

Crystallography and Crystal Chemistry  
X International School-Conference of  
Young Scientists 2025

## *Tutorial 4: How to visualize crystal structures: Jmol and Vesta*

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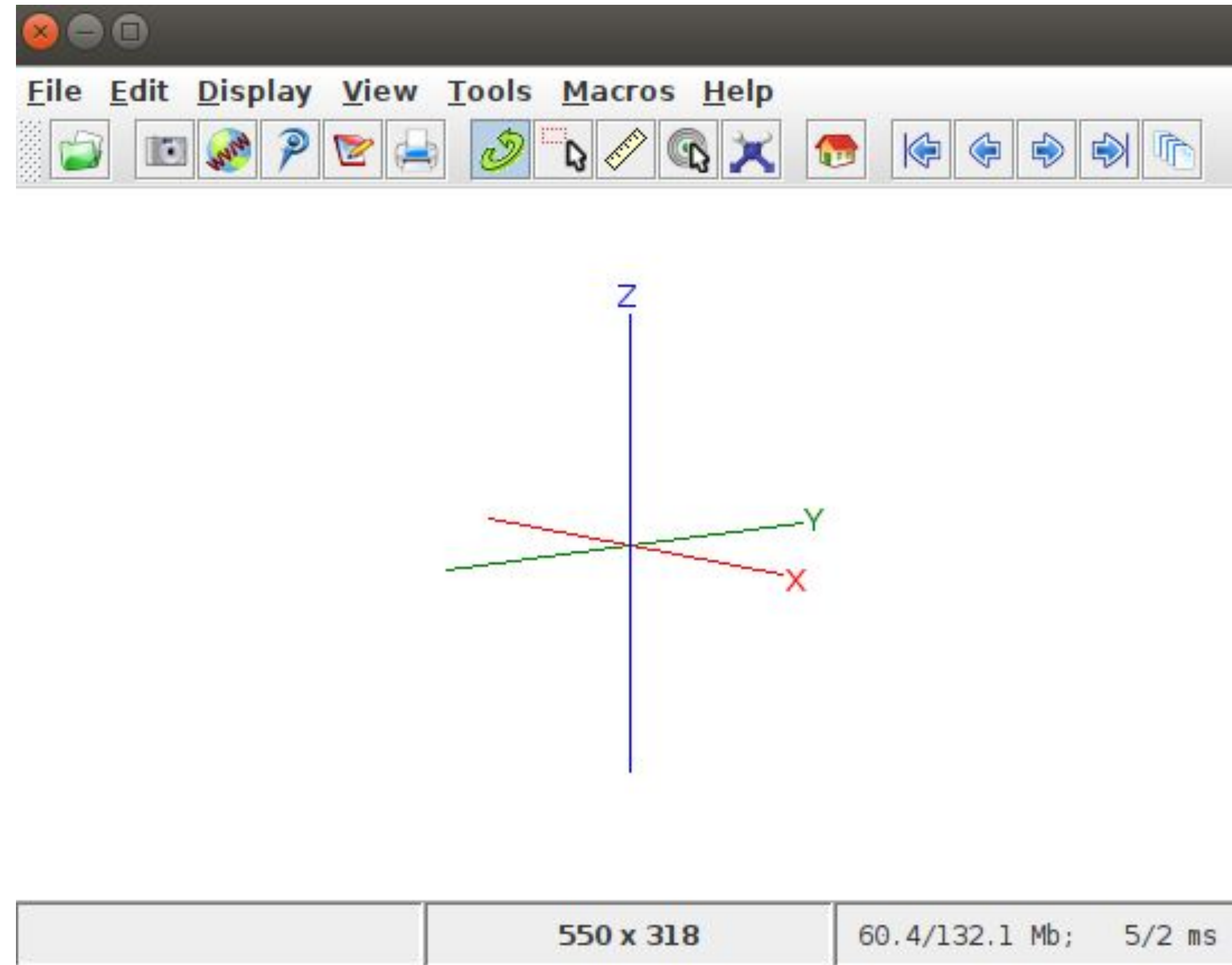
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# Jmol: an open-source Java viewer for chemical structures in 3D



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

[web\\_version](#)

# Jmol supports lots of structure file formats (~100)

Main of them are XYZ and Crystallographic Information File (cif)

```
24
Caffeine
H   -3.3804130   -1.1272367    0.5733036
N    0.9668296   -1.0737425   -0.8198227
C    0.0567293    0.8527195    0.3923156
N   -1.3751742   -1.0212243   -0.0570552
C   -1.2615018    0.2590713    0.5234135
C   -0.3068337   -1.6836331   -0.7169344
C    1.1394235    0.1874122   -0.2700900
N    0.5602627    2.0839095    0.8251589
O   -0.4926797   -2.8180554   -1.2094732
C   -2.6328073   -1.7303959   -0.0060953
O   -2.2301338    0.7988624    1.0899730
H    2.5496990    2.9734977    0.6229590
C    2.0527432   -1.7360887   -1.4931279
H   -2.4807715   -2.7269528    0.4882631
H   -3.0089039   -1.9025254   -1.0498023
H    2.9176101   -1.8481516   -0.7857866
H    2.3787863   -1.1211917   -2.3743655
H    1.7189877   -2.7489920   -1.8439205
C   -0.1518450    3.0970046    1.5348347
C    1.8934096    2.1181245    0.4193193
N    2.2861252    0.9968439   -0.2440298
H   -0.1687028    4.0436553    0.9301094
H    0.3535322    3.2979060    2.5177747
H   -1.2074498    2.7537592    1.7203047
```

```
1 # generated using pymatgen
2 data_LiCoO2
3 _symmetry_space_group_name_H-M 'P 1'
4 _cell_length_a 2.84289827
5 _cell_length_b 2.84289827
6 _cell_length_c 14.14561550
7 _cell_angle_alpha 90.00000000
8 _cell_angle_beta 90.00000000
9 _cell_angle_gamma 120.00000000
10 loop
11 _atom_site_type_symbol
12 _atom_site_label
13 _atom_site_symmetry_multiplicity
14 _atom_site_fract_x
15 _atom_site_fract_y
16 _atom_site_fract_z
17 _atom_site_occupancy
18 Li Li0 1 0.00000000 0.00000000 0.00000000 1.0
19 Li Li1 1 0.66666667 0.33333333 0.33333333 1.0
20 Li Li2 1 0.33333333 0.66666667 0.66666667 1.0
21 Co Co3 1 0.33333333 0.66666667 0.16666667 1.0
22 Co Co4 1 0.00000000 0.00000000 0.50000000 1.0
23 Co Co5 1 0.66666667 0.33333333 0.83333333 1.0
24 O O6 1 0.00000000 0.00000000 0.23958700 1.0
25 O O7 1 0.66666667 0.33333333 0.09374633 1.0
26 O O8 1 0.66666667 0.33333333 0.57292033 1.0
27 O O9 1 0.33333333 0.66666667 0.42707967 1.0
28 O O10 1 0.33333333 0.66666667 0.90625367 1.0
29 O O11 1 0.00000000 0.00000000 0.76041300 1.0
```

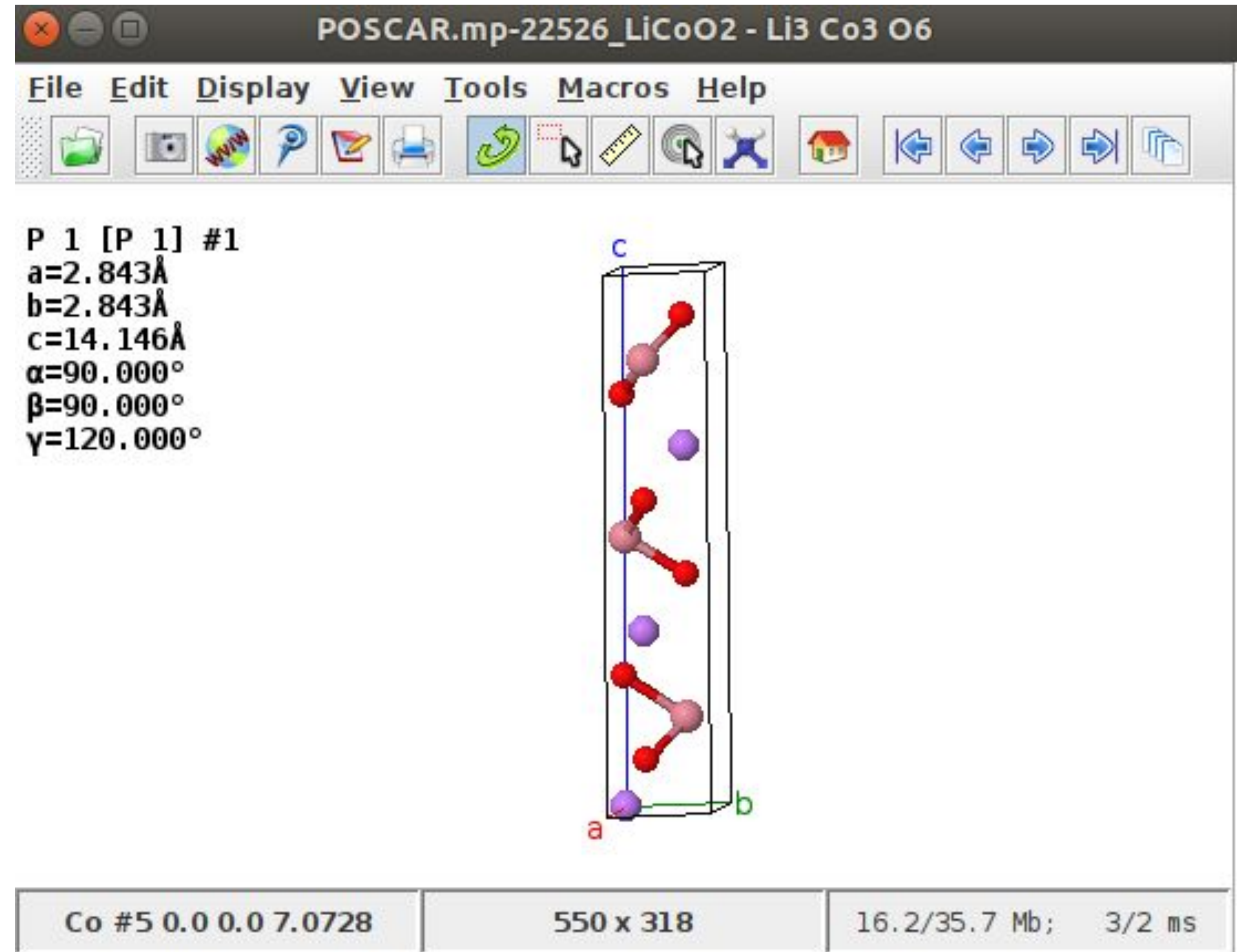
# But we love Jmol for VASP files supporting

**POSCAR** – input structure file

**CONTCAR** – output structure file

```
1  Li3 Co3 O6
2  1.0
3  2.842898 0.000000 0.000000
4  -1.421449 2.462022 0.000000
5  0.000000 0.000000 14.145615
6  Li Co O
7  3 3 6
8  direct
9  0.000000 0.000000 0.000000 Li
10 0.666667 0.333333 0.333333 Li
11 0.333333 0.666667 0.666667 Li
12 0.333333 0.666667 0.166667 Co
13 0.000000 0.000000 0.500000 Co
14 0.666667 0.333333 0.833333 Co
15 0.000000 0.000000 0.239587 O
16 0.666667 0.333333 0.093746 O
17 0.666667 0.333333 0.572920 O
18 0.333333 0.666667 0.427080 O
19 0.333333 0.666667 0.906254 O
20 0.000000 0.000000 0.760413 O
```

And even **OUTCAR** – output VASP file, which includes all the information about DFT calculation.

