May 10th, 1:00 PM - 3:00 PM

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

Paul R. DeStefano
*Portland State University*

Peter Moeck
*Portland State University*

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

Paul R. DeStefano
Nano-Crystallography Group
Portland State University

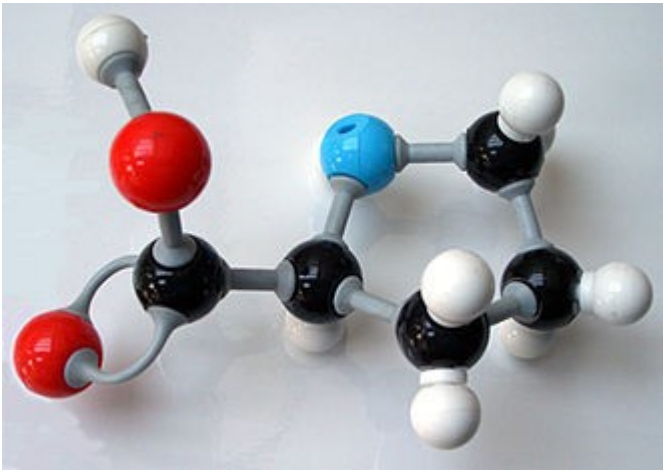
# 3D Printing Your Favorite Atomic Structures

