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Find, Build, and Export Information for 3D Printing of Your Favorite Molecules and Crystal Structures at Two Dedicated Websites

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Find, Edit, and 3D Print Your Favorite Atomic Structures From A Web-Site

Paul R. DeStefano
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Portland State University

3D Printing Your Favorite Atomic Structures

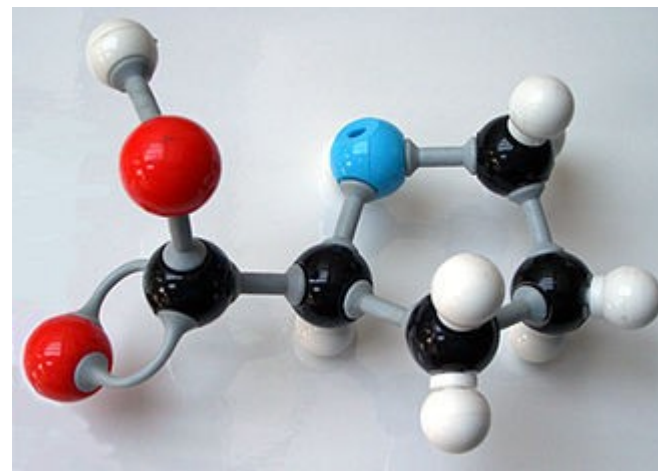
- Motivation
 - A New Web-Based Tool for 3D Visualizations
- Finding Atomic Structures (in COD, Mirror COD)
- Database information (in CIF)
- The software (Jmol/JSmol)
- Producing 3D Print Data (STL/VRML)
- Conclusion

3D Printing Your Favorite Atomic Structures

- Motivation
 - Primarily, education/study



Diamond model, W. H. Bragg, Museum of the Royal Institution, London. Photo, André Authier.



Modern plastic ball and stick model of proline.

3D Printing Your Favorite Atomic Structures

- Motivation

- Now, data is abundant (Crystallographic Dbs)
 - e.g. > 370,000 entries in COD
- Easy to find precise structure descriptions
- But, how to visualize/study these detailed descriptions?

3D Printing Your Favorite Atomic Structures

- Motivation
 - Enter 3D Printing (Additive Manufacturing)
 - Now we have a device produces precise 3D models



3D printing a hyperboloid

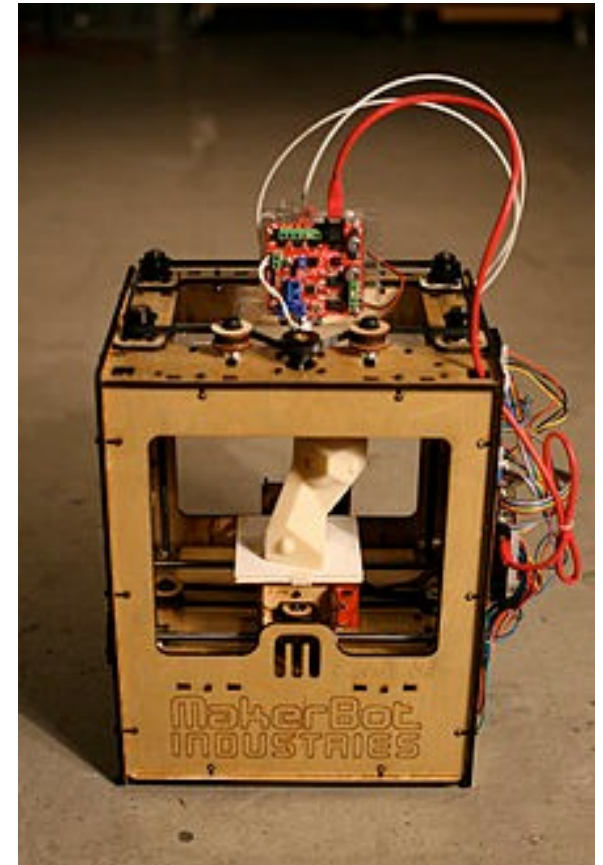
3D Printing Your Favorite Atomic Structures

- 3D Printing (Additive Manufacturing)
 - 3D printers combine small amounts of material, precisely
 - 250DPI, O(100-10) micrometer layer thickness
 - Requires: 3D Print File Formats
 - STL (Stereolithography)
 - VRML/X3D



3D Printing Your Favorite Atomic Structures

- 3D Printing (Additive Manufacturing)
 - 3D Print Files Formats
 - STL (Stereolithography)
 - Original 3D Printing Format
 - Most compatible
 - Monochrome
 - VRML/X3D
 - “Web-Enabled”
 - Polychrome, multicolor
 - X3D: ISO standard successor to VRML



3D Printing Your Favorite Atomic Structures

- Motivation
 - What is needed is a tool that:
 - Can interpret data from these databases (CIF data format)
 - Is integrated with at least one large (open) database
 - Is not limited to a particular software platform
 - Understands useful ways to visualize atomic structures
 - **Can convert to or export 3D print files**

3D Printing Your Favorite Atomic Structures

- Finding Atomic Structures: Databases (COD)
 - <http://nanocrystallography.org/> (mirror, North America)



The screenshot shows the homepage of the Crystallography Open Database (COD). The browser address bar displays "nanocrystallography.org". The page features the COD logo, which consists of three spheres: a cyan one with a black 'C', a green one with a black 'O', and a pink one with a black 'D'. The main heading reads "Crystallography Open Database". On the left side, there is a navigation menu with three sections: "COD Home" (with links for "Home" and "What's new?"), "Accessing COD Data" (with links for "Browse" and "Search"), and "Add Your Data" (with links for "Deposit your data", "Manage depositions", "Manage/release", and "prepublications"). In the center, there is a larger version of the COD logo. Below the logo, the text states: "Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding [biopolymers](#)". A note below that says: "All data on this site have been placed in the public domain by the contributors." At the bottom, a small line of text reads: "COD Advisory Board thanks [The Research Council of Lithuania](#) for their financial support of the