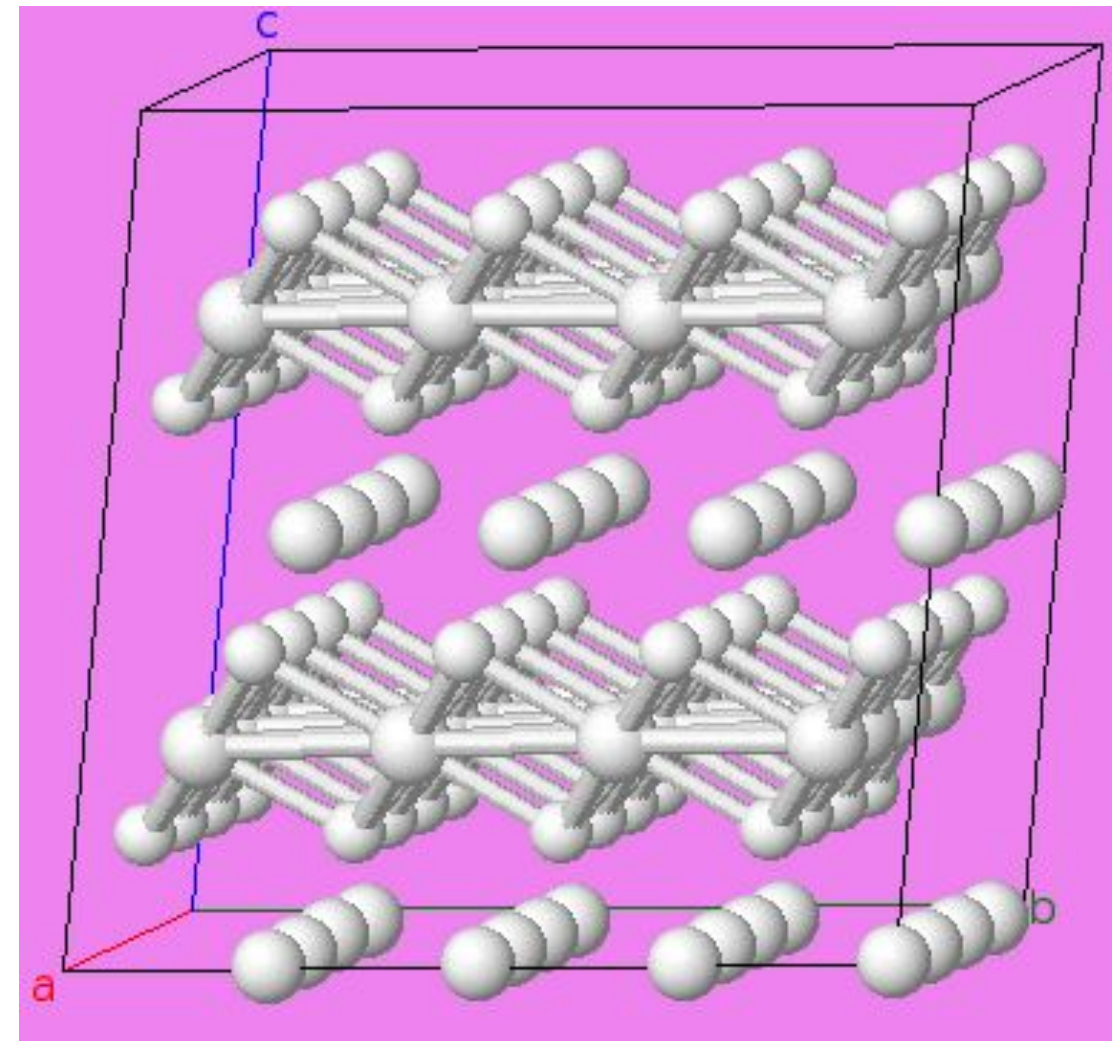
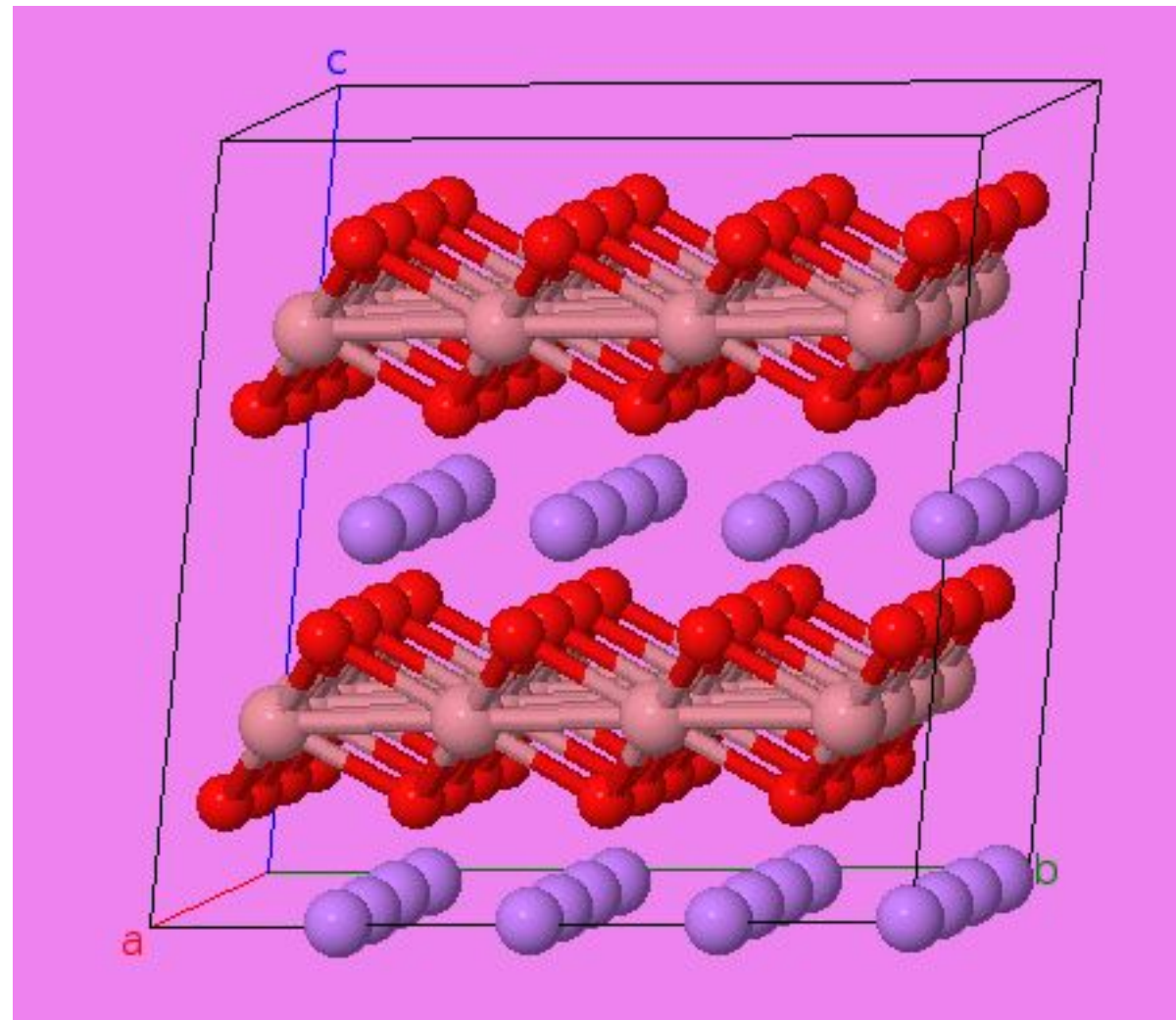


# Some useful tools in Jmol

Using **Jmol console** (*File*→*Console*) you are able to color background and atoms in your favorite colors. But do not get carried away too much, remember about the formal style when preparing figures for your scientific paper

```
$ color background violet
```

```
$ color atoms white
```

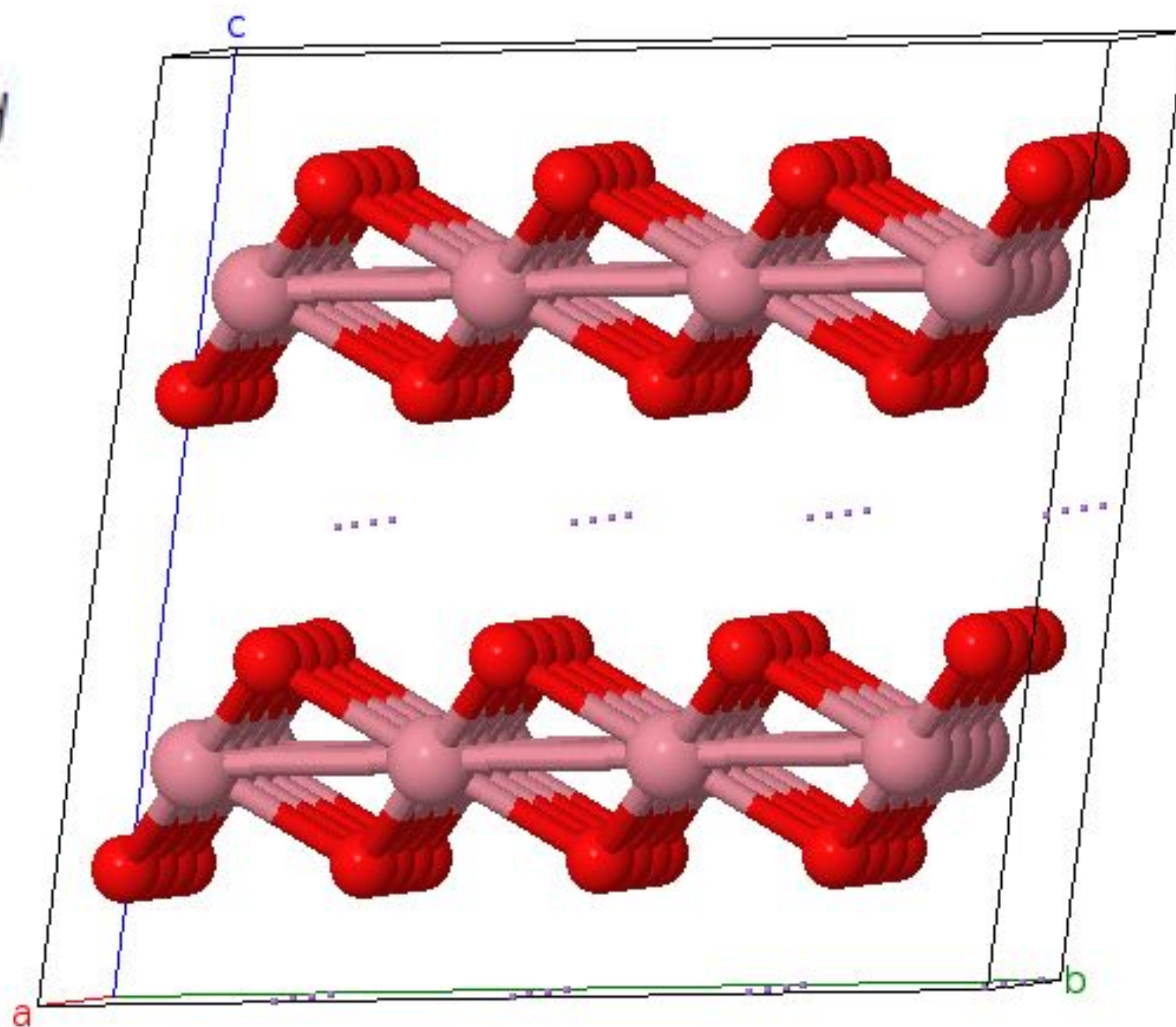


```
$ select li  
32 atoms selected  
$ color green  
$ select co  
32 atoms selected  
$ color red  
$ select o  
64 atoms selected  
$ color yellow
```

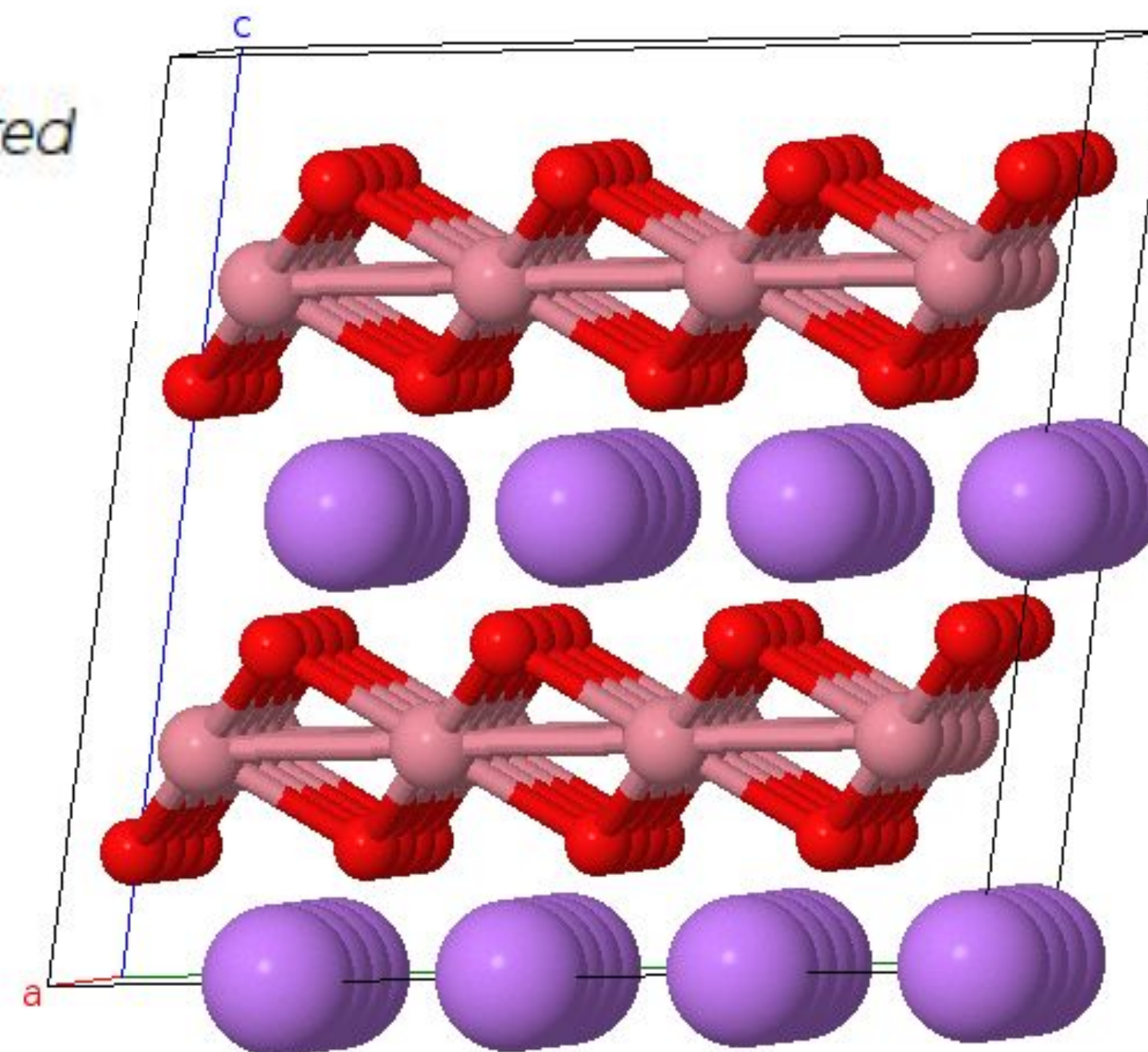
# Some useful tools in Jmol

Using console you can manage the atomic size.

```
$ select li  
32 atoms selected  
$ cpk 10
```

