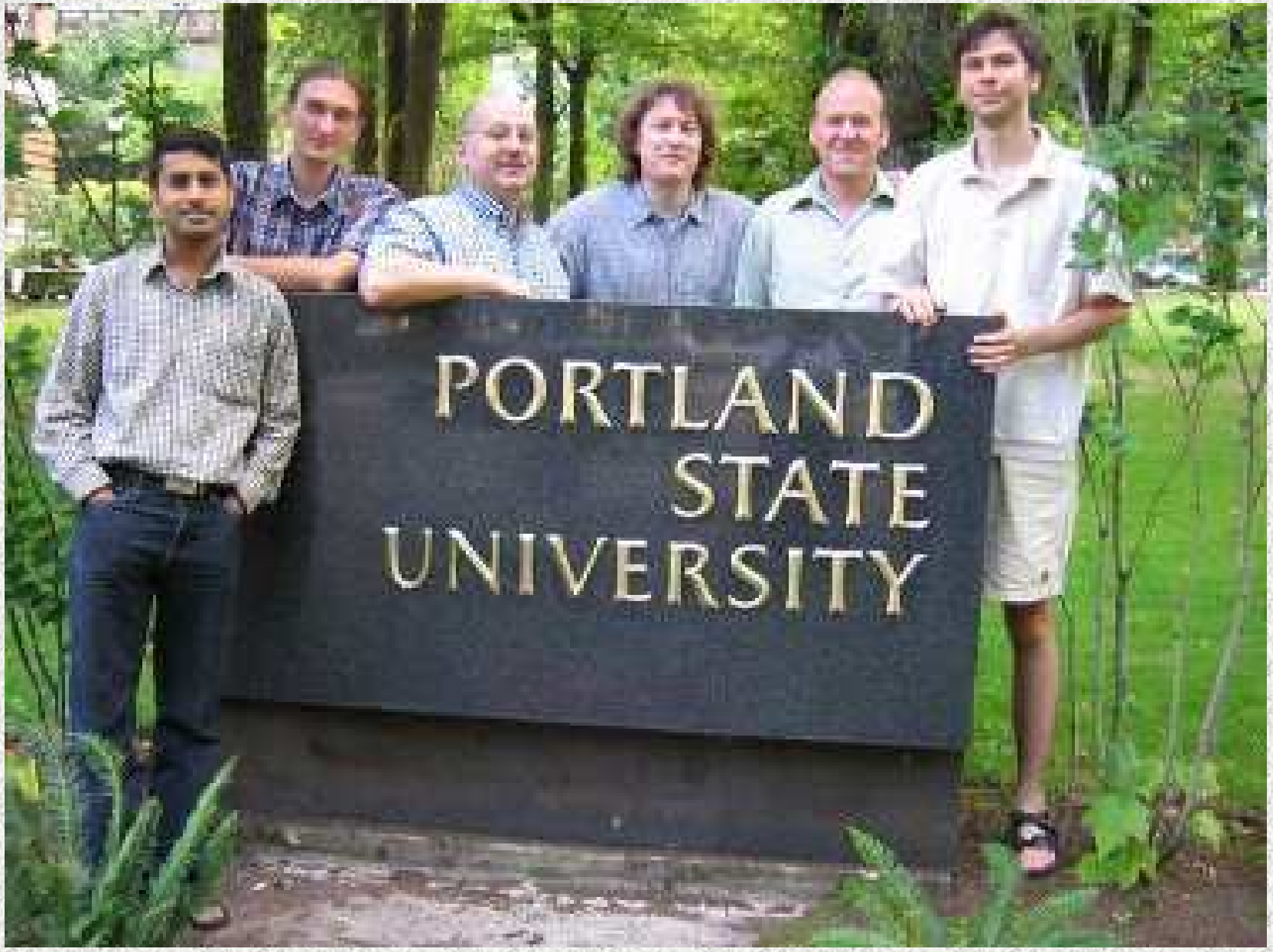
Aberration-corrected translation-symmetry averaged STEM Z-contrast, H. Yang et al., Phil. Mag. 2012, 1-11, iFirst Article.



only pure O columns are located at interface

Frieze Group *p11g*

$SrTiO_3$ Σ = 13a, (510)/[001], 22.6° tilt boundary in [001] projection, sectioned at ¼ [510], large disks Sr columns, medium disks pure O columns, small disks mixed O and Ti columns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