3D Printing Your Favorite Atomic Structures

- Finding Atomic Structures: Databases (OACP)
 - Open Access Crystallography Project
 - <http://nanocrystallography.research.pdx.edu/search/codmirror/>

The screenshot shows the COD Mirror website interface. At the top, there is a search bar and the URL nanocrystallography.research.pdx.edu/search/co. The page features the Portland State University logo and the title "COD Mirror". A sidebar on the left lists various databases and tools, including "Open Access Crystallography", "Interactive Databases", "Nano-Crystallography Group", and "Tools". The main content area displays a periodic table with elements color-coded by groups. Below the periodic table, there are search filters: "Include these elements:", "Exclude these elements:", "Strict number of elements:", "Text (1 or 2 words):", "Unit Cell (UC) Volume (Å³) min:", "UC Volume (Å³) max:", "UC Edge a (Å) min:", "UC Edge a (Å) max:", and "UC Edge b (Å) min:". A "Search" button is located at the bottom of the filter section.

Open Access
Crystallography Project
Interface



3D Printing Your Favorite Atomic Structures

- Finding Atomic Structures: Search

Include these elements:

*Select elements from periodic table.
Or enter properly formatted comma seperated list ex: Si, O*

Exclude these elements:

Shift+Click elements from periodic table

Strict number of elements:

Text (1 or 2 words):

Unit Cell (UC) Volume (\AA^3) min:

UC Volume (\AA^3) max:

UC Edge a (\AA) min:

UC Edge a (\AA) max:

UC Edge b (\AA) min:

UC Edge b (\AA) max:

UC Edge c (\AA) min:

UC Edge c (\AA)max:

UC Angle Aplha ($^\circ$) min:

UC Angle Alpha ($^\circ$) max:

UC Angle Beta ($^\circ$) min:

UC Angle Beta($^\circ$) max:

UC Angle Gamma ($^\circ$) min:

UC Angle Gamma ($^\circ$) max:

Include these elements:

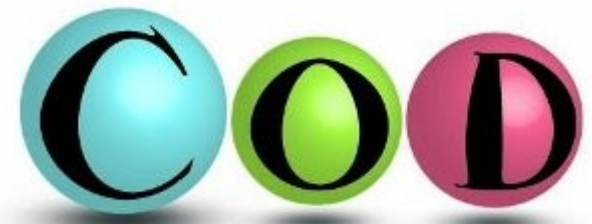
*Select elements from periodic table.
Or enter properly formatted comma seperated list ex: Si, O*

Exclude these elements:

Shift+Click elements from periodic table

Strict number of elements:

Text (1 or 2 words):



3D Printing Your Favorite Atomic Structures

- Finding Atomic Structures: Search

Portland State UNIVERSITY COD Mirror

Open Access Crystallography There are 77 results.

Interactive Databases

COD Mirror
EDU-COD
Crystal Morphology Databases

Formula:- Al Li O4 Si -
Cell Parameters: $a = 10.4971\text{\AA}$ $b = 10.4971\text{\AA}$ $c = 11.19513\text{\AA}$ $\alpha = 90.0^\circ$ $\beta = 90.0^\circ$ $\gamma = 120.0^\circ$
Cell Volume = 1068.31\AA^3

[View CIF](#) [Download CIF](#) [View Structure in JSmol with HTML 5](#)

nanocrystallography.research.pdx.edu/search/co Search

Formula:- O2 Si -
Cell Parameters: $a = 4.916\text{\AA}$ $b = 4.916\text{\AA}$ $c = 5.4054\text{\AA}$ $\alpha = 90.0^\circ$ $\beta = 90.0^\circ$ $\gamma = 120.0^\circ$
Cell volume = 113.131\AA^3

[View CIF](#) [Download CIF](#) [View Structure in JSmol with HTML 5](#)
[View Structure in Jmol V12 with Java](#)

Crystallography in the World
Facets of Electron Crystallography 2010
MRS Tutorial and Seminars 2009
3D Print Files
Links
Login
Upload

[View Structure in Jmol V12 with Java](#)

Formula:- Al_{0.155} Li_{0.155} O₂ Si_{0.845} -
Cell Parameters: $a = 5.0865\text{\AA}$ $b = 5.0865\text{\AA}$ $c = 5.4451\text{\AA}$ $\alpha = 90.0^\circ$ $\beta = 90.0^\circ$ $\gamma = 120.0^\circ$
Cell Volume = 122.004\AA^3

[View CIF](#) [Download CIF](#) [View Structure in JSmol with HTML 5](#)
[View Structure in Jmol V12 with Java](#)

Formula:- Al_{0.2} Ca_{1.8} F_{0.66} Fe_{0.06} K_{0.12} Mg_{4.94} Na_{0.38} O_{23.34} Si_{7.8} -
Cell Parameters: $a = 9.85145\text{\AA}$ $b = 18.02911\text{\AA}$ $c = 5.273416\text{\AA}$ $\alpha = 90.0^\circ$ $\beta = 104.757^\circ$ $\gamma = 90.0^\circ$
Cell Volume = 905.733\AA^3

[View CIF](#) [Download CIF](#) [View Structure in JSmol with HTML 5](#)
[View Structure in Jmol V12 with Java](#)