- 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

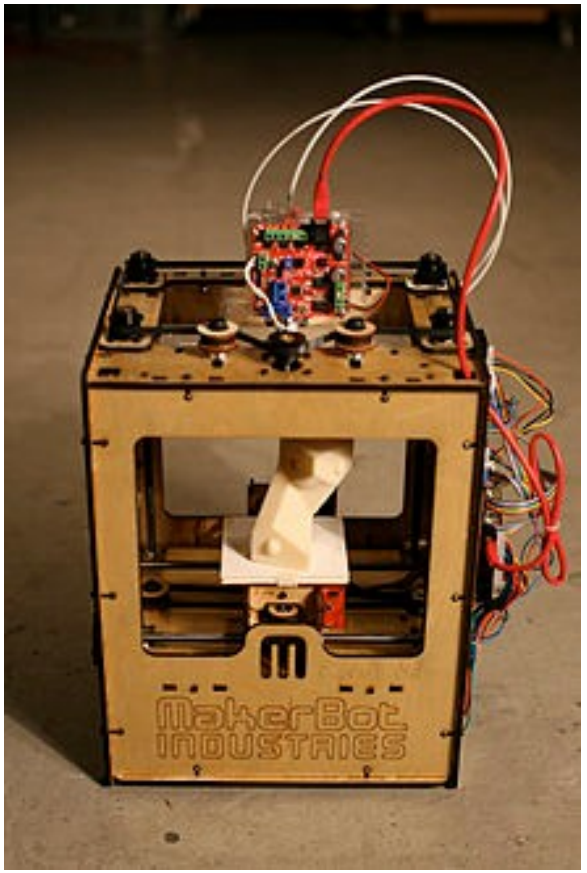
3D printing a hyperboloid

# 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

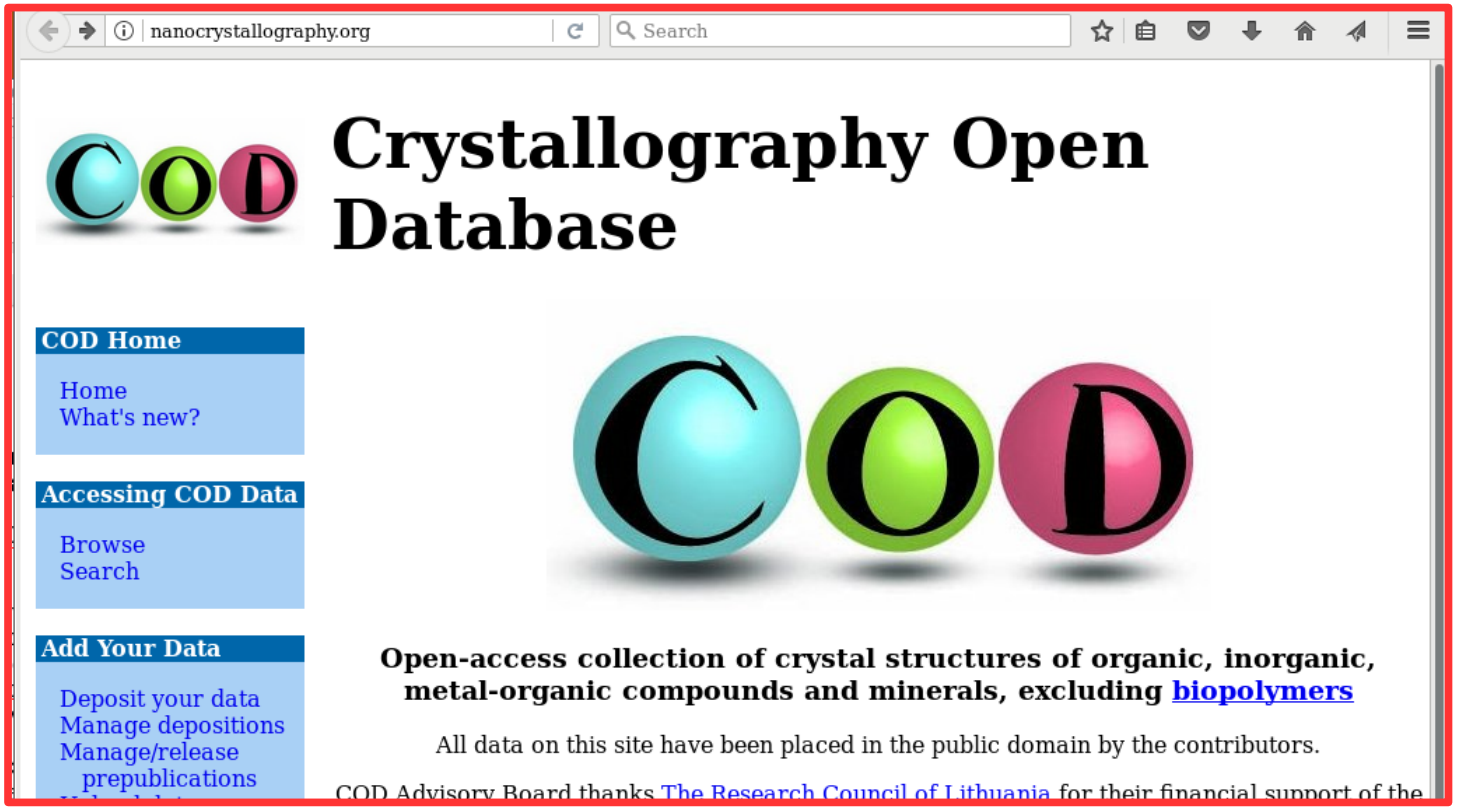


# 3D Printing Your Favorite Atomic Structures

- 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**

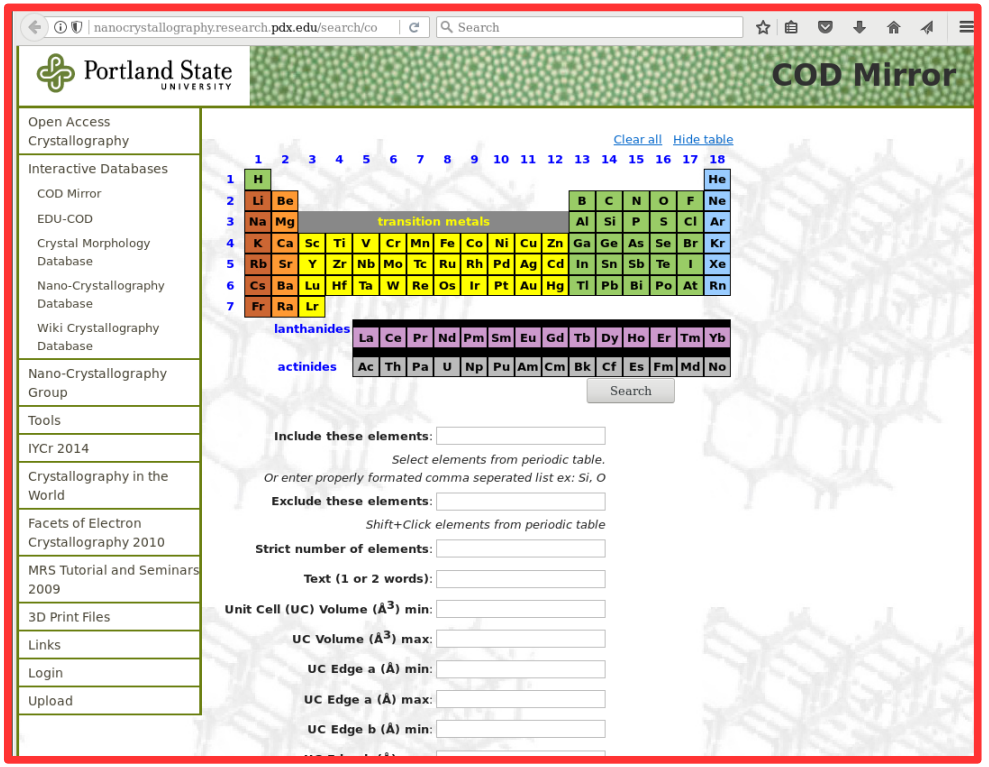
# 3D Printing Your Favorite Atomic Structures

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



# 3D Printing Your Favorite Atomic Structures

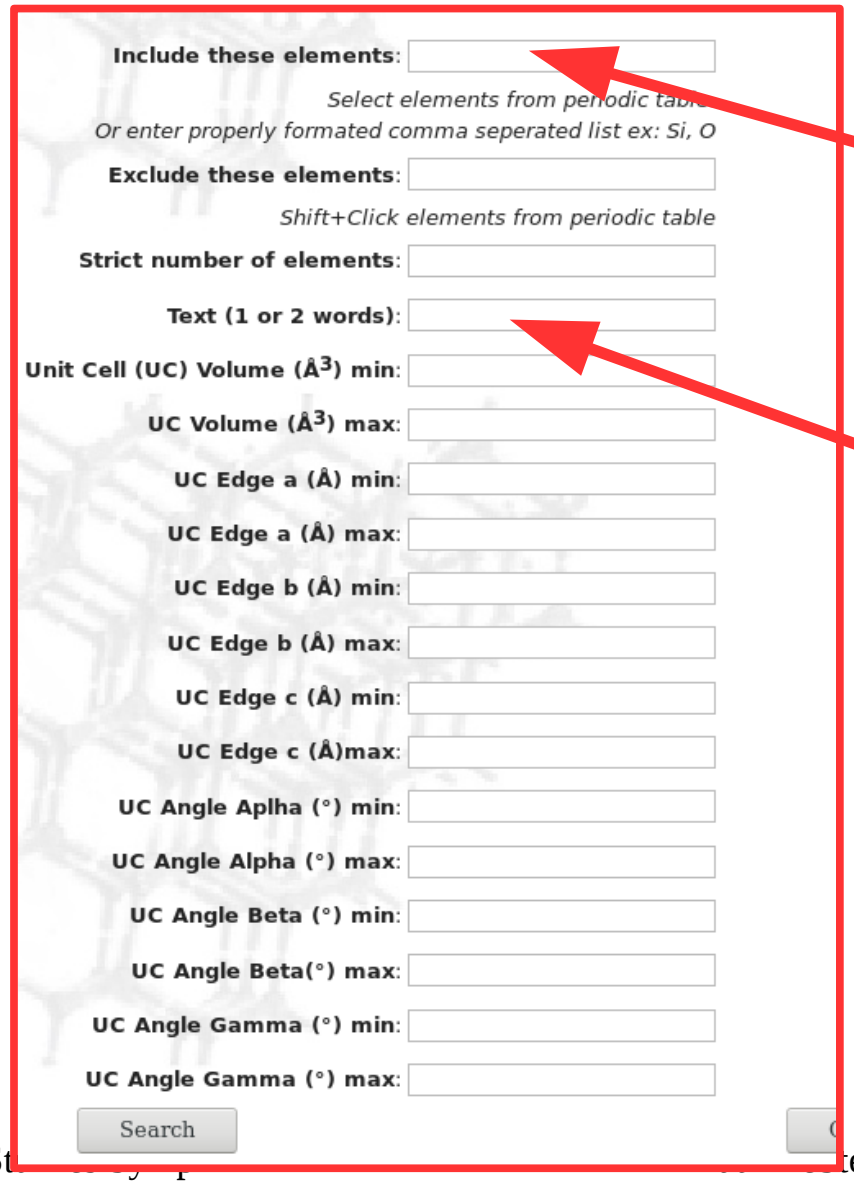
- Finding Atomic Structures: Databases (OACP)
  - Open Access Crystallography Project
  - http://nanocrystallography.research.pdx.edu/search/codmirror/