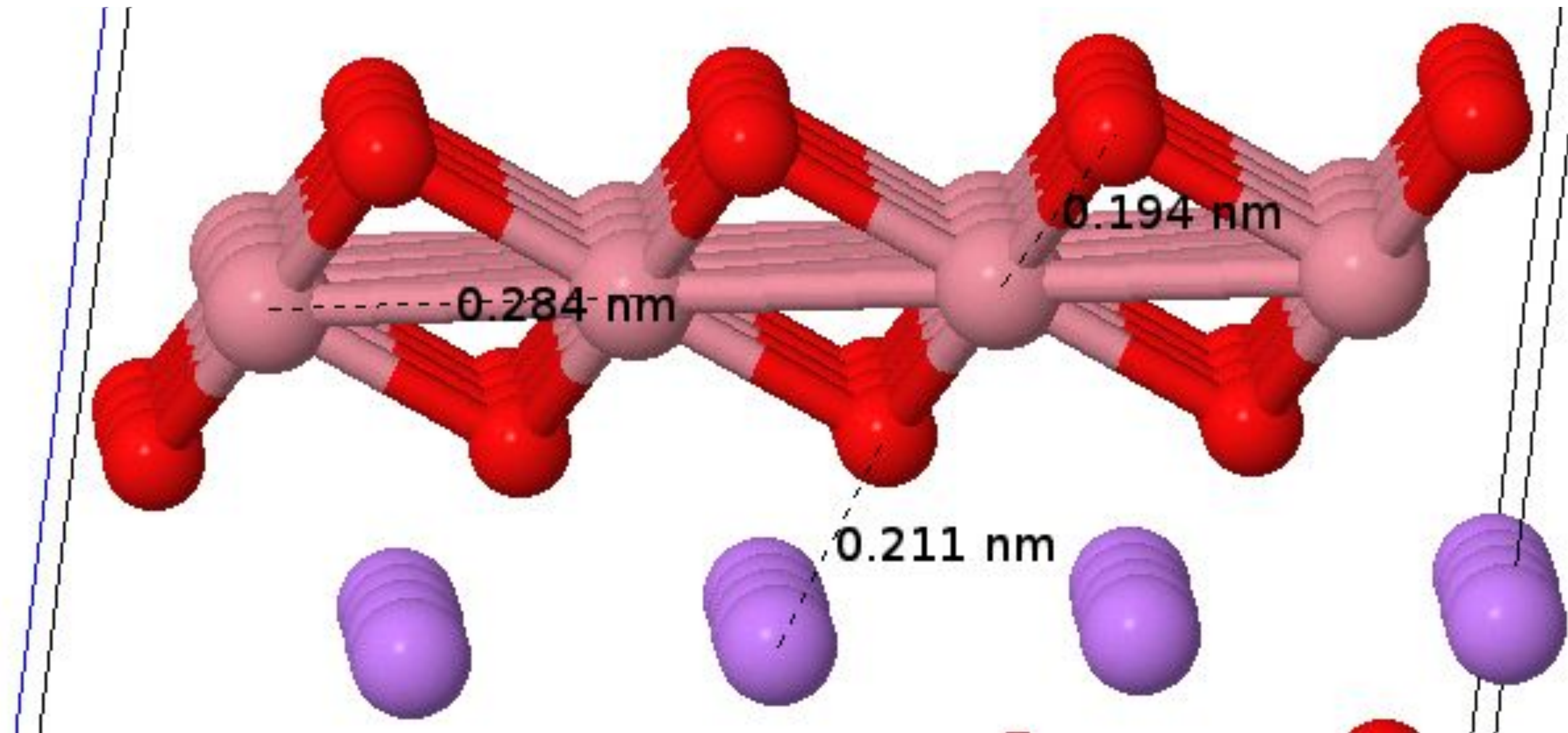


```
$ select li  
32 atoms selected  
$ cpk 10  
$ cpk 200
```



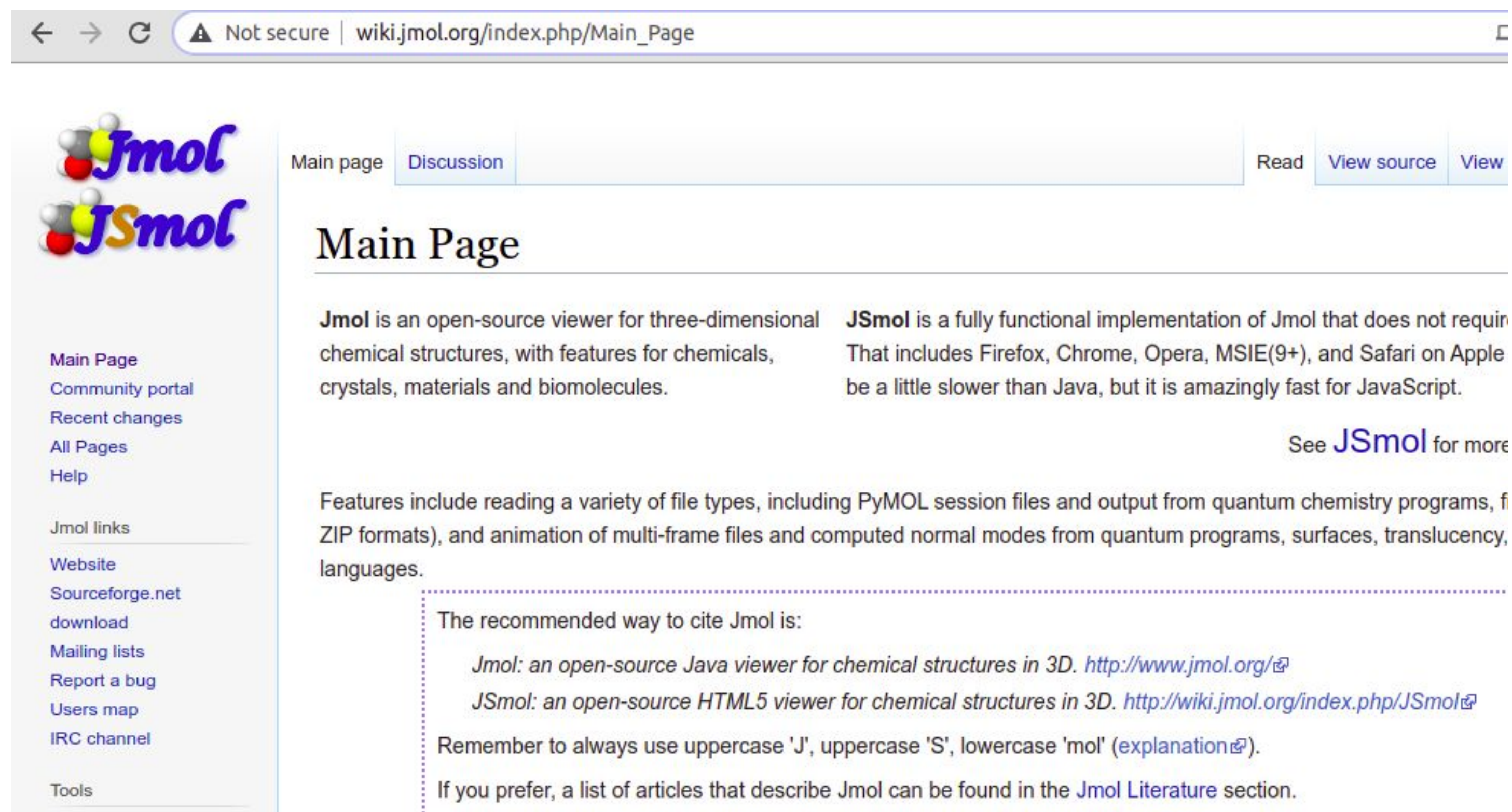
# Some useful tools in Jmol

Double left-clicking on two atoms you can measure interatomic distance between them.





# Some useful tools in Jmol

There was a little portion of Jmol's capabilities, but it has a very wide functionality, which you can find on the package webpage.



The screenshot shows a web browser window with the URL `wiki.jmol.org/index.php/Main_Page`. The page features the Jmol and JSmol logos on the left. The main content area is titled "Main Page" and contains two columns of text. The left column describes Jmol as an open-source viewer for three-dimensional chemical structures. The right column describes JSmol as a fully functional implementation of Jmol that does not require Java. Below this, there is a section for "Features" and a "Citation" section with a dashed border. The citation section provides the recommended way to cite Jmol and JSmol, along with their respective URLs. A note at the bottom of the citation section reminds users to use uppercase 'J', uppercase 'S', and lowercase 'mol' in citations.

← → ↻ ⚠ Not secure | wiki.jmol.org/index.php/Main\_Page

Main page Discussion Read View source View

## Main Page

**Jmol** is an open-source viewer for three-dimensional chemical structures, with features for chemicals, crystals, materials and biomolecules.

**JSmol** is a fully functional implementation of Jmol that does not require Java. That includes Firefox, Chrome, Opera, MSIE(9+), and Safari on Apple. It may be a little slower than Java, but it is amazingly fast for JavaScript.

See [JSmol](#) for more

Features include reading a variety of file types, including PyMOL session files and output from quantum chemistry programs, file formats (e.g., CIF, PDB, MOL, XYZ, etc.), and animation of multi-frame files and computed normal modes from quantum programs, surfaces, translucency, and other features.

The recommended way to cite Jmol is:

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

*JSmol: an open-source HTML5 viewer for chemical structures in 3D.* <http://wiki.jmol.org/index.php/JSmol>

Remember to always use uppercase 'J', uppercase 'S', lowercase 'mol' ([explanation](#)).

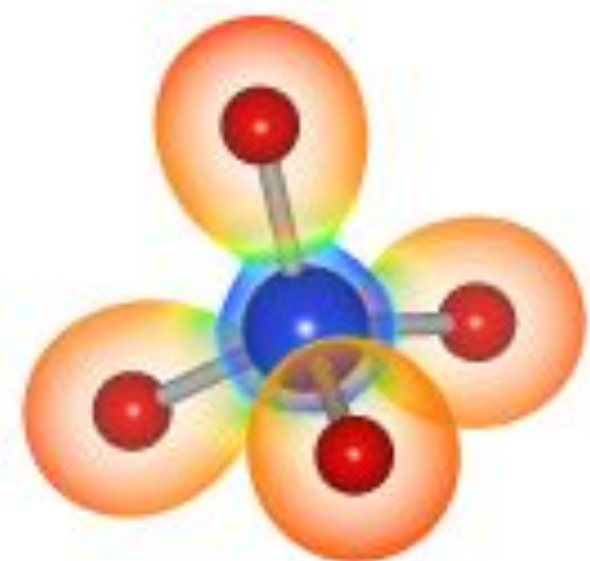
If you prefer, a list of articles that describe Jmol can be found in the [Jmol Literature](#) section.