Formula:- Al_{0.25} Li_{0.25} O₂ Si_{0.75} -



<http://nanocrystallography.research.pdx.edu/viewmcod/9000775>

3D Printing Your Favorite Atomic Structures

- Crystallographic Information File (CIF)
 - Most Complete & Compact Format >25 years

```
#-----  
#$Date: 2016-02-16 14:49:47 +0200 (Tue, 16 Feb 2016) $  
#$Revision: 176465 $  
#$URL: svn://www.crystallography.net/cod/cif/9/00/07/9000775.cif $  
#-----  
#
```

```
# This file is available in the Crystallography Open Database (COD),  
# http://www.crystallography.net/. The original data for this entry  
# were provided the American Mineralogist Crystal Structure Database,  
# http://ruff.geo.arizona.edu/AMS/amcsd.php  
#
```

```
# The file may be used within the scientific community so long as  
# proper attribution is given to the journal article from which the  
# data were obtained.  
#
```

```
data_9000775  
loop_  
_publ_author_name  
'Levien, L.'  
'Prewitt, C. T.'  
'Weidner, D. J.'  
_publ_section_title  
;
```

```
Structure and elastic properties of quartz at pressure  
P = 1 atm  
;
```

```
_journal_name_full      'American Mineralogist'  
_journal_page_first    920  
_journal_page_last     930  
_journal_volume        65  
_journal_year          1980  
_chemical_formula_sum  'O2 Si'  
_chemical_name_mineral Quartz
```

```
_symmetry_space_group_name_H-M 'P 32 2 1'  
_cell_angle_alpha      90  
_cell_angle_beta      90  
_cell_angle_gamma     120  
_cell_length_a        4.916  
_cell_length_b        4.916  
_cell_length_c        5.4054  
_cell_volume          113.131  
_diffrn_ambient_pressure 100  
_exptl_crystal_density_diffrn 2.646  
_cod_original_formula_sum 'Si O2'  
_cod_database_code      9000775
```

```
loop_  
_symmetry_equiv_pos_as_xyz  
x,y,z  
y,x,2/3-z  
-y,x-y,2/3+z  
-x,-x+y,1/3-z  
-x+y,-x,1/3+z  
x-y,-y,-z
```

```
loop_  
_atom_site_aniso_label  
_atom_site_aniso_U_11  
_atom_site_aniso_U_22  
_atom_site_aniso_U_33  
_atom_site_aniso_U_12  
_atom_site_aniso_U_13  
_atom_site_aniso_U_23  
Si 0.00854 0.00716 0.00725 0.00358 -0.00001 -0.00002  
O 0.01745 0.01322 0.01229 0.00973 -0.00291 -0.00408
```

```
loop_  
_atom_site_label  
_atom_site_fract_x  
_atom_site_fract_y  
_atom_site_fract_z  
Si 0.46970 0.00000 0.00000  
O 0.41350 0.26690 0.11910
```

3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Software

Bob Hanson, Author

- <http://jmol.sourceforge.net/>

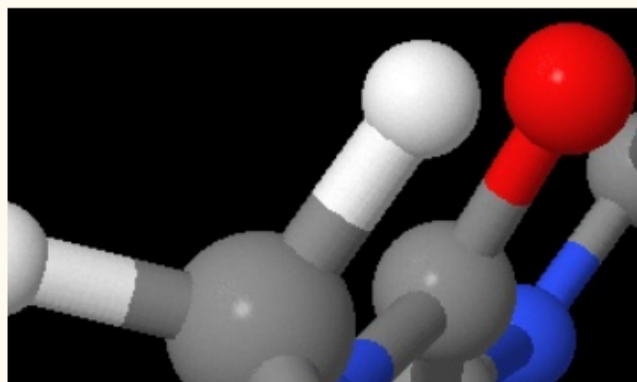


[Documentation](#) | [View](#)
[Browser check](#) | [Download](#)

Jmol



Jmol: an open-source Java viewer for chemical structures in 3D
with features for chemicals, crystals, materials and biomolecules



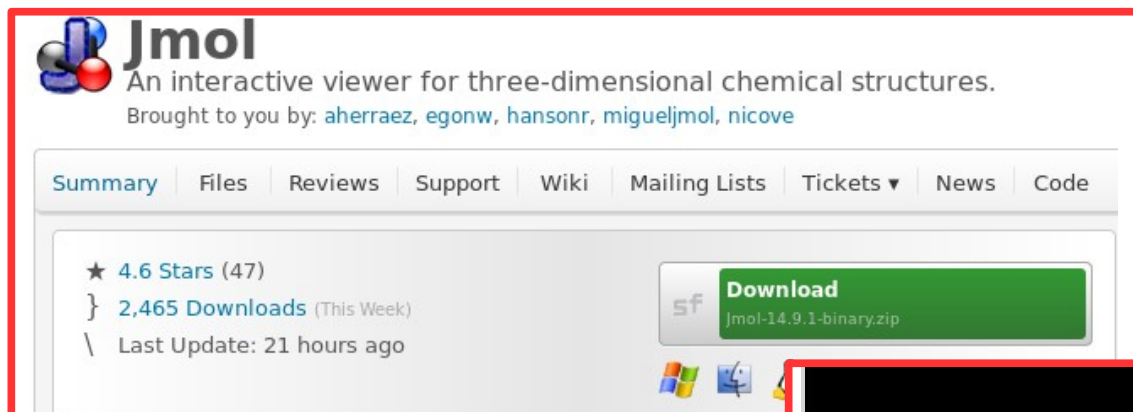
Jmol is an interactive web browser applet.

This is a still image, but you can get an animated display of Jmol abilities by clicking [here](#).