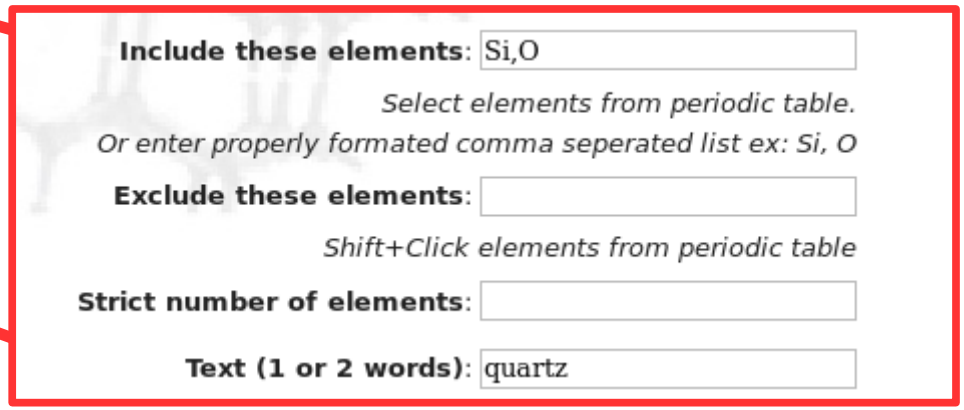



Open Access Crystallography Project Interface

# 3D Printing Your Favorite Atomic Structures

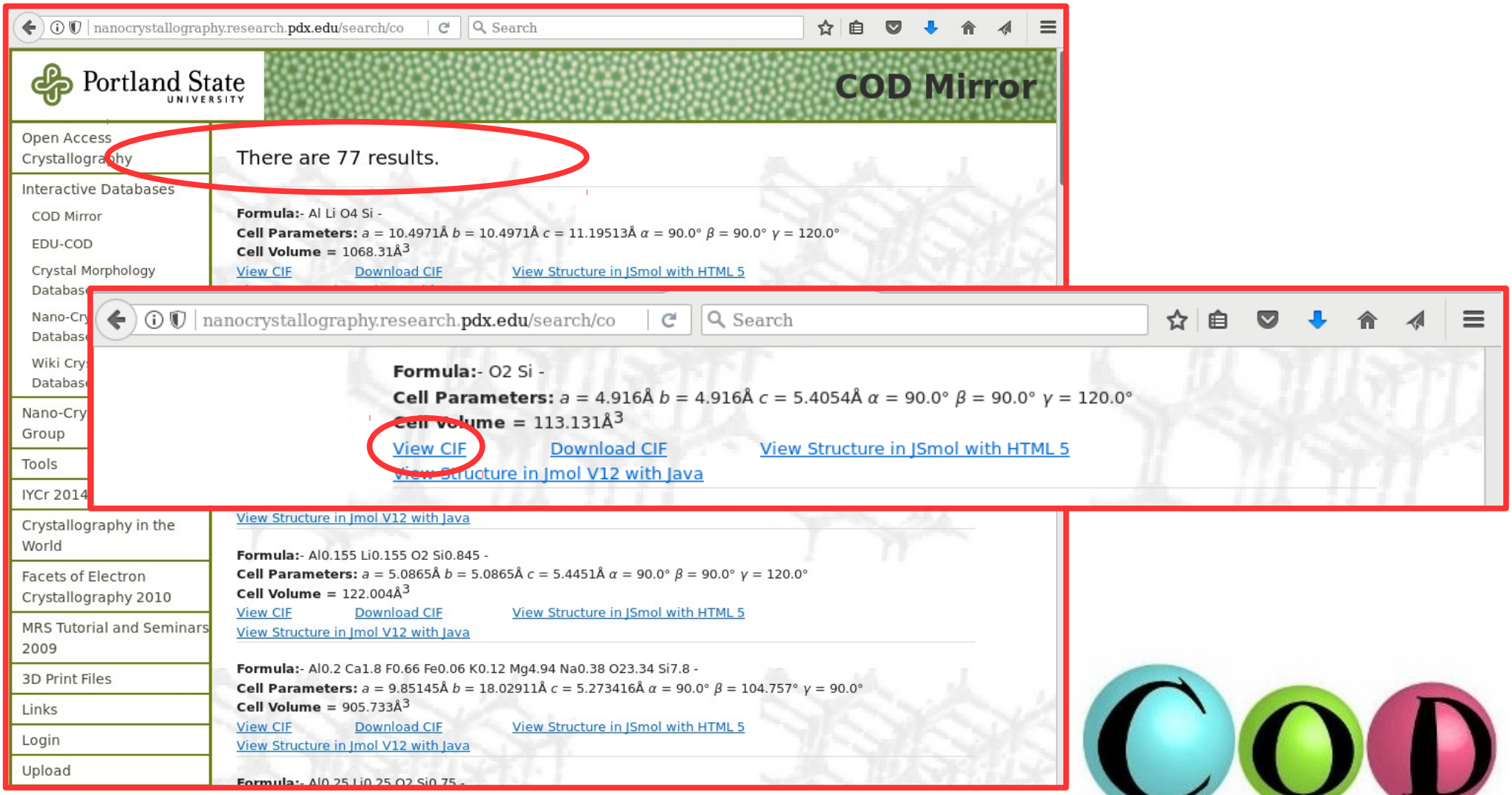
- Finding Atomic Structures: Search




# 3D Printing Your Favorite Atomic Structures

- Finding Atomic Structures: Search




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