Main Page  
Community portal  
Recent changes  
All Pages  
Help

Jmol links

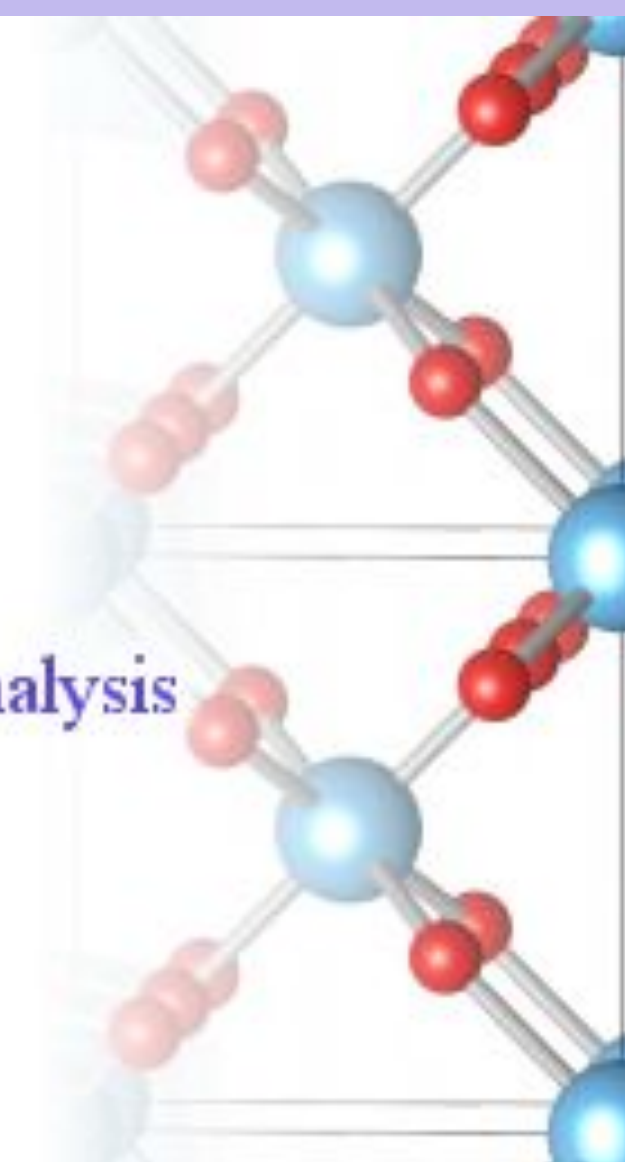
Website  
Sourceforge.net  
download  
Mailing lists  
Report a bug  
Users map  
IRC channel