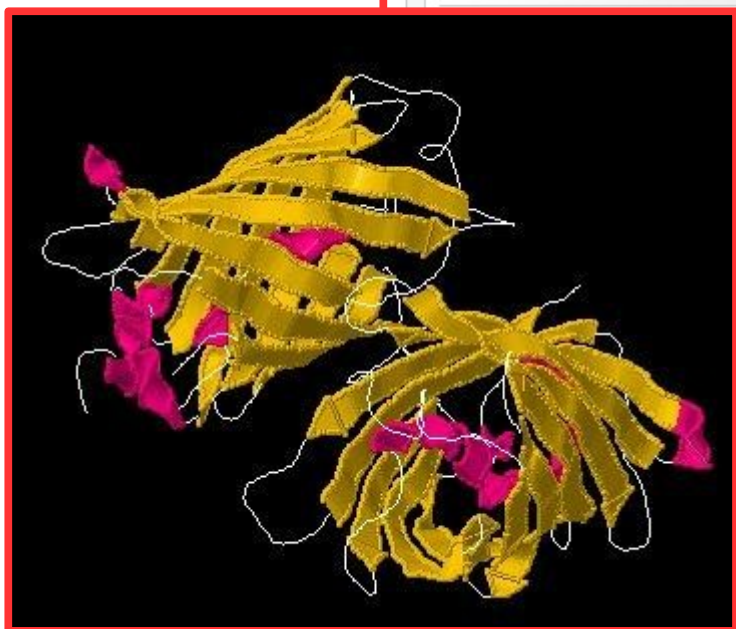
V. Scalfani et al., J Cheminform 8, 66 (2016), doi:10.1186/s13321-016-0181-z

3D Printing Your Favorite Atomic Structures

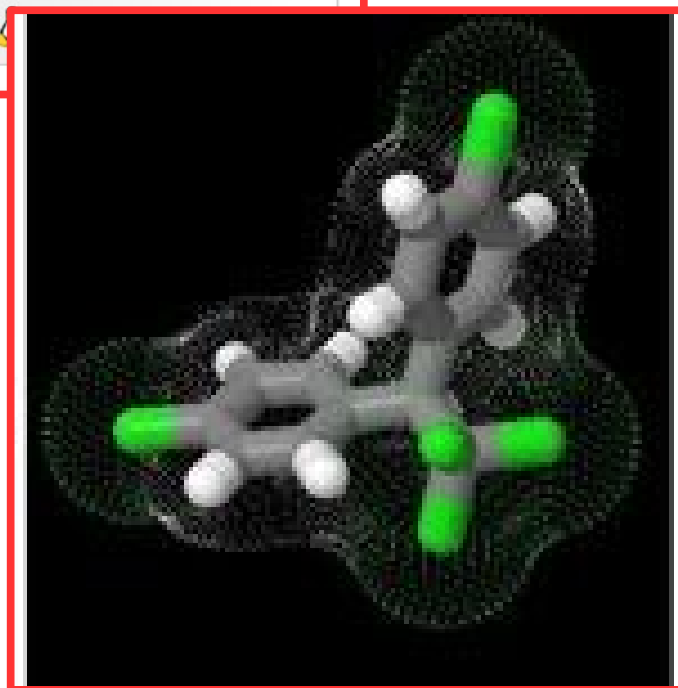
- Jmol/JSmol Software in Active Development
 - <https://sourceforge.net/projects/jmol/?source=navbar>



The screenshot shows the SourceForge project page for Jmol. At the top left is the Jmol logo, a stylized 'J' with a blue and red sphere. To its right, the text reads "Jmol An interactive viewer for three-dimensional chemical structures. Brought to you by: aherraez, egonw, hansonr, migueljmol, nicove". Below this is a navigation bar with links for Summary, Files, Reviews, Support, Wiki, Mailing Lists, Tickets, News, and Code. A statistics section shows "4.6 Stars (47)", "2,465 Downloads (This Week)", and "Last Update: 21 hours ago". A green "Download" button is visible, labeled "Download" and "jmol-14.9.1-binary.zip".



PSU Stu Res Symp

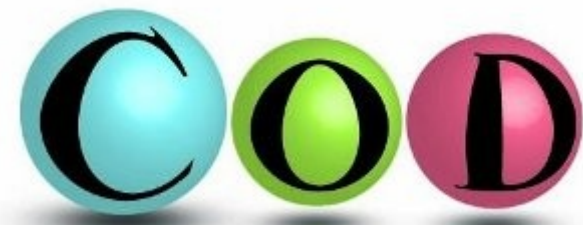


Paul DeStefano, PSU

3D Printing Your Favorite Atomic Structures

- Proposed, New Web-Based Tool for 3D Printing
 - Click Link

Formula:- C₈ H₁₀ N₄ O₂ -
Cell Parameters: $a = 14.9372\text{\AA}$ $b = 14.9372\text{\AA}$ $c = 6.898\text{\AA}$ $\alpha = 90.0^\circ$ $\beta = 90.0^\circ$ $\gamma = 120.0^\circ$
Cell Volume = 1332.88\AA^3
[View CIF](#) [Download CIF](#) [View Structure in JSmol with HTML 5](#)
[View Structure in Jmol V12 with Java](#)