# 3D Printing Your Favorite Atomic Structures

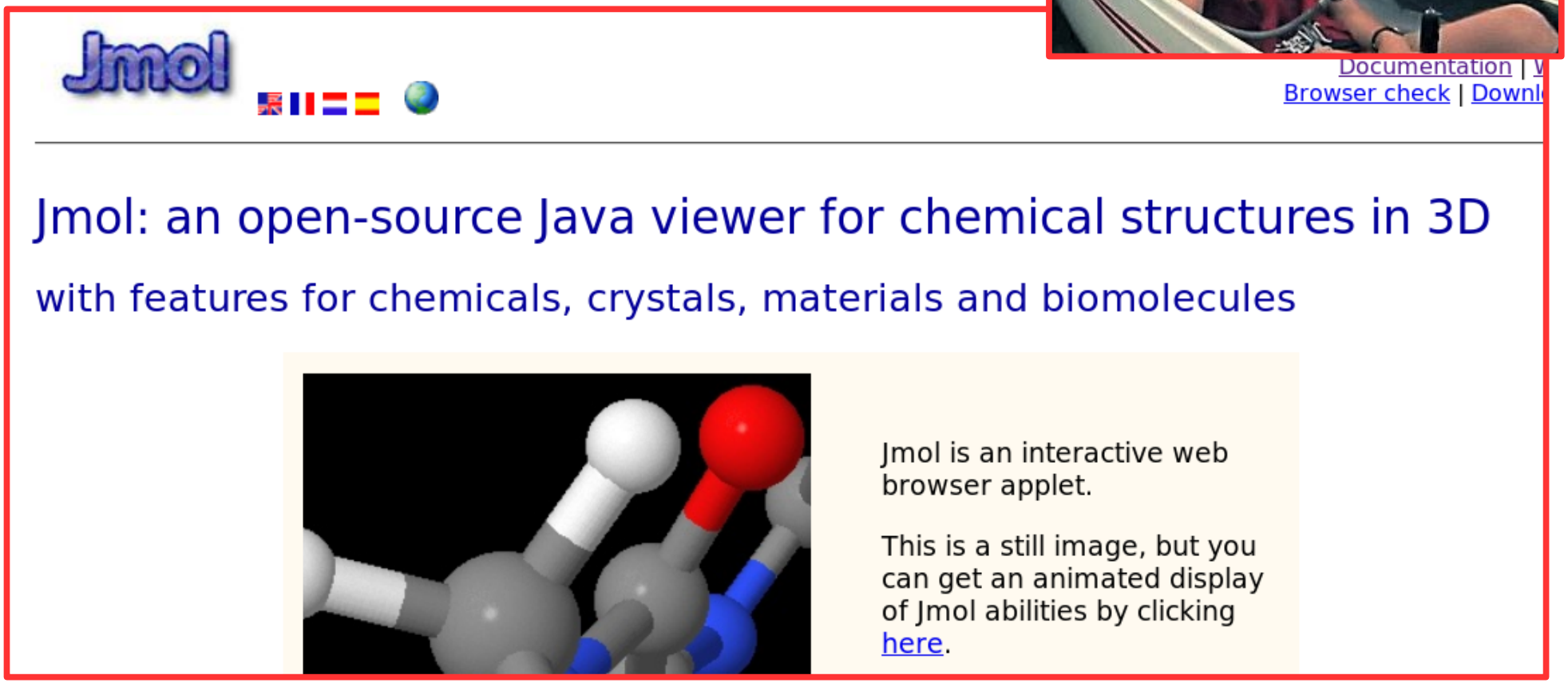
- Crystallographic Information File (CIF)
  - Most Complete & Compact Format >25 years

```
#------------------------------------------------------------------------------
#$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://rruff.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
  - http://jmol.sourceforge.net/