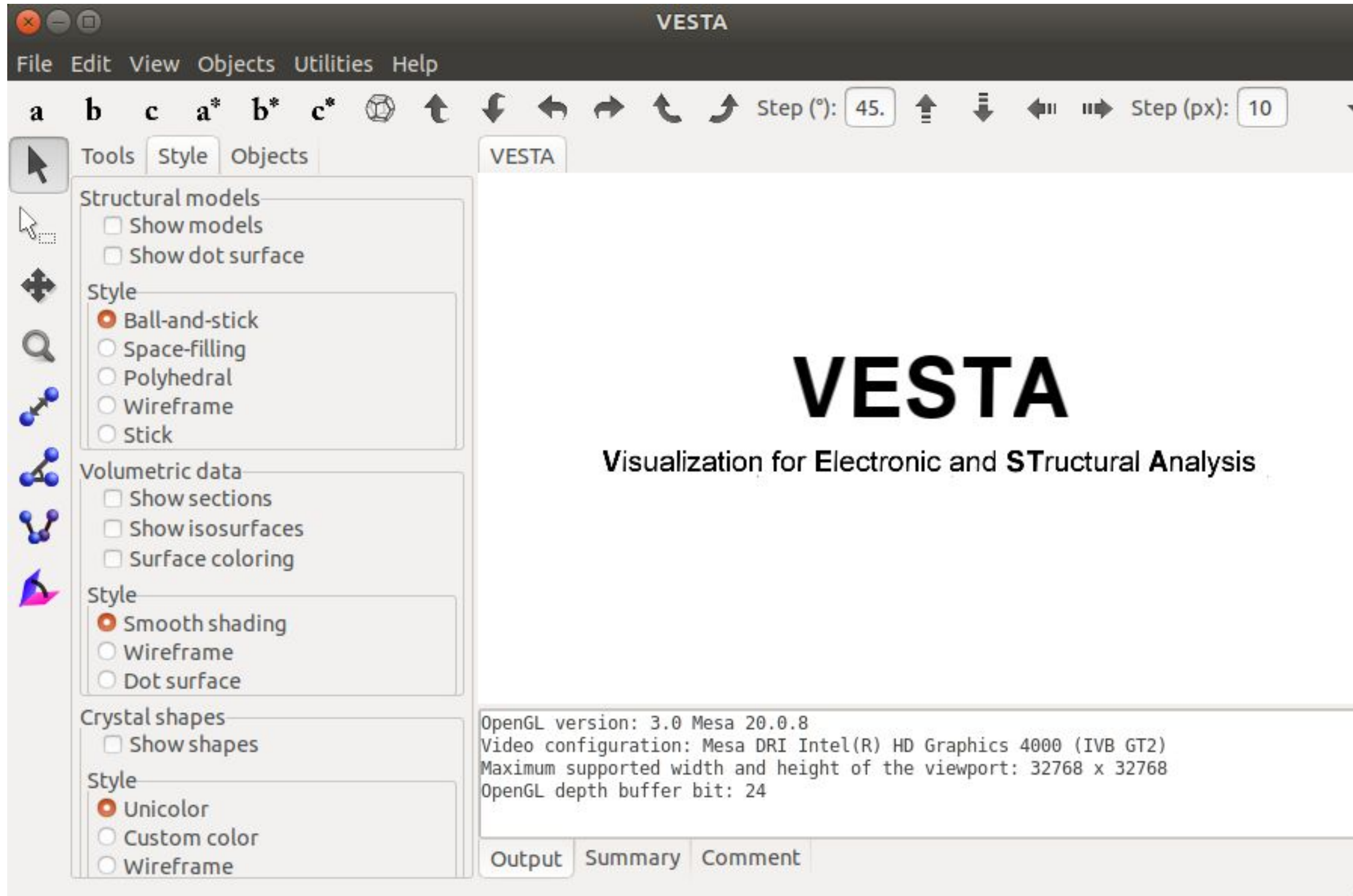
Tools



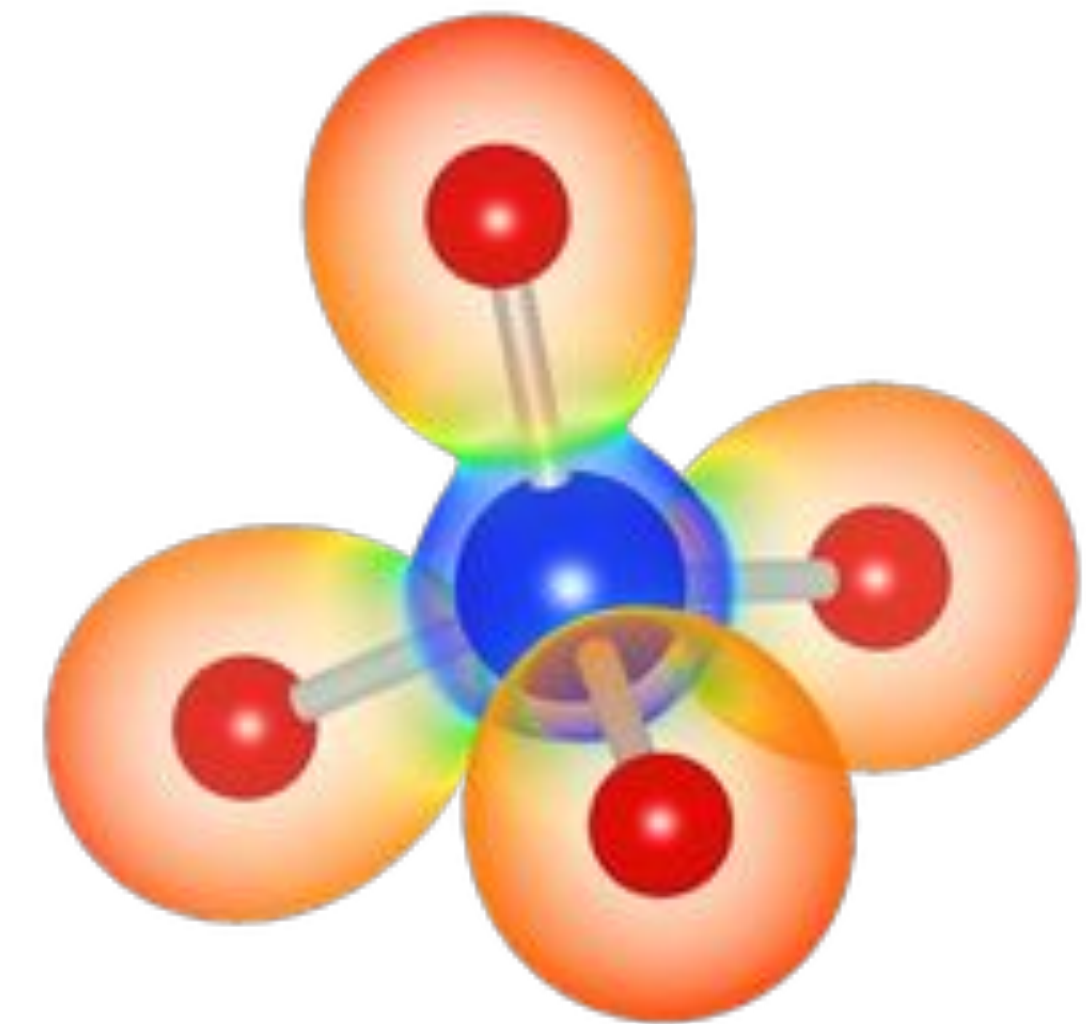
# VESTA

Visualization for Electronic and STructural Analysis





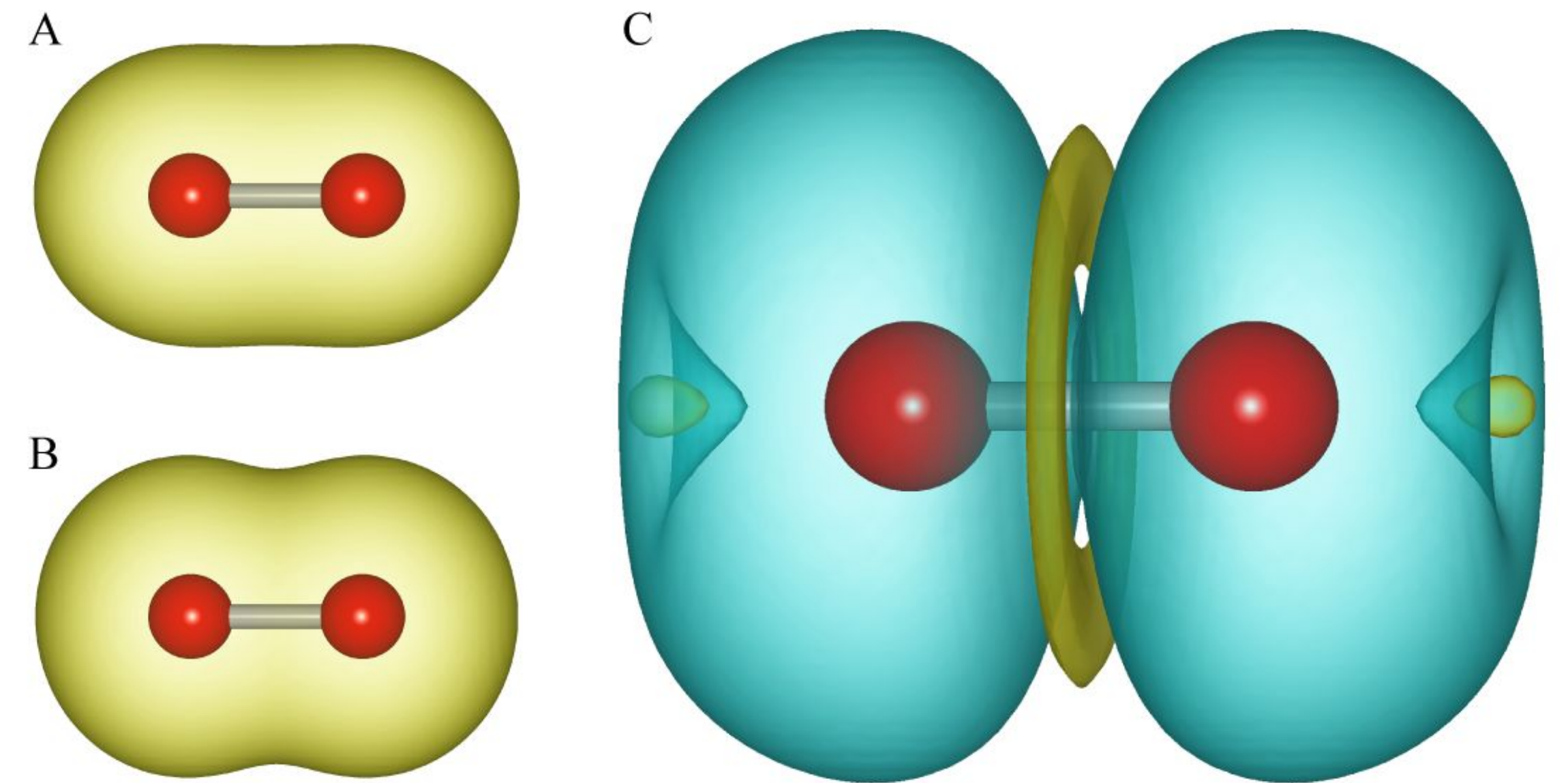
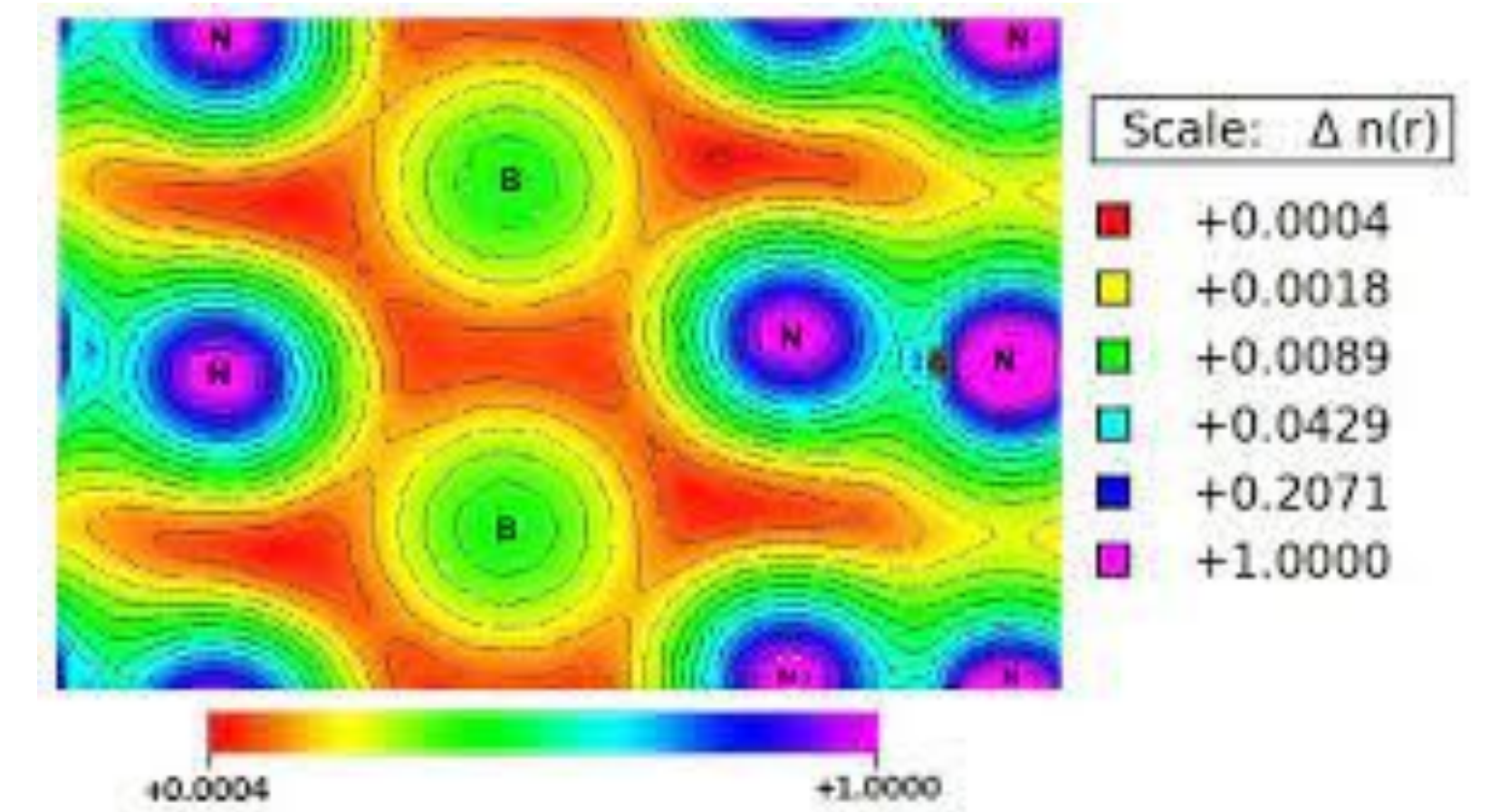
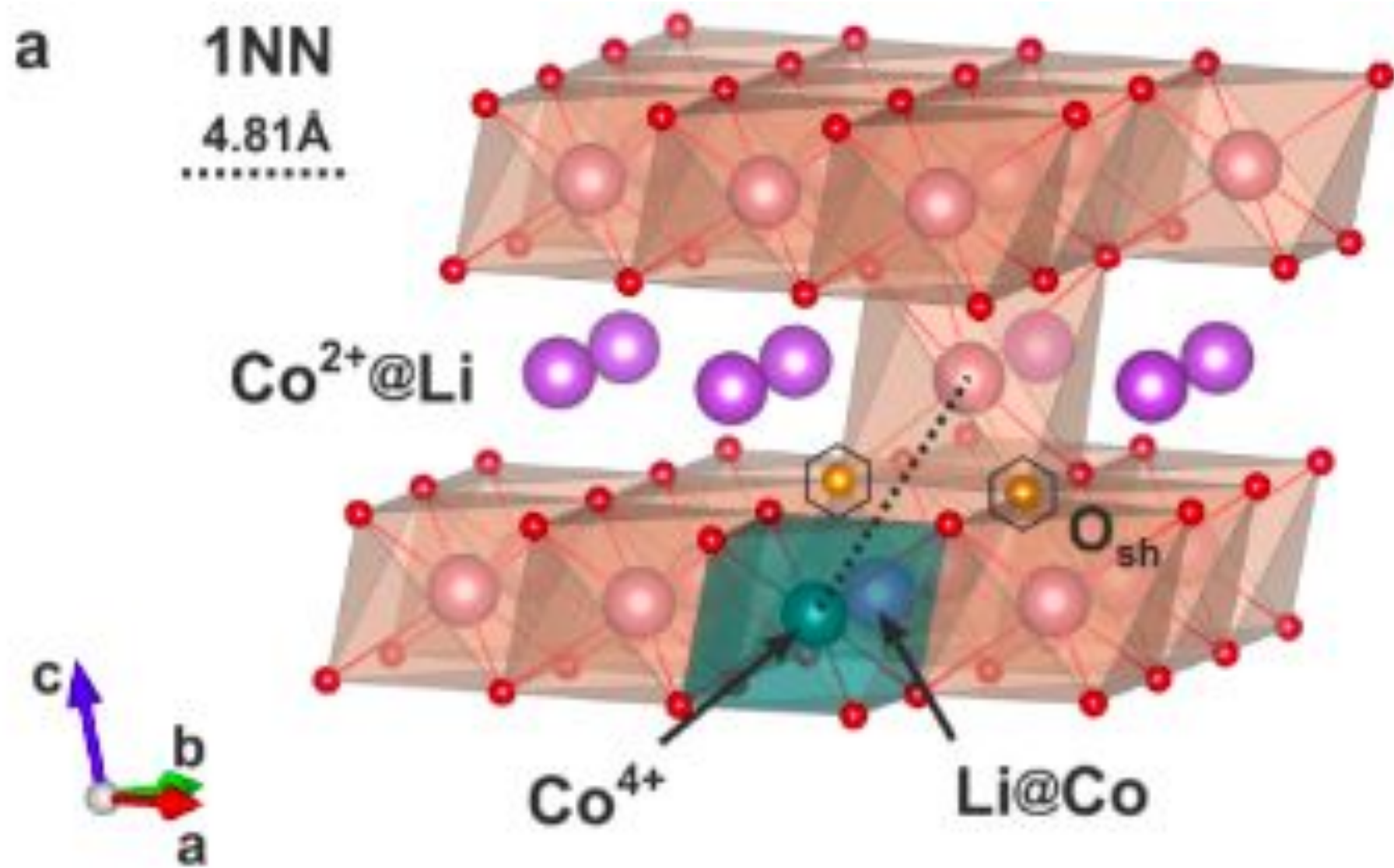
VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies.



<https://jp-minerals.org/vesta/en/>

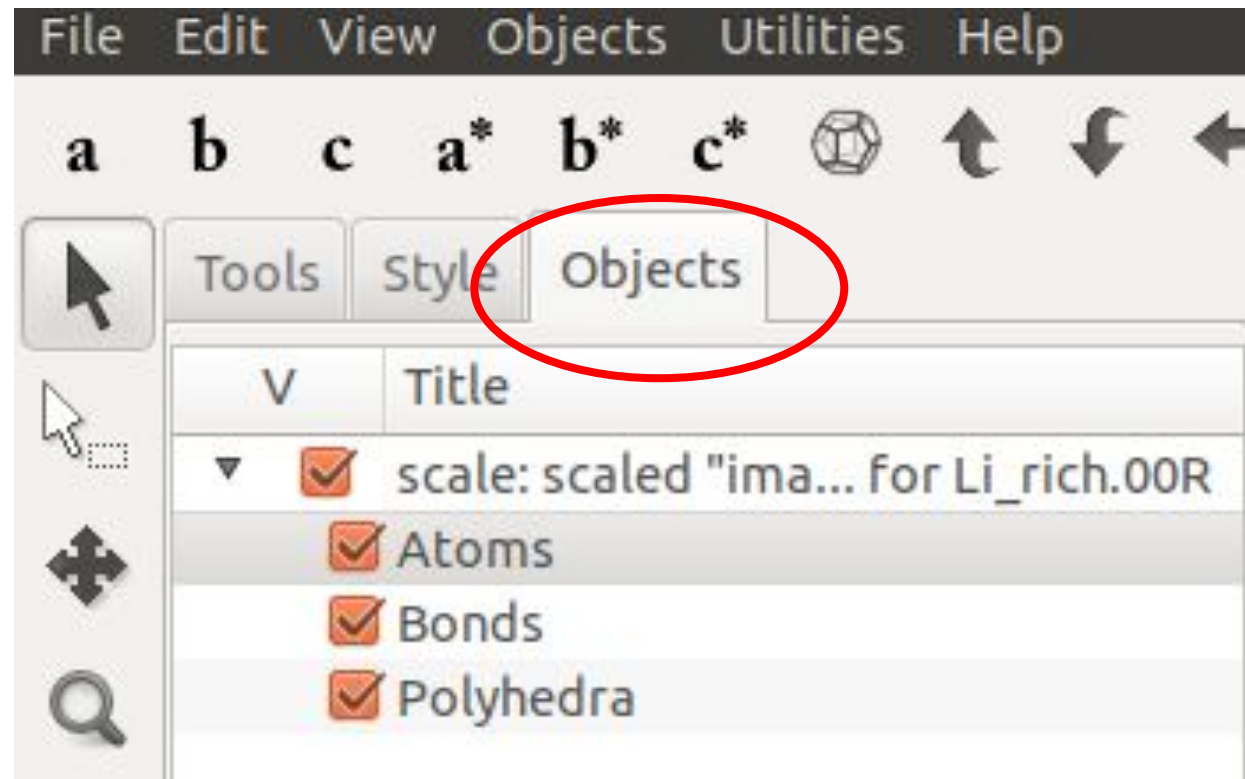
# VESTA's advantageous

- supporting CHG file format
- more beautiful pictures for papers



Distributions of electron densities and effective spin densities calculated with DVSCAT for the  $O_2$  molecule. A: up-spin electron density; B: down-spin electron density; C: effective spin density (A - B) calculated with VESTA. Isosurface levels were set at  $0.01a_0^{-3}$  (A and B) and  $0.001a_0^{-3}$  (C), respectively.