3D Printing Your Favorite Atomic Structures

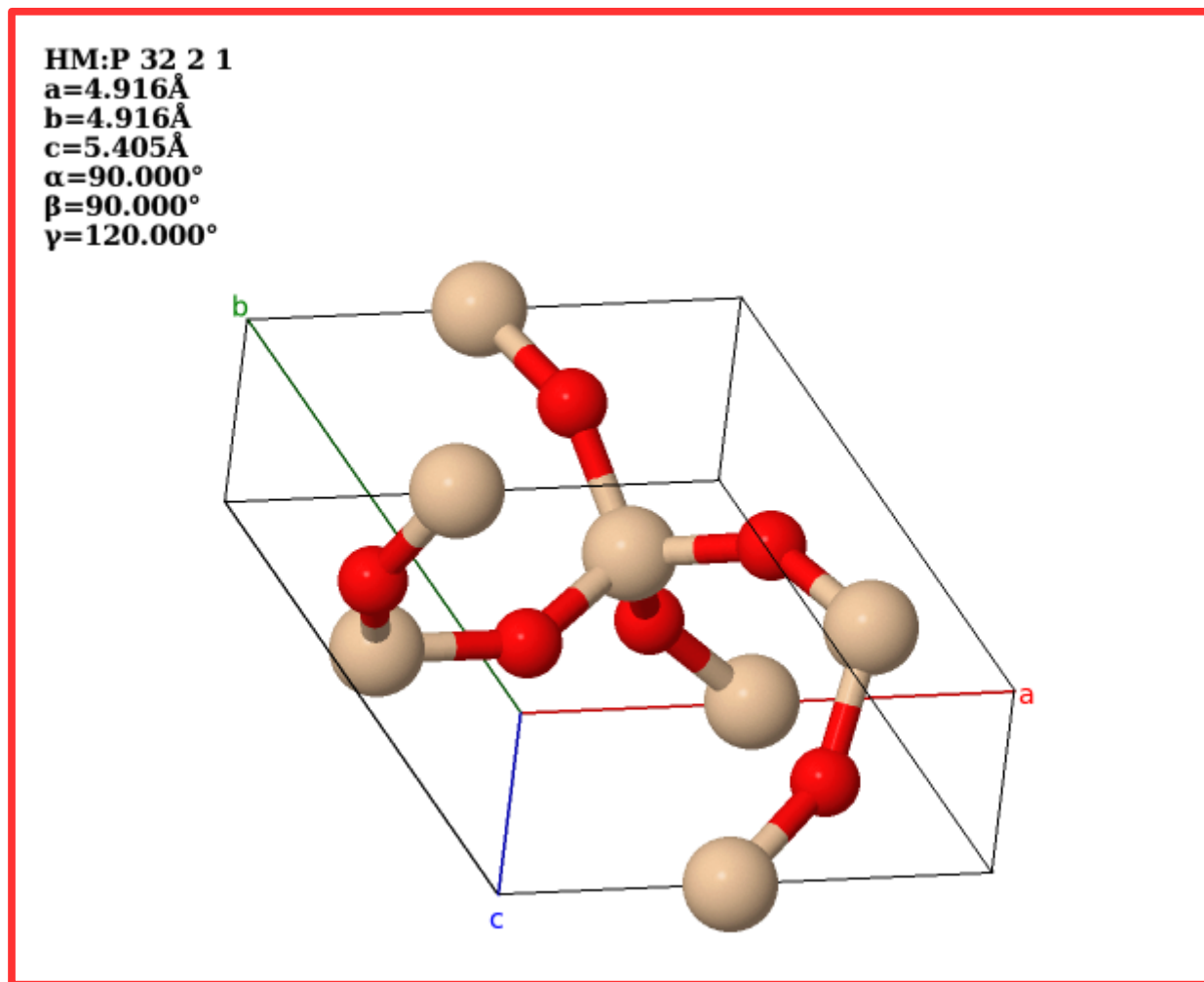
- Jmol/JSmol Feature: View

The screenshot displays the Jmol Crystal Symmetry Explorer interface. The central 3D model shows a quartz unit cell with atoms represented as red and white spheres. The unit cell axes are labeled 'a', 'b', and 'c'. The interface includes several control panels:

- Jmol Crystal Symmetry Explorer**: HM:P 32 2 1, a=4.916Å, b=4.916Å, c=5.405Å, α=90.000°, β=90.000°, γ=120.000°.
- load options**: molecular units, unpacked cell, packed cell, 3x1x1 set, 1x3x1 set, 1x1x3 set, 3x3x1 plane, 3x1x3 plane, 1x3x3 plane, 3x3x3 cube, 20-Angstrom cube.
- display options**: switch background, toggle unitcell, molecule by number, largest molecule, all molecules, center displayed.
- model options**: quartz (dropdown), Hermann-Mauguin symbol: ? (dropdown), 6 operators (dropdown), select a symmetry operation (dropdown), 1-x,1-y,1-z (input), #1 Si { 0.47 0.00 0.00/1 } (dropdown), show atoms opacity: 20% (dropdown).
- 3D printing options**: Set Scale, Save VRML, Save X3D, Save STL.
- console**: load ../data/quartz.cif packed, Execute.