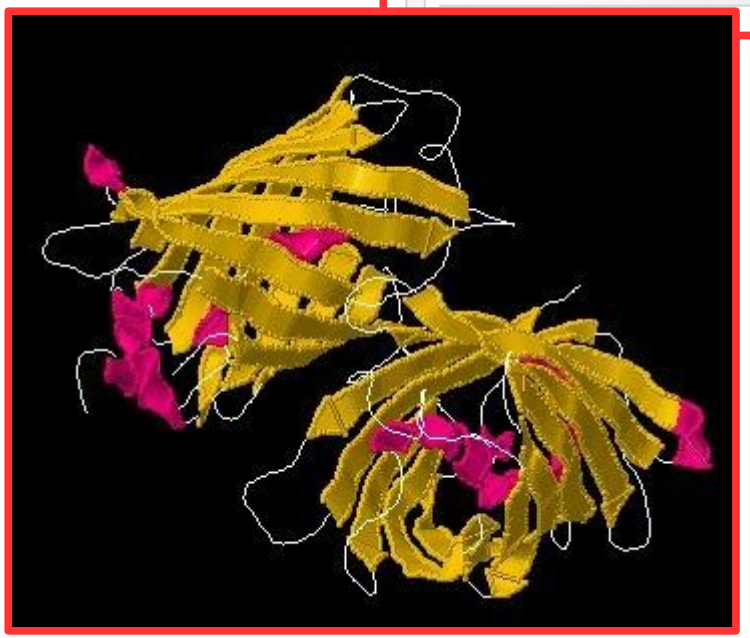
Bob Hanson, Author

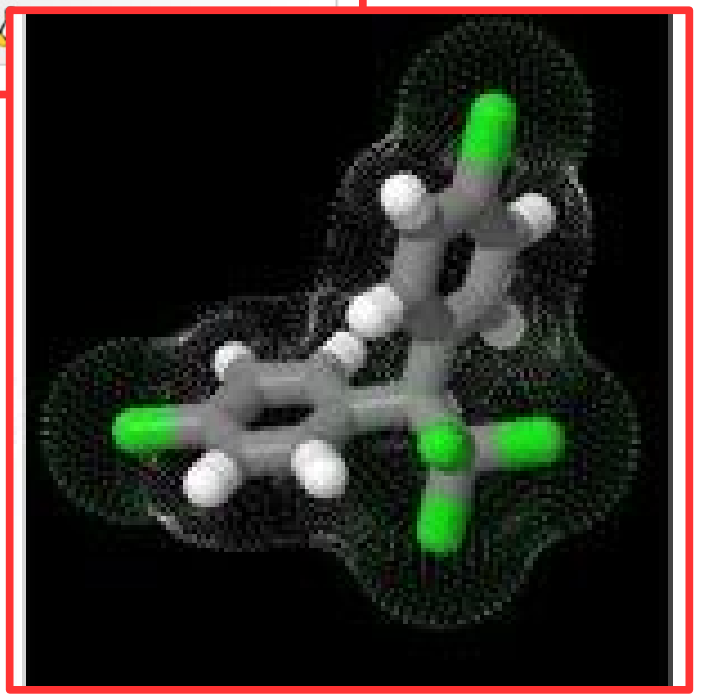



V. Scalfani et al., J Cheminform 8, 66 (2016), doi:10.1186/s13321-016-0181-z

# 3D Printing Your Favorite Atomic Structures

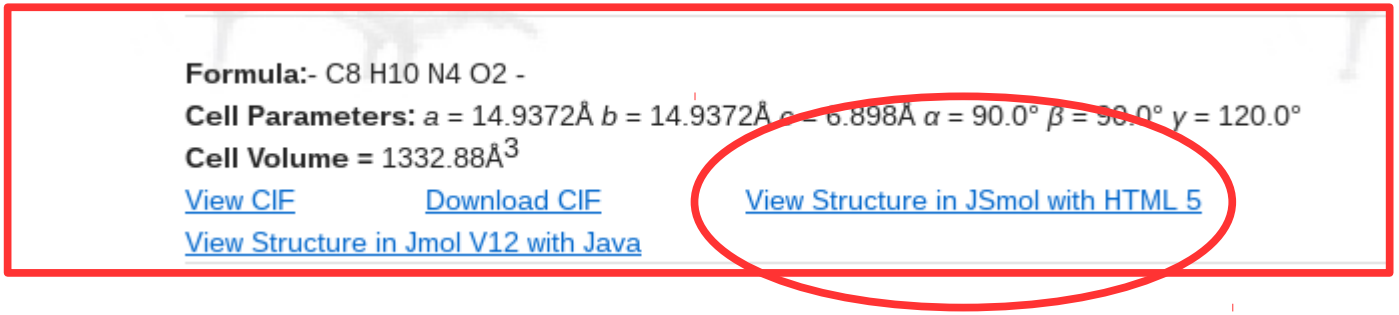
- Jmol/JSmol Software in Active Development
  - https://sourceforge.net/projects/jmol/?source=navbar



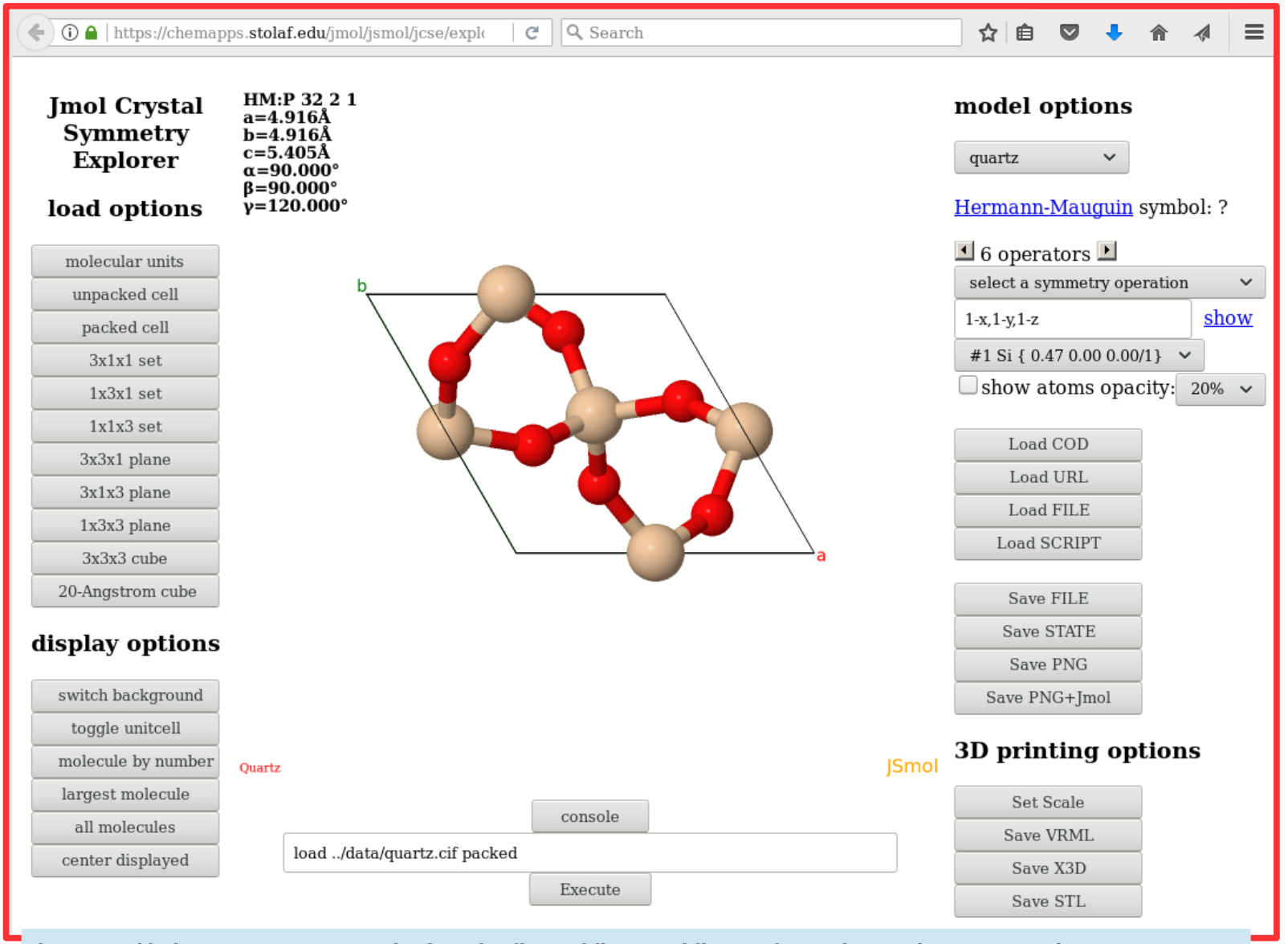