# VESTA: style options



Objects tab allows us to manage style

1) Atoms: you can change atomic radii and colors

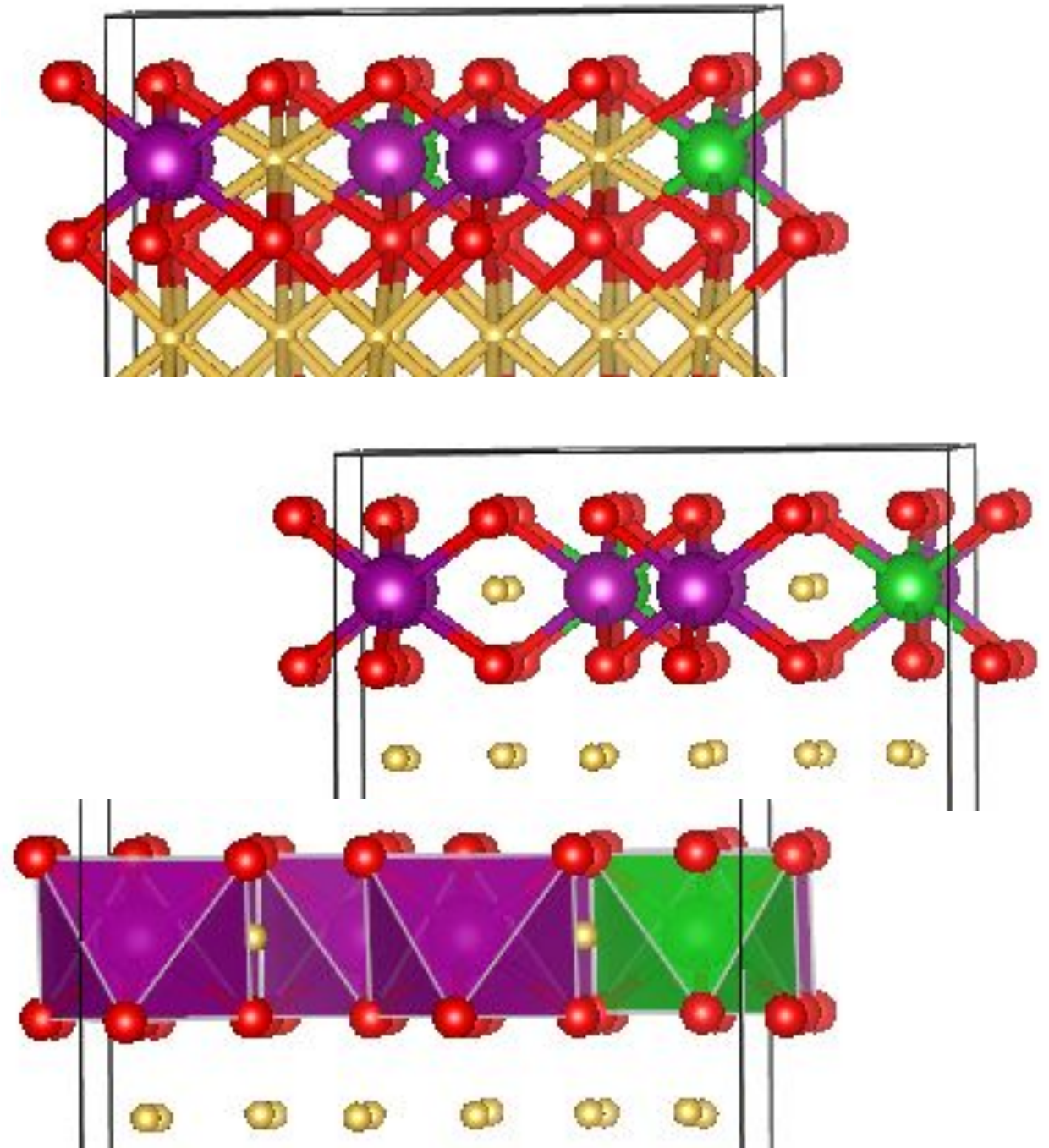
2) Bonds: you can change bond color, thickness and even switch off some of them

3) Polyhedra: you can change its color and switch off some of them

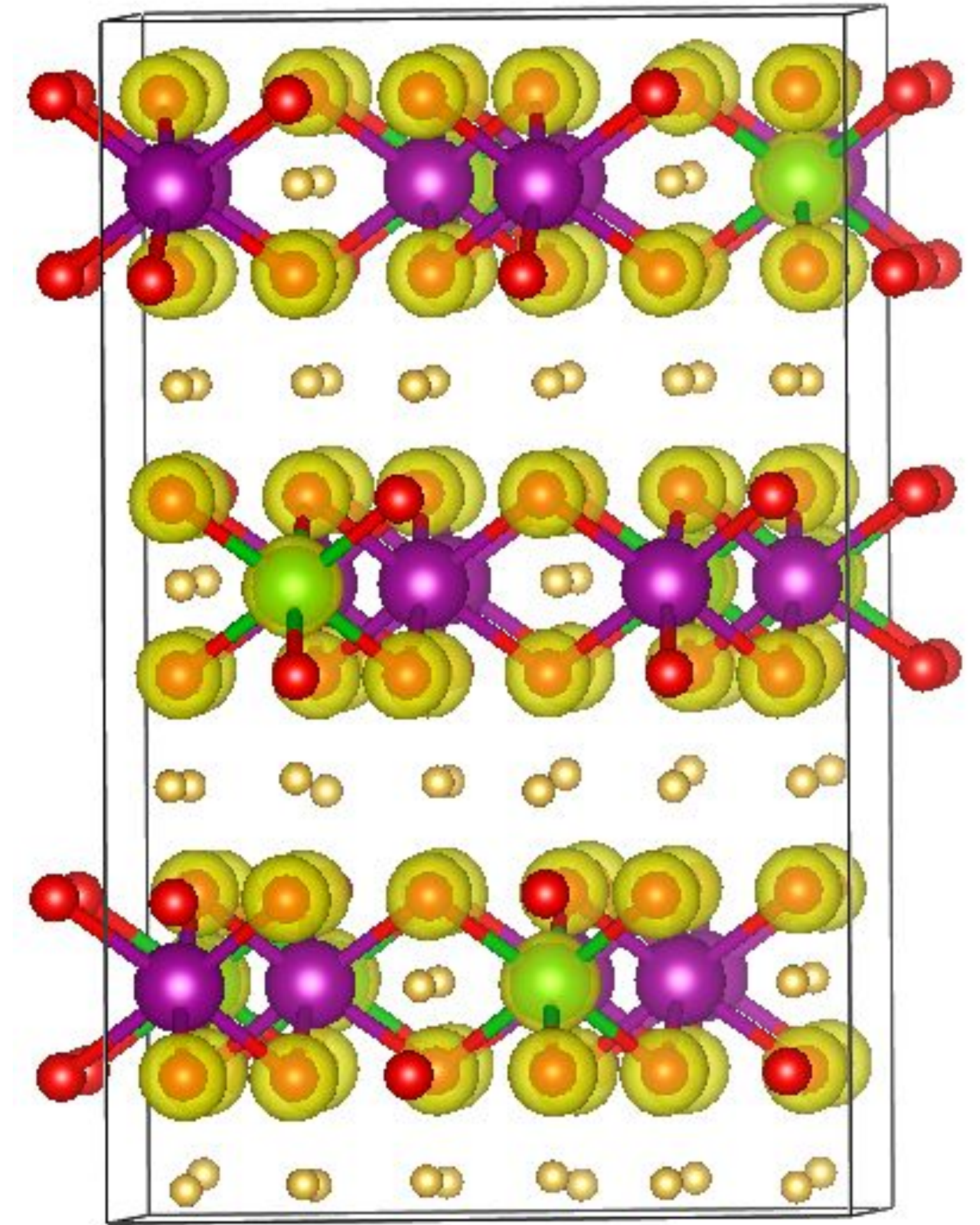
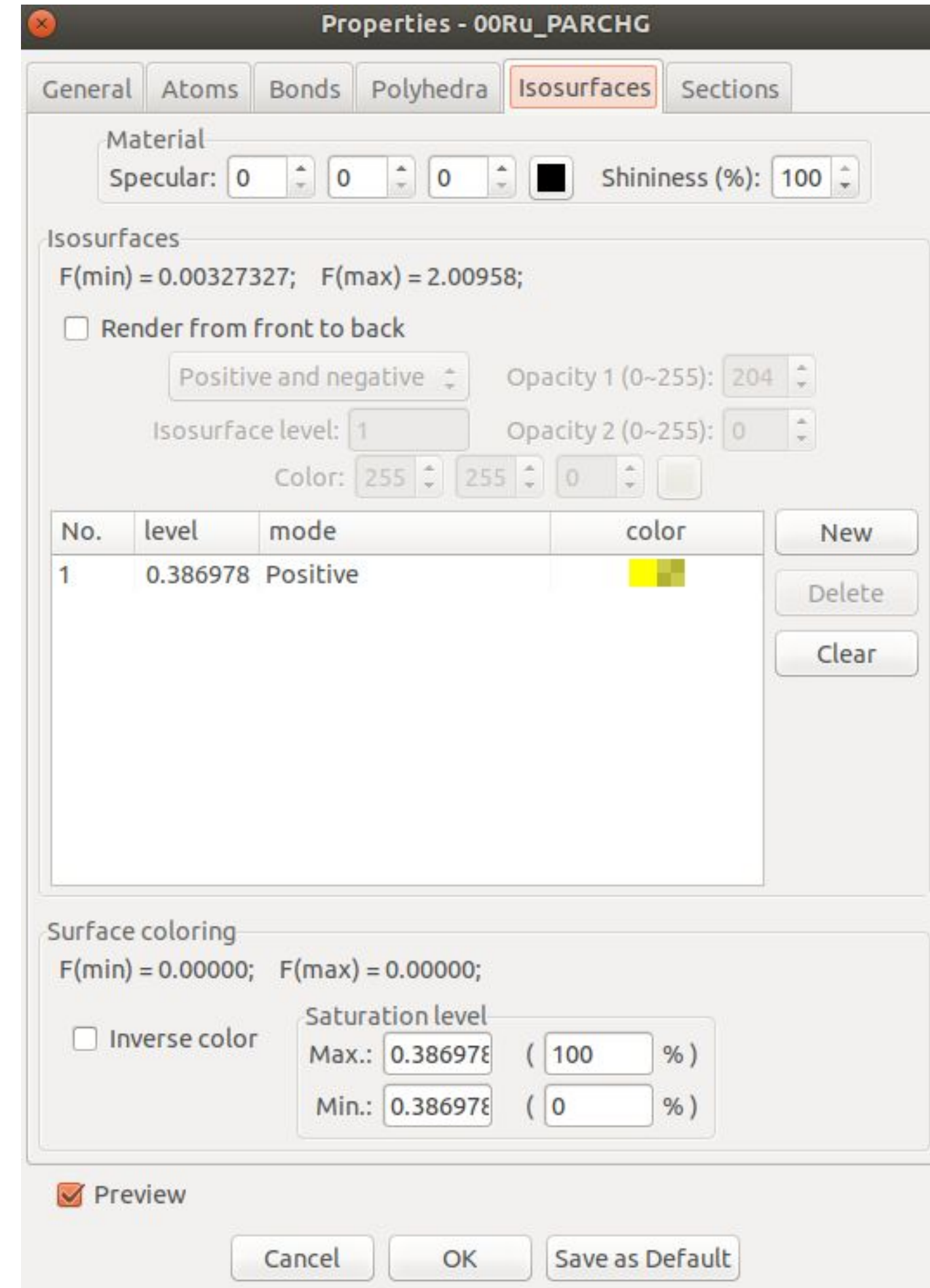
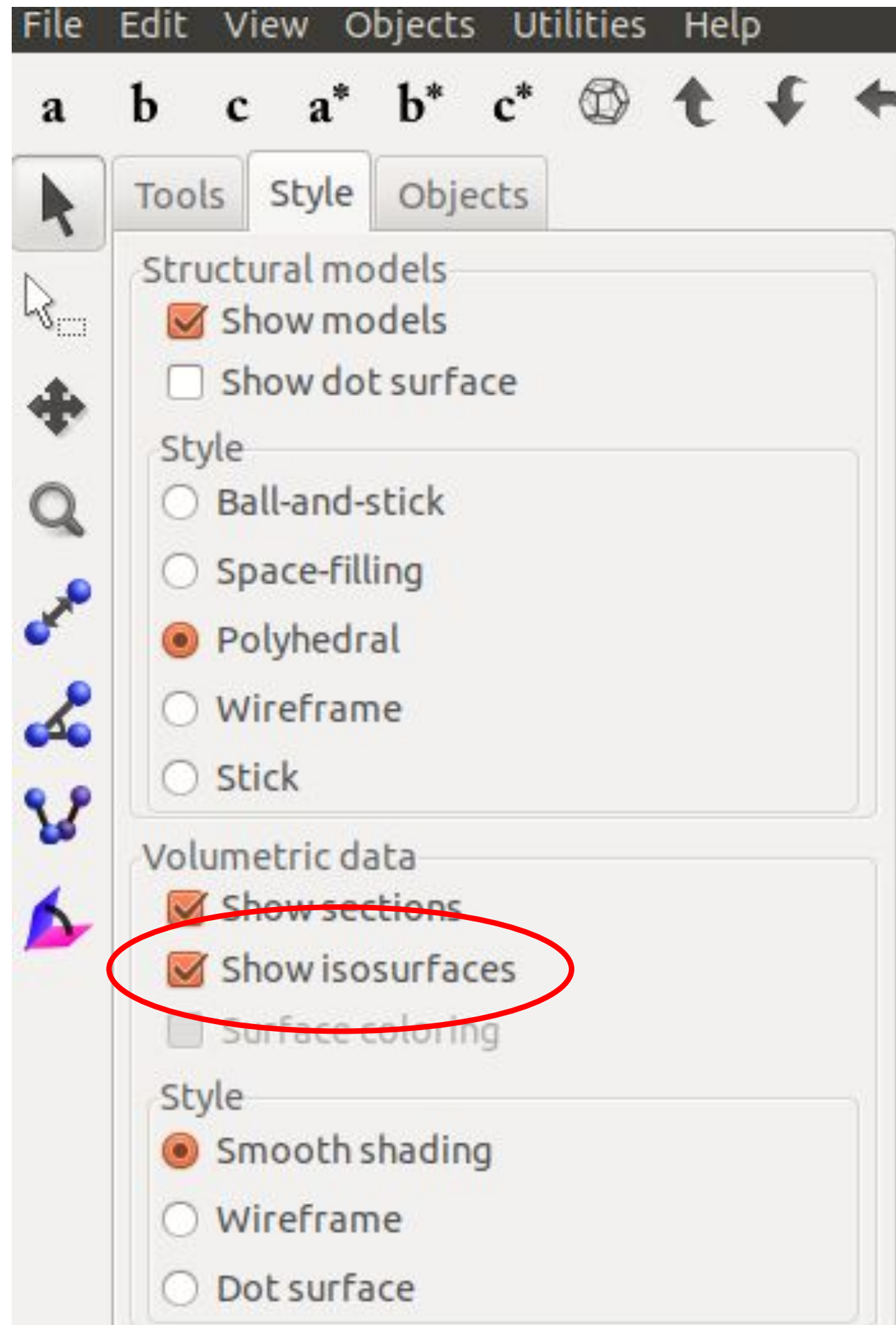
Site	r (Å)	C	L	S	V
▶ Li	0.50		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ Mn	1.37		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ O	0.74		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ Ni	1.25		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Bond	S	r/w	C	S	V
Li-O	2	0.25 Å		<input type="checkbox"/>	<input checked="" type="checkbox"/>
Mn-O	2	0.25 Å		<input type="checkbox"/>	<input checked="" type="checkbox"/>
Ni-O	2	0.25 Å		<input type="checkbox"/>	<input checked="" type="checkbox"/>