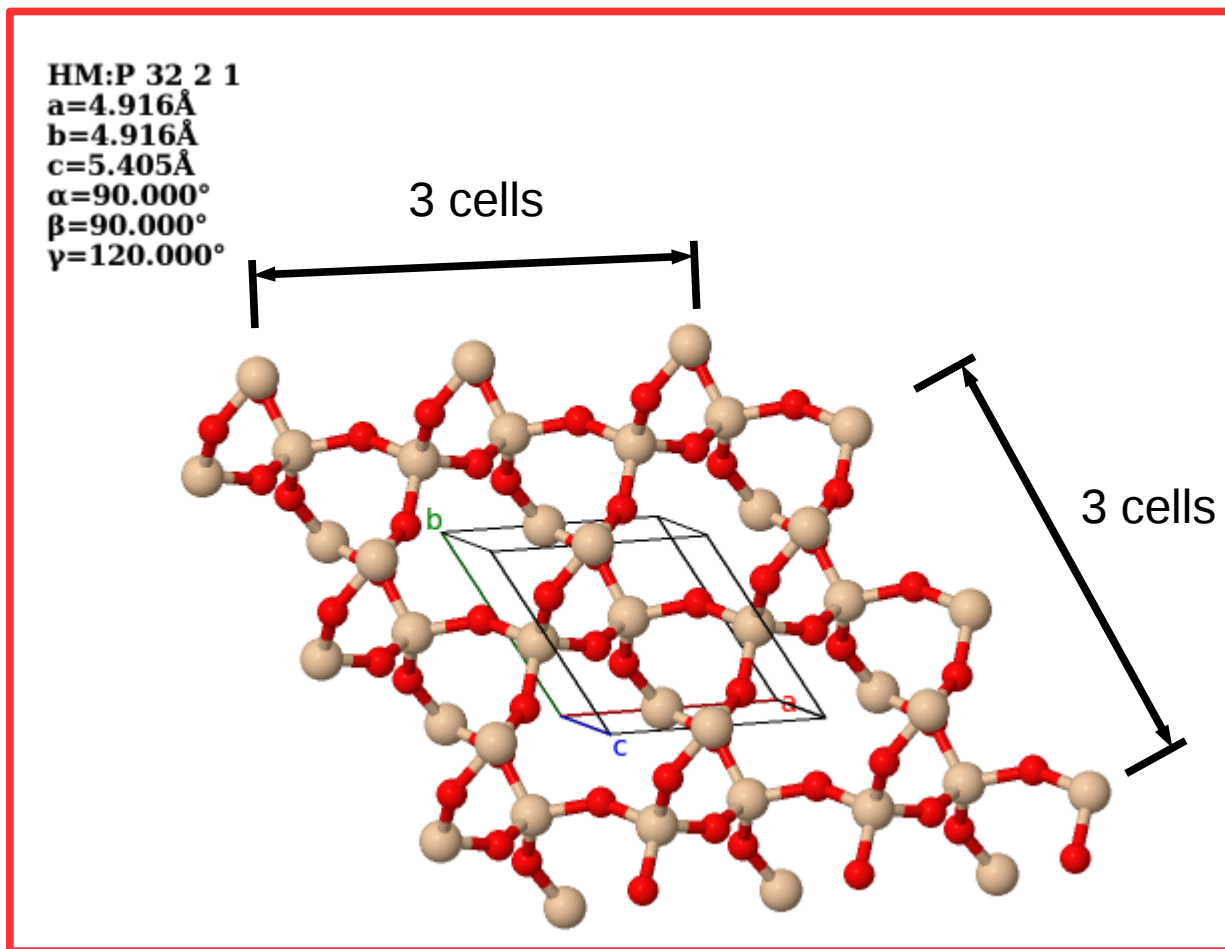
3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Feature: View



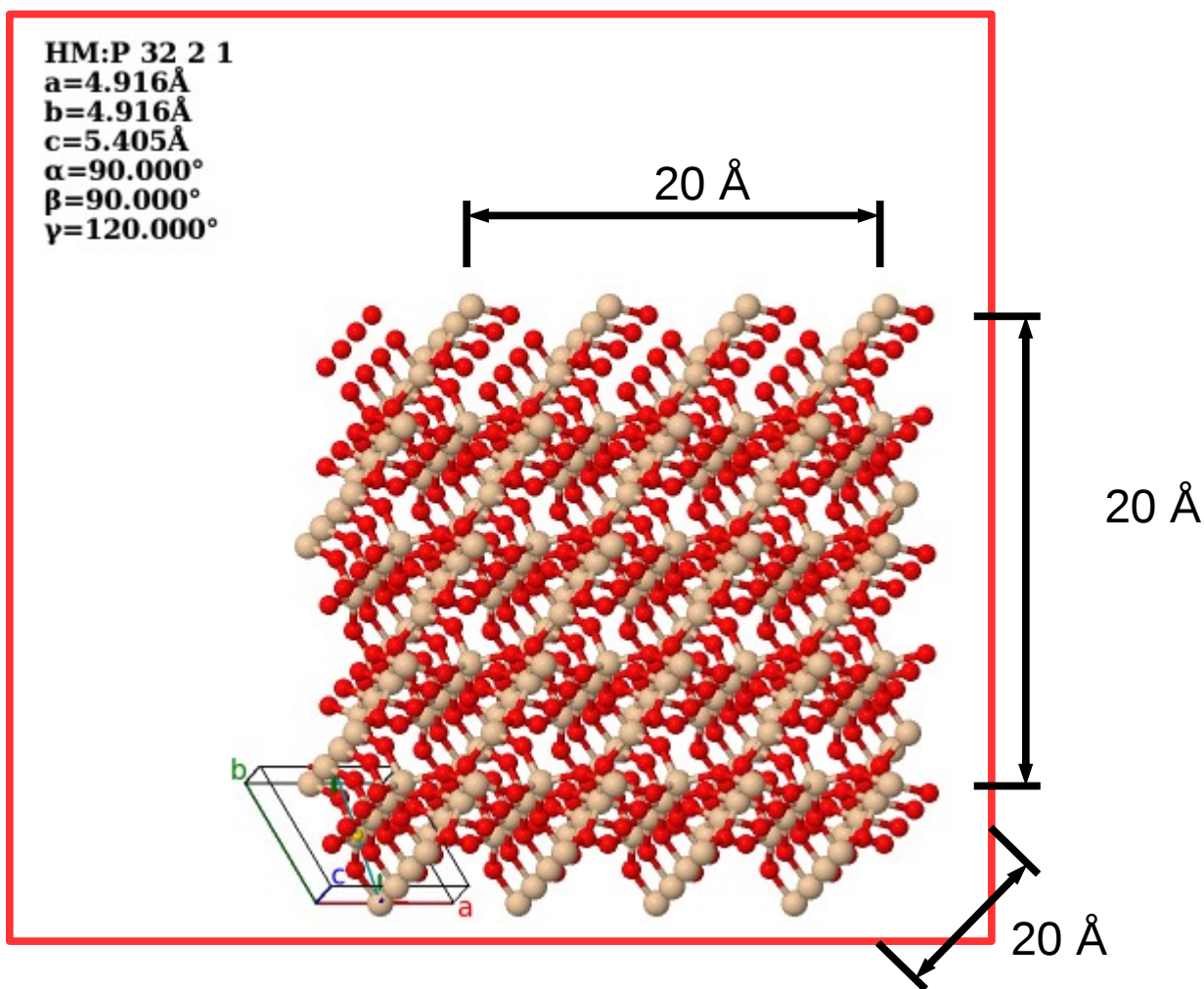
3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Feature: Render Options (1x3x3 Plane)



