

# Crystallography and Crystal Chemistry VIII International School-Conference of Young Scientists 2023

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



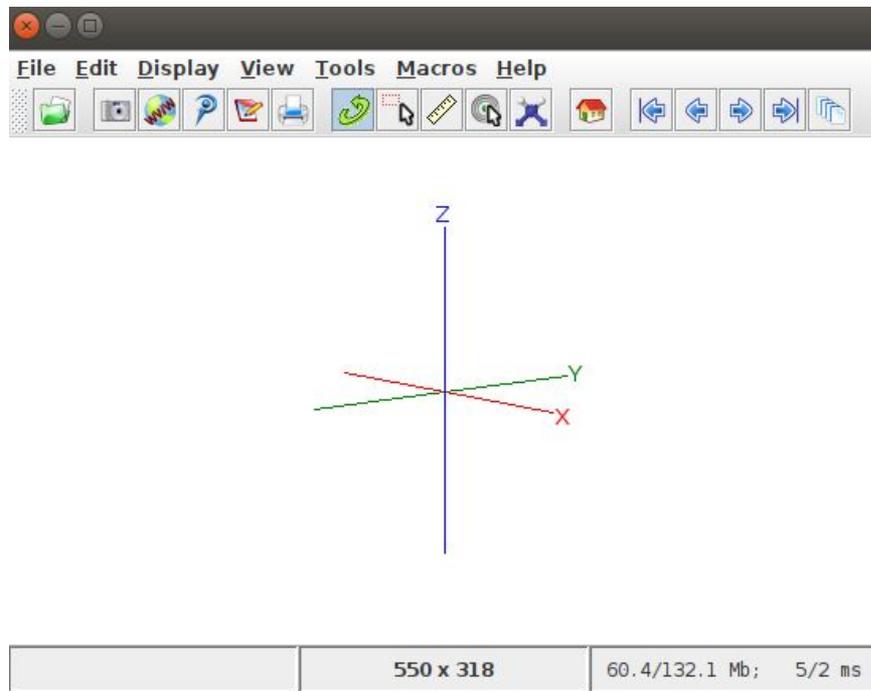
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**Center for Energy Science and Technology**  
**Skoltech, Moscow, Russian Federation**

**November 10<sup>th</sup>,  
2023**



# 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
```

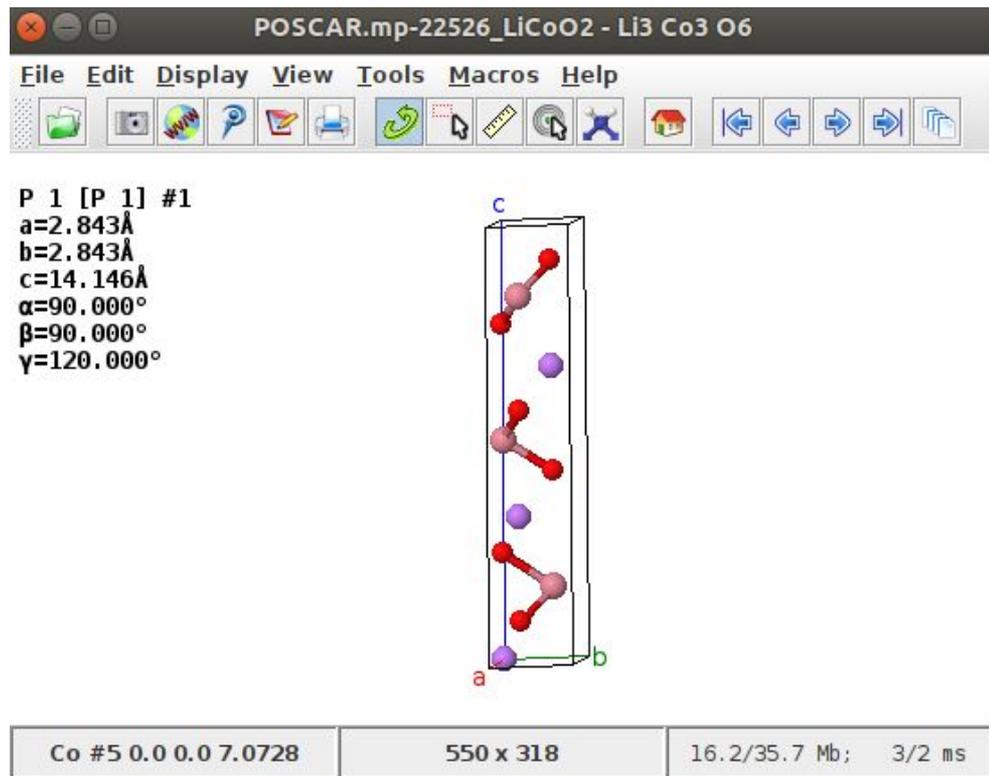
# But we love Jmol for VASP files supporting

**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
```