Polyhedra	C	S	V
▶ Li		<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ Mn		<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ Ni		<input type="checkbox"/>	<input checked="" type="checkbox"/>

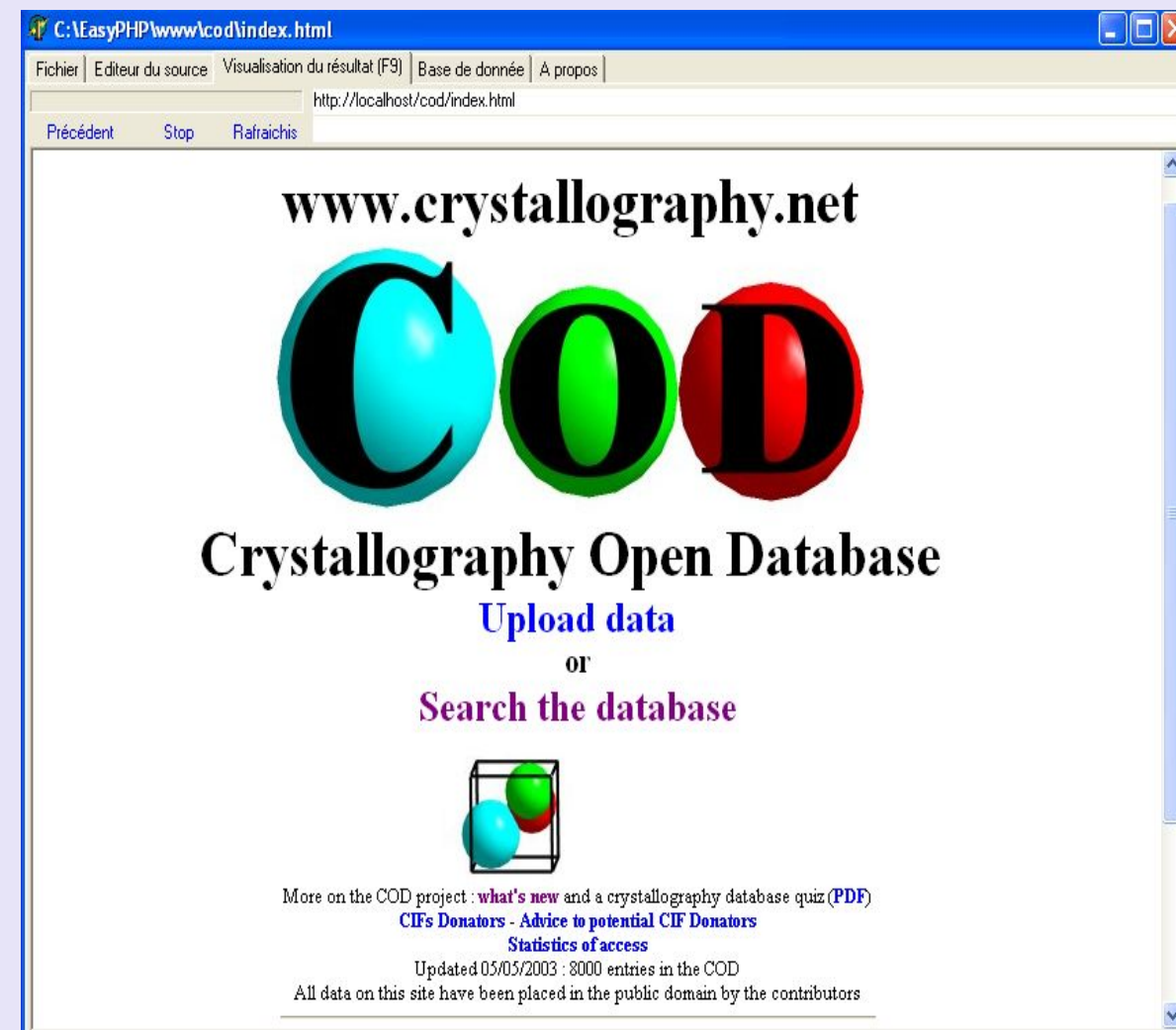


# VESTA: Charge isosurface visualization



# Crystal structure databases

## Experimental



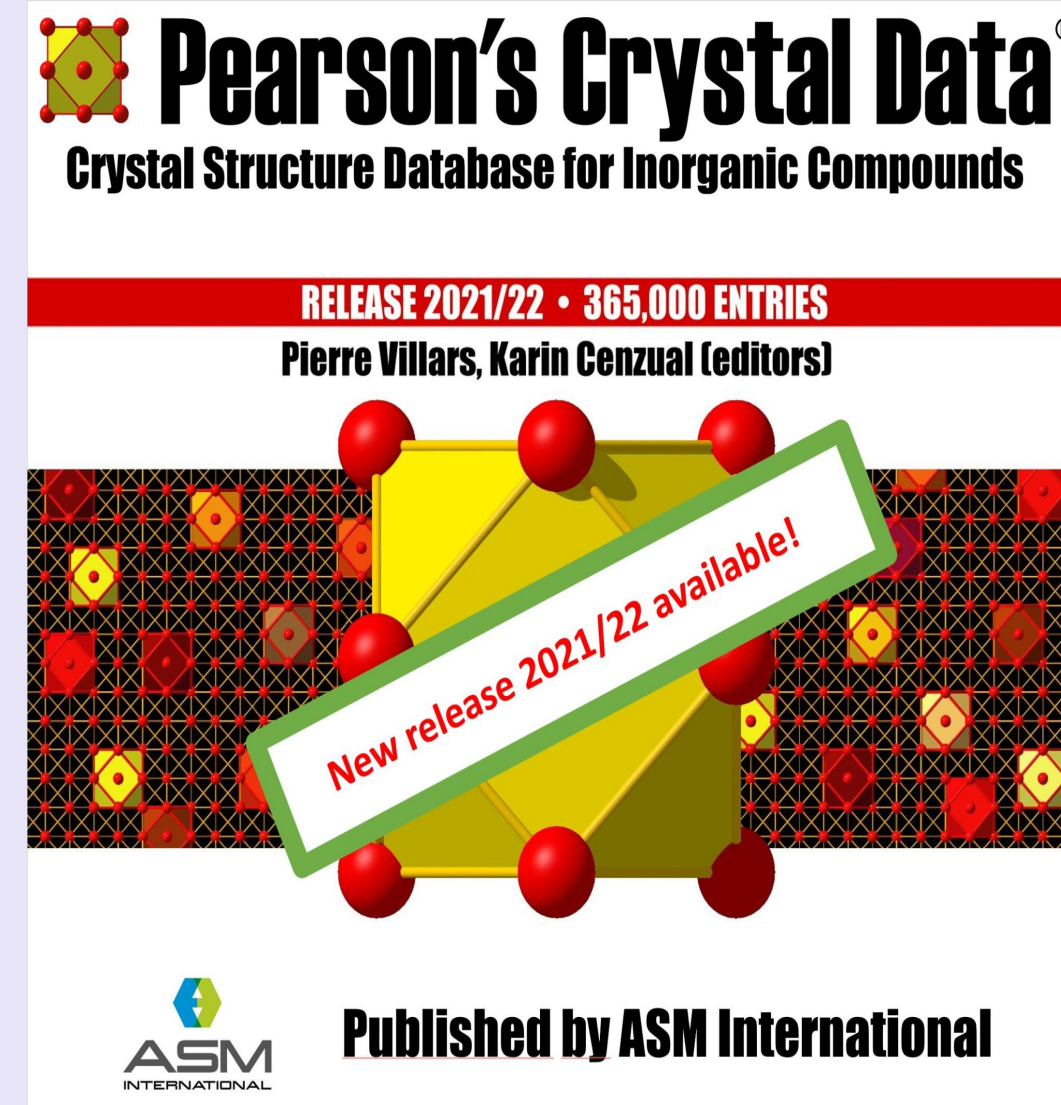
www.crystallography.net

**COD**

Crystallography Open Database

Upload data  
or  
Search the database

More on the COD project: [what's new](#) and a crystallography database quiz (PDF)  
[CIFs Donators - Advice to potential CIF Donators](#)  
[Statistics of access](#)  
Updated 05/05/2003: 8000 entries in the COD  
All data on this site have been placed in the public domain by the contributors

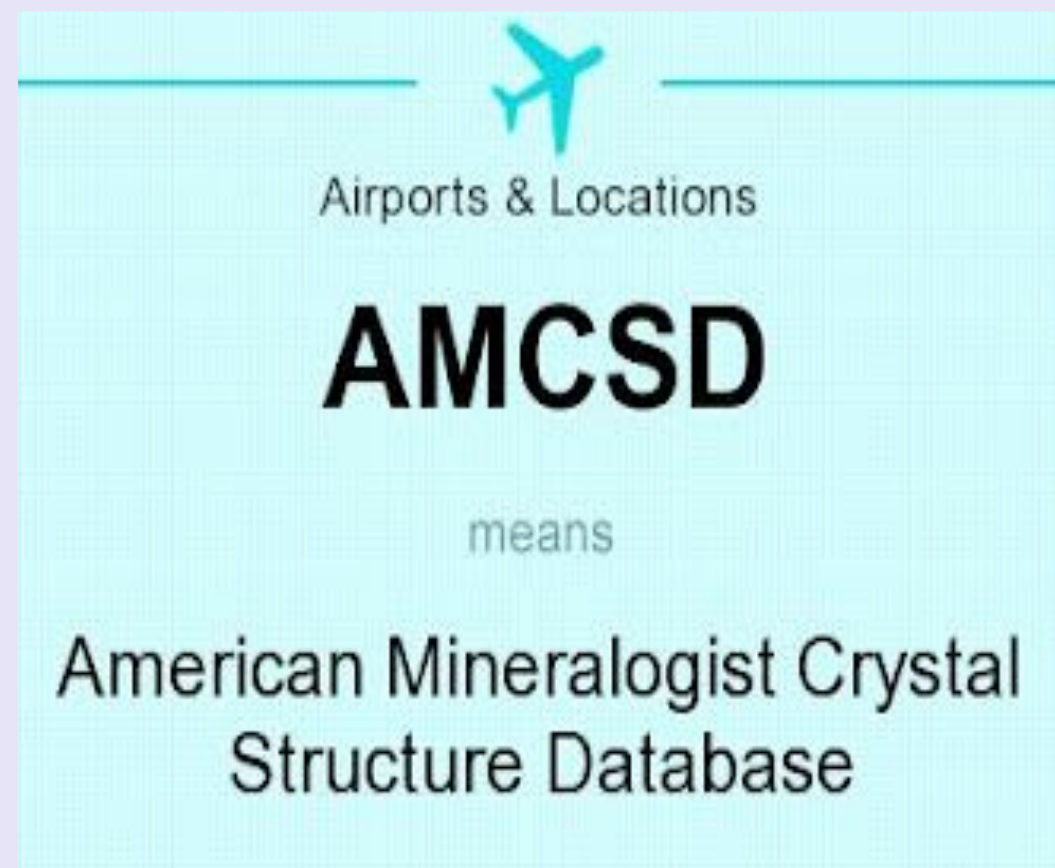


**Pearson's Crystal Data**  
Crystal Structure Database for Inorganic Compounds

RELEASE 2021/22 • 365,000 ENTRIES  
Pierre Villars, Karin Cenzual (editors)

New release 2021/22 available!