3D Printing Your Favorite Atomic Structures

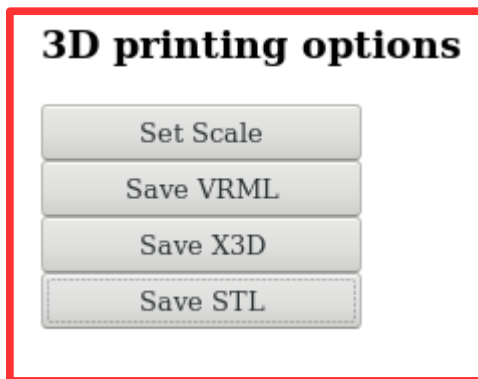
- Jmol/JSmol Feature: Render Options (20Å Cube)



Structure Larger than One Unit Cell is Apparent

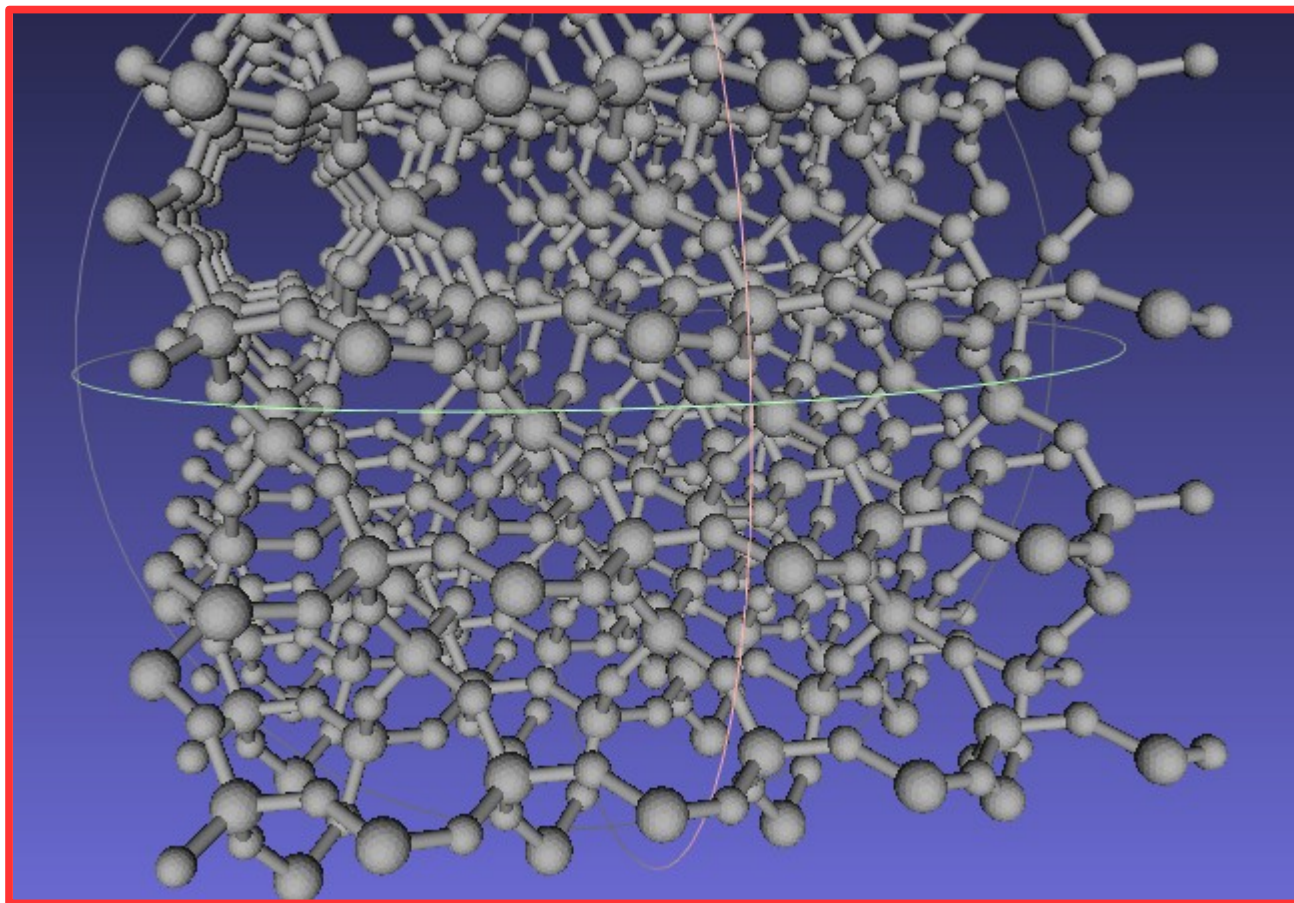
3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Feature: Save to 3D Print File