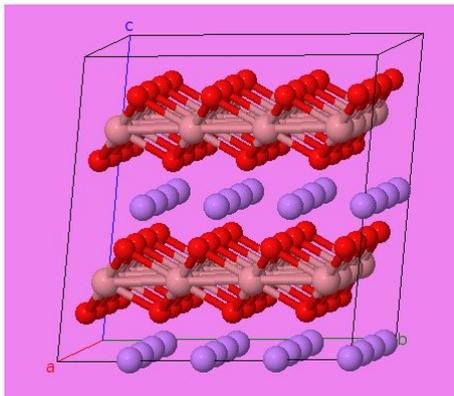
and even **OUTCAR** - output VASP file,  
which includes all the information about  
DFT calculation



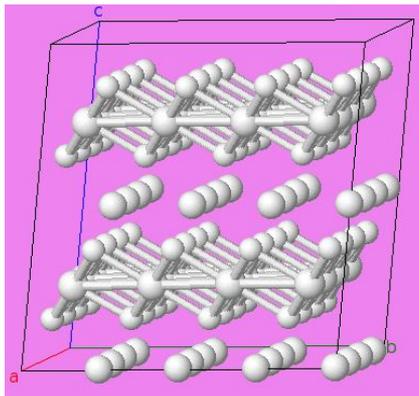
# Some useful tools in Jmol

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

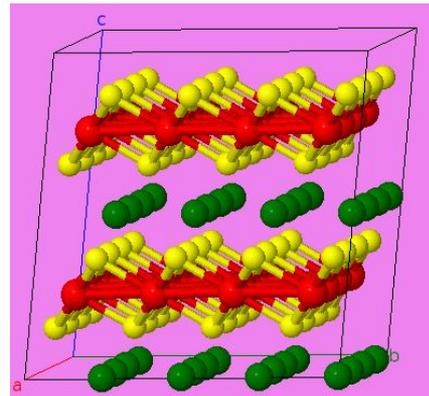
```
$ color background violet
```



```
$ color atoms white
```



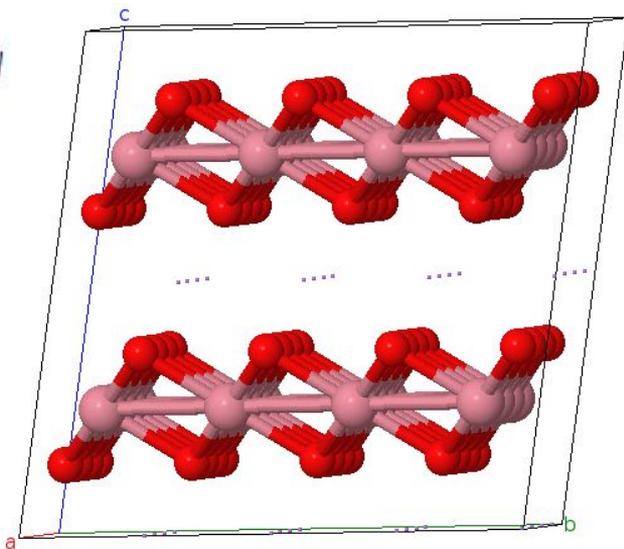
```
$ select li  
32 atoms selected  
$ color green  
$ select co  
32 atoms selected  
$ color red  
$ select o  
64 atoms selected  
$ color yellow
```