Published by ASM International



Airports & Locations

**AMCSD**

means

American Mineralogist Crystal Structure Database



**ICSD**

FIZ Karlsruhe

## Computational



**AFLOW**  
Automatic - FLOW for Materials Discovery



**The Materials Project**



**OQMD**  
The Open Quantum Materials Database

# Materials Project



The image shows the Materials Project website interface. At the top, there is a navigation bar with links for Home, About, Apps, Documentation, Forum, API, Tutorials, and Dashboard. Below this is a search bar with a magnifying glass icon and a text input field containing "Na-O". To the right of the search bar is a button labeled "search".








The main content area features a periodic table of elements. The search results are displayed in the table, with elements Na, O, and their combinations highlighted in red. The search bar also includes a dropdown menu labeled "by Elements" and a "search" button.

On the right side of the interface, there is a sidebar with several filter options:

- # of elements:** A text input field containing "e.g., 4 or >2 & <6".
- excluded elements:** A text input field containing "Cl Br".
- Submit:** A blue button.
- External Provenance:** Two checkboxes: "ICSD" and "Exptl. ICSD".
- Material Tags:** A text input field containing "imgreite".
- Band Gap (eV):** A slider control with a range from 0 to 10.
- Energy Above Hull:** A label at the bottom of the sidebar.

# Materials Project database: LiCoO<sub>2</sub>

100 records per page  Batch Structures  Edit Structures Show / hide columns  Print Export

Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Volume	Nsites	Density (gm/cc)	
mp-22526	LiCoO <sub>2</sub>	R $\bar{3}m$	-1.752	0	0.733 	33.003	4	4.924	<input type="checkbox"/>
mp-849273	LiCoO <sub>2</sub>	Fd $\bar{3}m$	-1.72	0.032	0.000 	138.634	16	4.689	<input type="checkbox"/>
mp-853240	LiCoO <sub>2</sub>	Imma	-1.715	0.037	1.884 	138.594	16	4.691	<input type="checkbox"/>
mp-1097885	LiCoO <sub>2</sub>	C2/m	-1.708	0.043	2.013 	138.978	16	4.678	<input type="checkbox"/>
mp-867664	LiCoO <sub>2</sub>	P $\bar{1}$	-1.666	0.085	0.442 	167.512	20	4.851	<input type="checkbox"/>
mp-753473	LiCoO <sub>2</sub>	P6 <sub>3</sub> mc	-1.659	0.093	0.896	73.734	8	4.408	<input type="checkbox"/>
mp-1222334	LiCoO <sub>2</sub>	P4/mmm	-1.541	0.211	0.000 	34.567	4	4.702	<input type="checkbox"/>

# Materials Project database: $\text{LiCoO}_2$ ( $R\bar{3}m$ ) card

Zoom in/out    Shift + Drag cursor  
Rotate along the center axis    Option + Drag cursor

**Edit Crystal**    **Generate Phase Diagram**

**Tags:** Lithium cobalt(III) dioxide Lithium cobalt dioxide Lithium iron(III) oxide  
High pressure experimental phase Lithium cobalt oxide Lithium cobalt(III) oxide  
Lithium cobalt oxide (1/1/2) Lithium cobaltate(III)

**Hermann Mauguin**  
 $R\bar{3}m$  [166]

**Hall**  
-R 3 2"

**Point Group**  
 $\bar{3}m$

**Crystal System**  
trigonal

**File Formats**

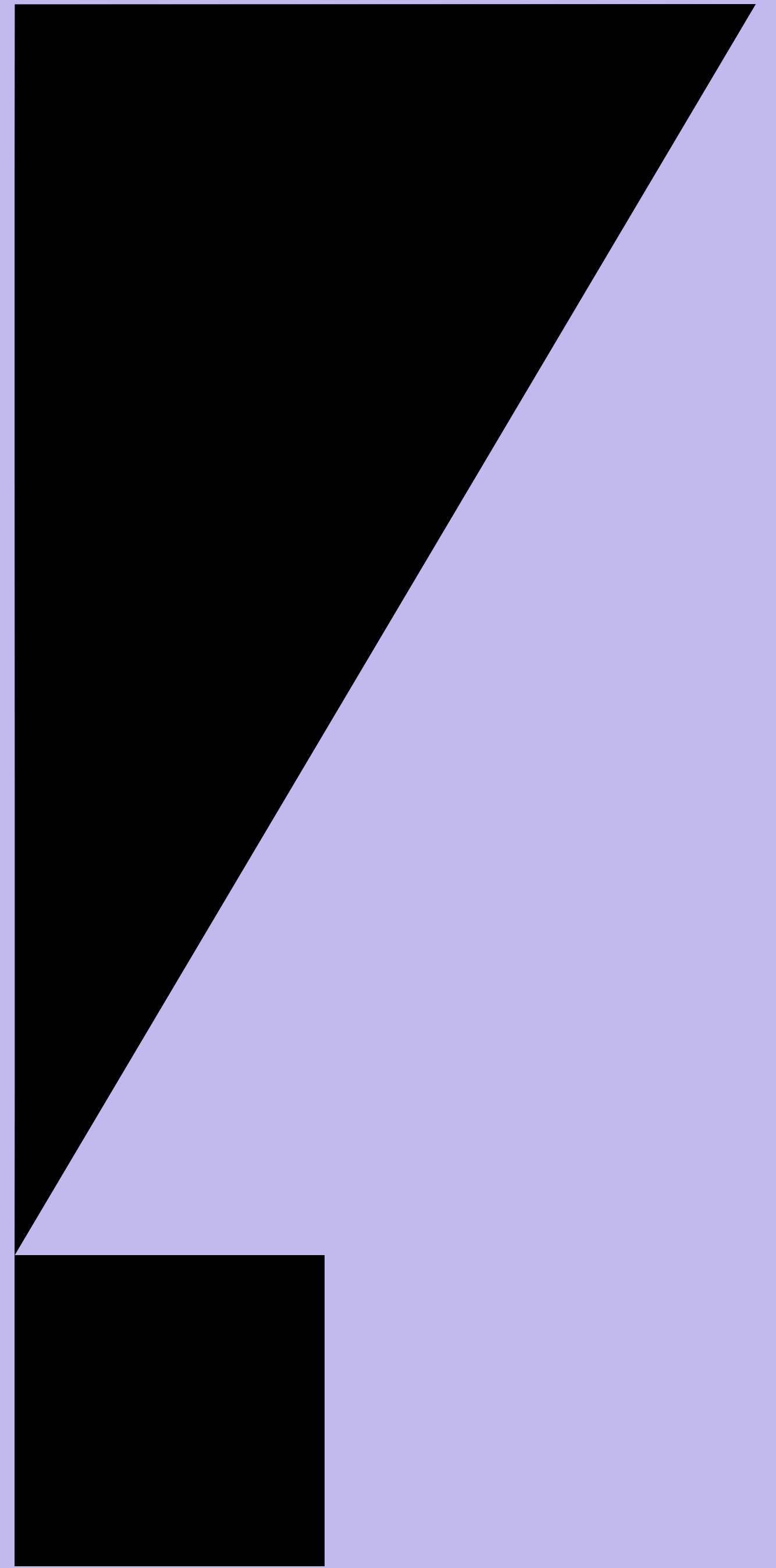
- CIF
- VASP
- POSCAR
- CSSR
- JSON

We have not yet calculated a detailed bandstructure for this material

**T**

**h**

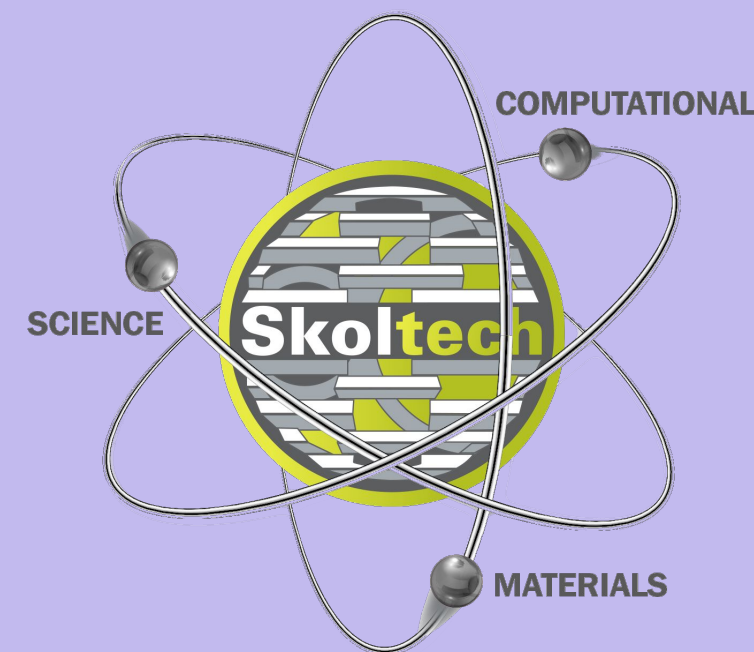
**x**



# Acknowledgement

**Skoltech**  
Energy

Center for  
Energy Science  
and Technology

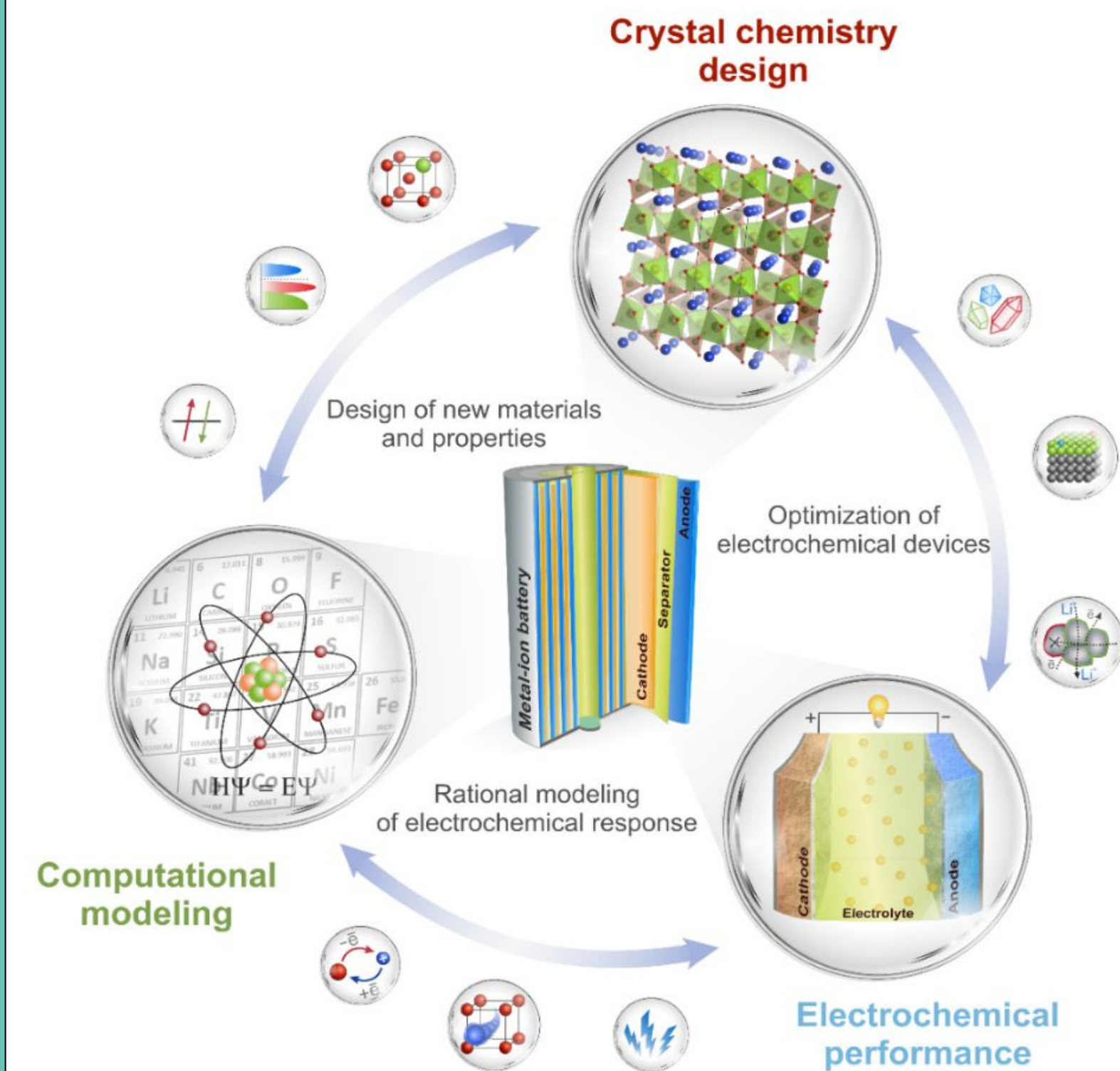


Russian Science  
Foundation

# Our group

## Storion Research Lab

Center for Energy Science and Technology at Skoltech, Moscow



★ [MatSolver](#) - a web-service for predicting materials properties.