# 3D Printing Your Favorite Atomic Structures

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



# 3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Feature: View

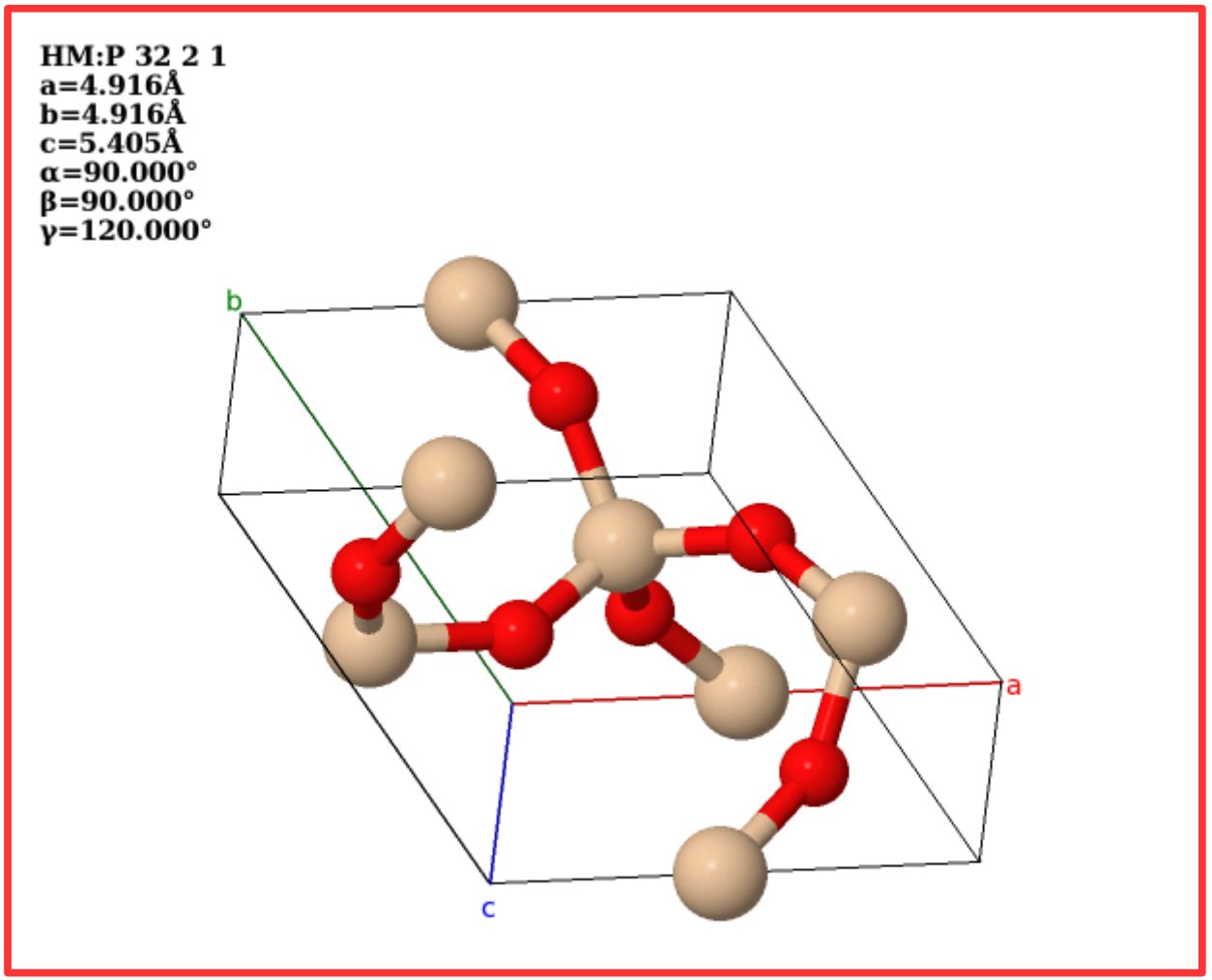




https://chemapps.stolaf.edu/jmol/jsmol/jcse/explore.htm?cod=1100887

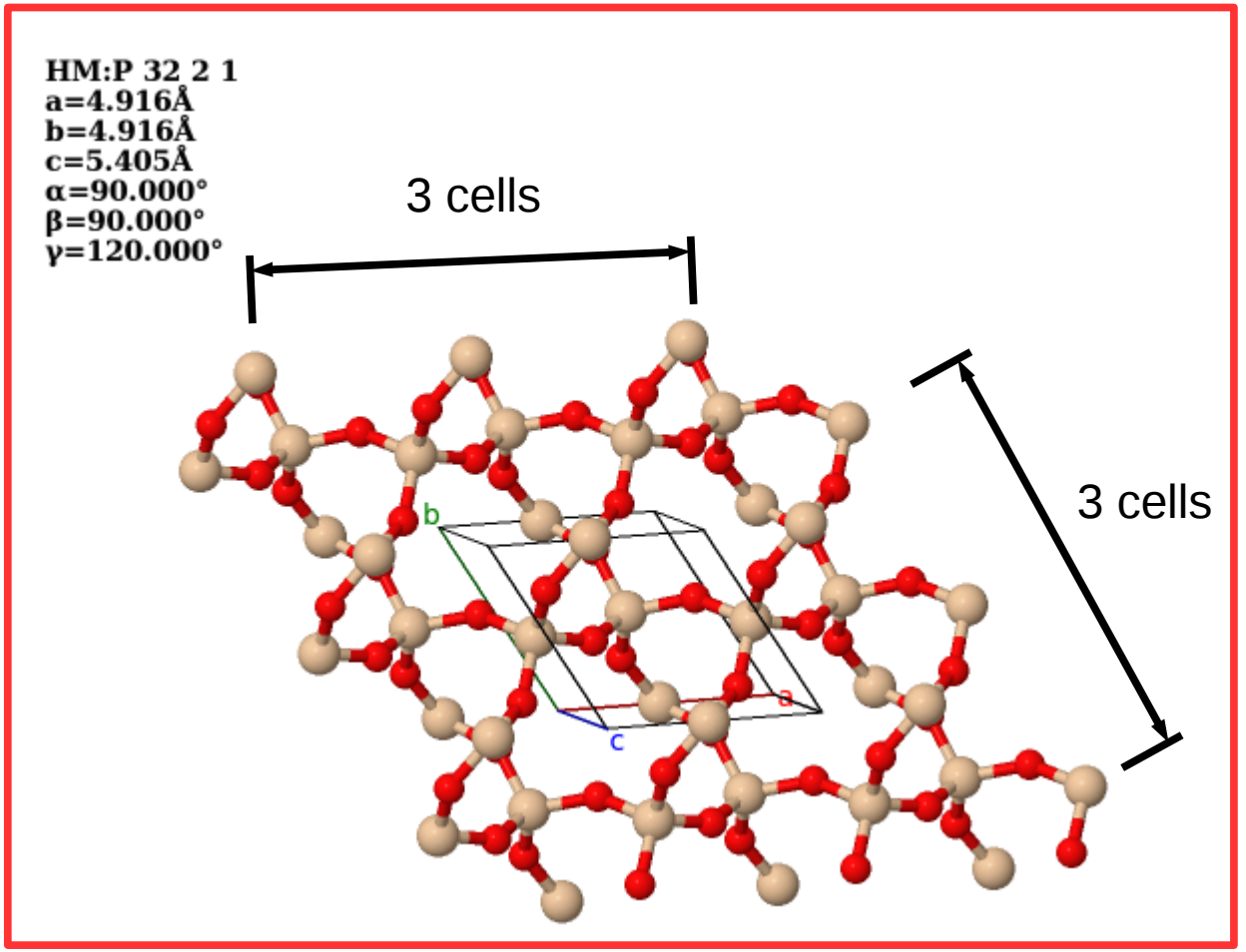
# 3D Printing Your Favorite Atomic Structures

- Jmol/JSmol Feature: View