3D Printing Your Favorite Atomic Structures

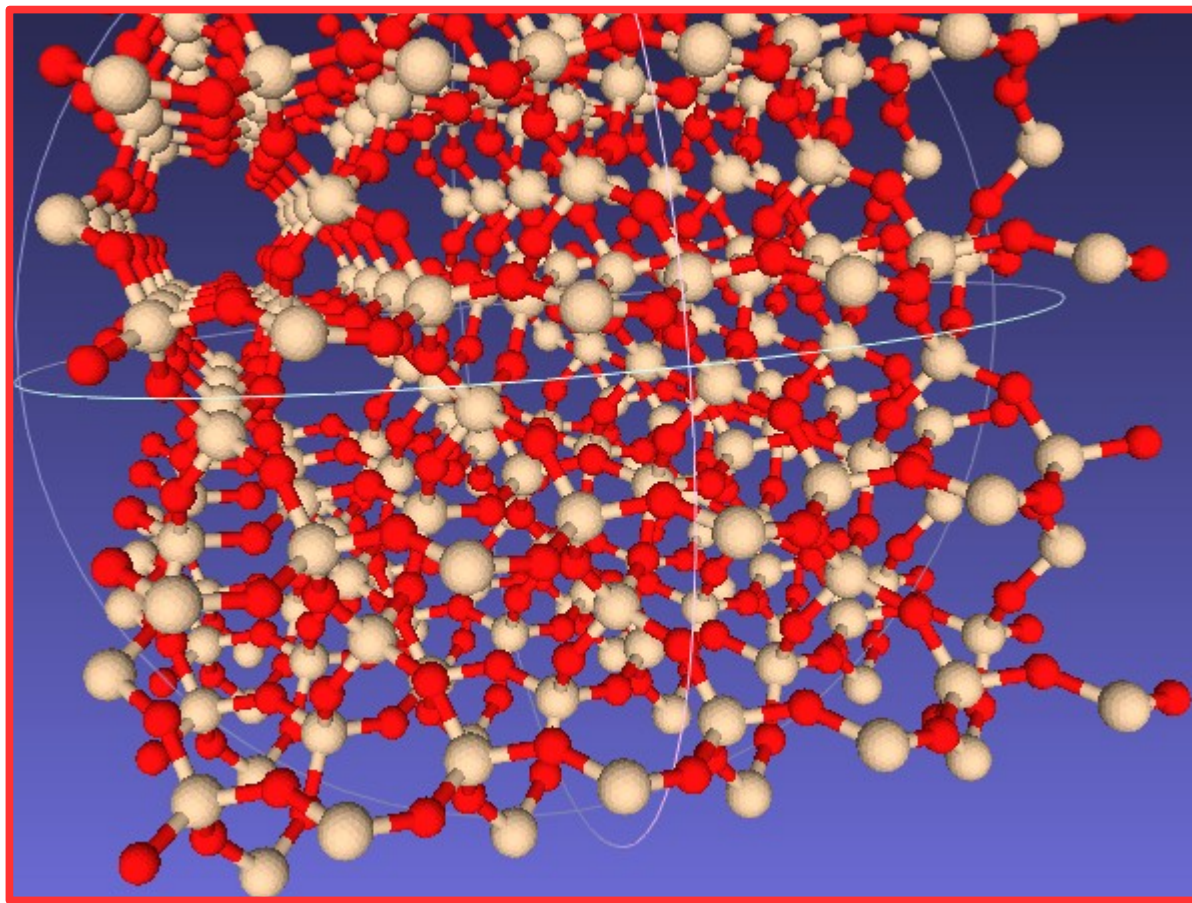
- Jmol/JSmol Feature: Save to 3D Print File (STL)



3D Graphics Viewer (Meshlab) Screenshot

3D Printing Your Favorite Atomic Structures

- Jmol/JSmol: Save to 3D Print File (X3D,VRML)



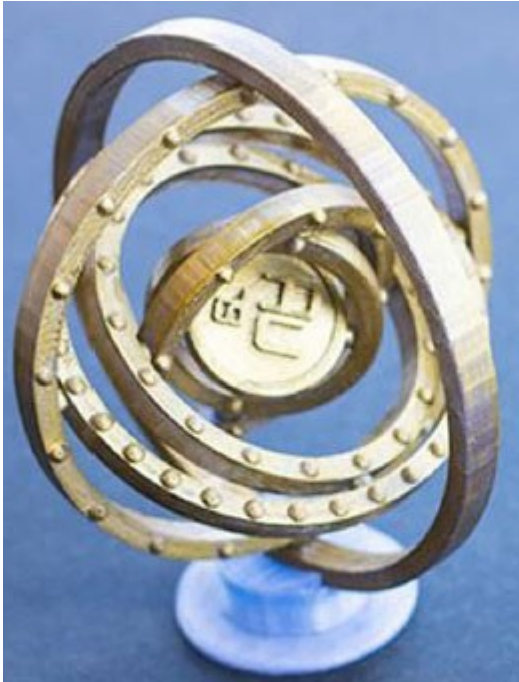
X3D succeeds the
ISO standard VRML

3D Printing Your Favorite Atomic Structures

- Summary & Conclusions
 - A new web-based tool would be valuable
 - Combine Search, Edit, 3D Printing
 - Come to the tool with a molecule, leave with a 3D model file
 - My next task is to build this tool
 - On the PSU Open Access Crystallography Project Site, first
 - On the North American COD Mirror Site, to be incorporated...

Thank you!

3D Printing Your Favorite Atomic Structures



Thank you!

References

- J. Stone-Sundberg et al., 3D printed models of small and large molecules, structures and morphologies of crystals, as well as their anisotropic physical properties, *Crystal Res. & Tech.*, 5 March 2015
- V. Scalfani et al., Programmatic conversion of crystal structures into 3D printable files using Jmol, *J Cheminform* 8, 66 (2016), doi:10.1186/s13321-016-0181-z