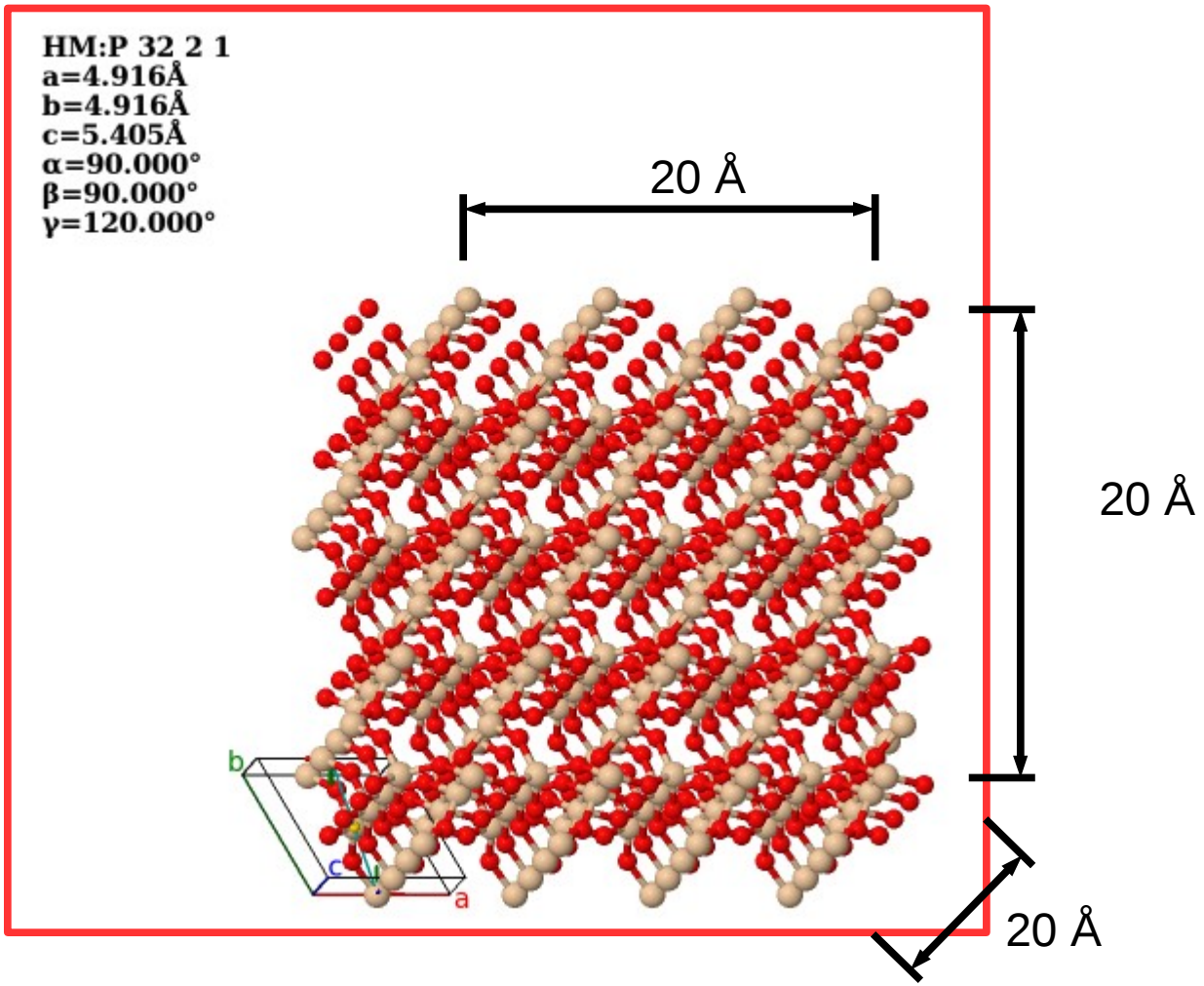
# 3D Printing Your Favorite Atomic Structures

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



# 3D Printing Your Favorite Atomic Structures

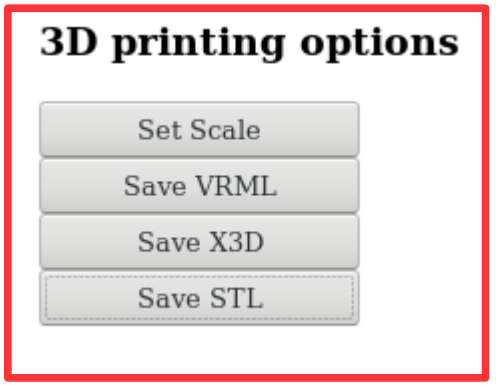
- Jmol/JSmol Feature: Render Options (20Å Cube)




Structure Larger than One Unit Cell is Apparent

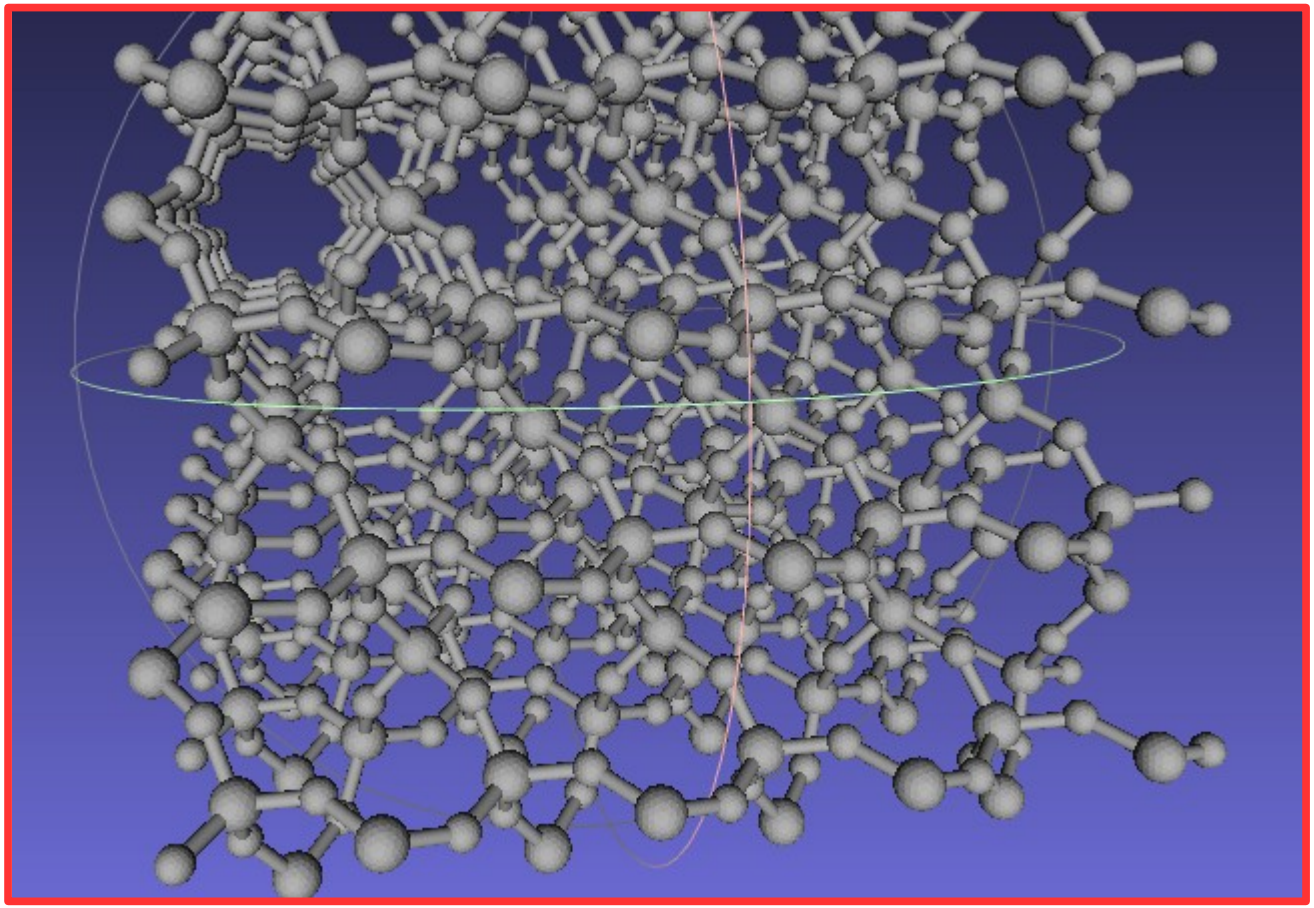
# 3D Printing Your Favorite Atomic Structures

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



# 3D Printing Your Favorite Atomic Structures

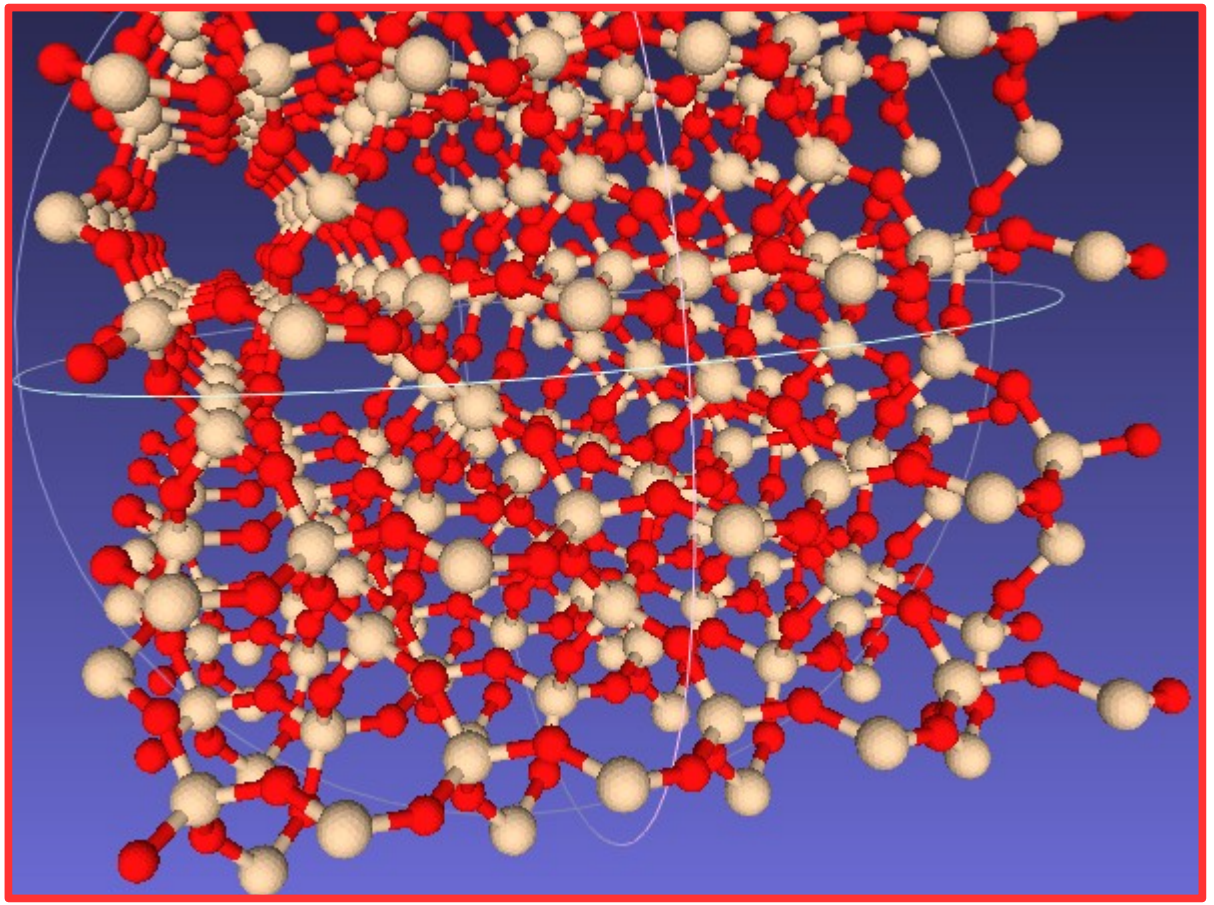
- Jmol/JSmol Feature: Save to 3D Print File (STL)



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 Graphics Viewer (Meshlab) Screenshot

# 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