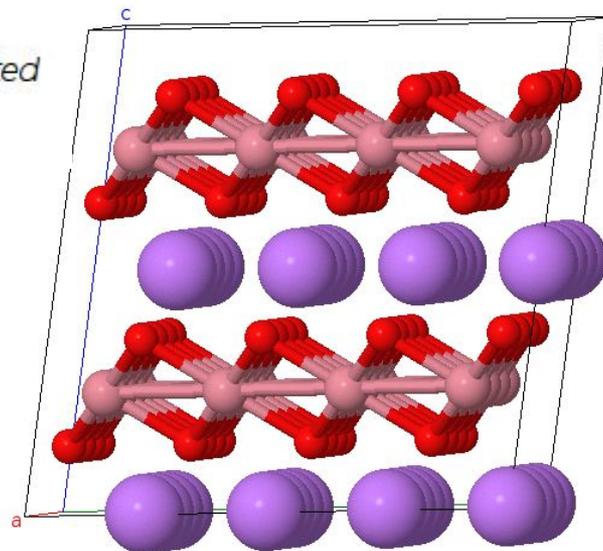
# Some useful tools in Jmol

Using console you can manage the atomic size

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

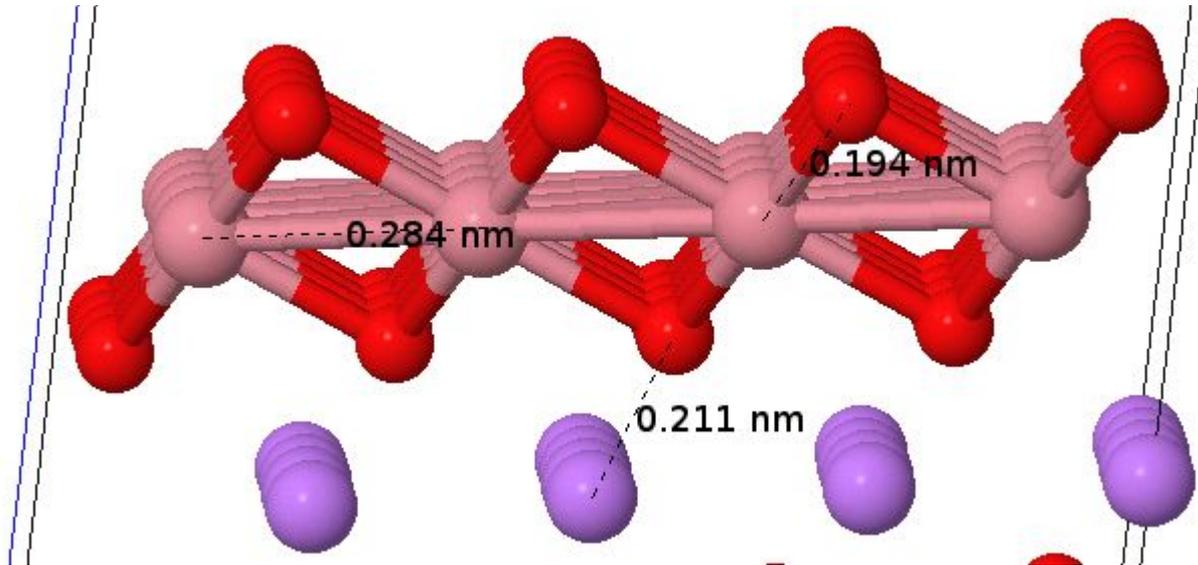


```
$ select li  
32 atoms selected  
$ cpk 10  
$ cpk 200
```



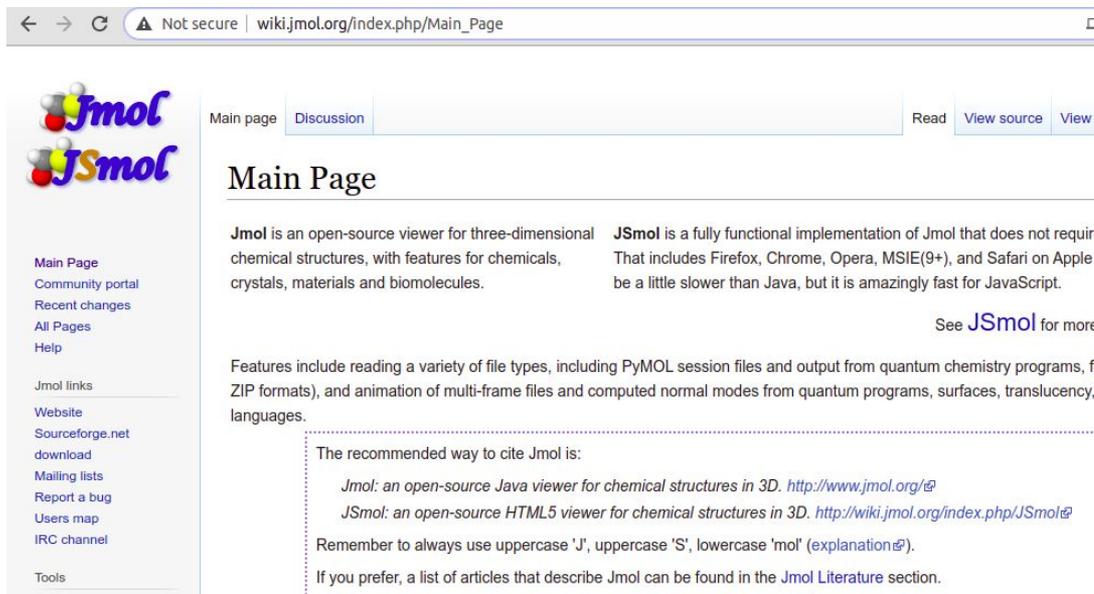
# Some useful tools in Jmol

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 address bar displaying "wiki.jmol.org/index.php/Main\_Page". The page content includes a navigation menu with "Main page" selected, and buttons for "Read", "View source", and "View". The main heading is "Main Page". The text describes Jmol as an open-source viewer for three-dimensional chemical structures and JSmol as a fully functional implementation. It lists features like reading PyMOL session files and animation. A section titled "The recommended way to cite Jmol is:" provides links for citing Jmol and JSmol. A note mentions using uppercase 'J', uppercase 'S', and lowercase 'mol'. A link to "Jmol Literature" is also provided.

← → ↻ 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 is 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, and animation of multi-frame files and computed normal modes from quantum programs, surfaces, translucency, and languages.

The recommended way to cite Jmol is:

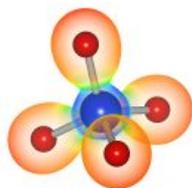
*Jmol: an open-source Java viewer for chemical structures in 3D.* <http://www.jmol.org/>

*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](#)).

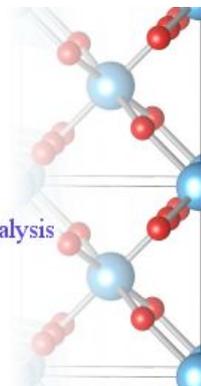
If you prefer, a list of articles that describe Jmol can be found in the [Jmol Literature](#) section.

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Community portal  
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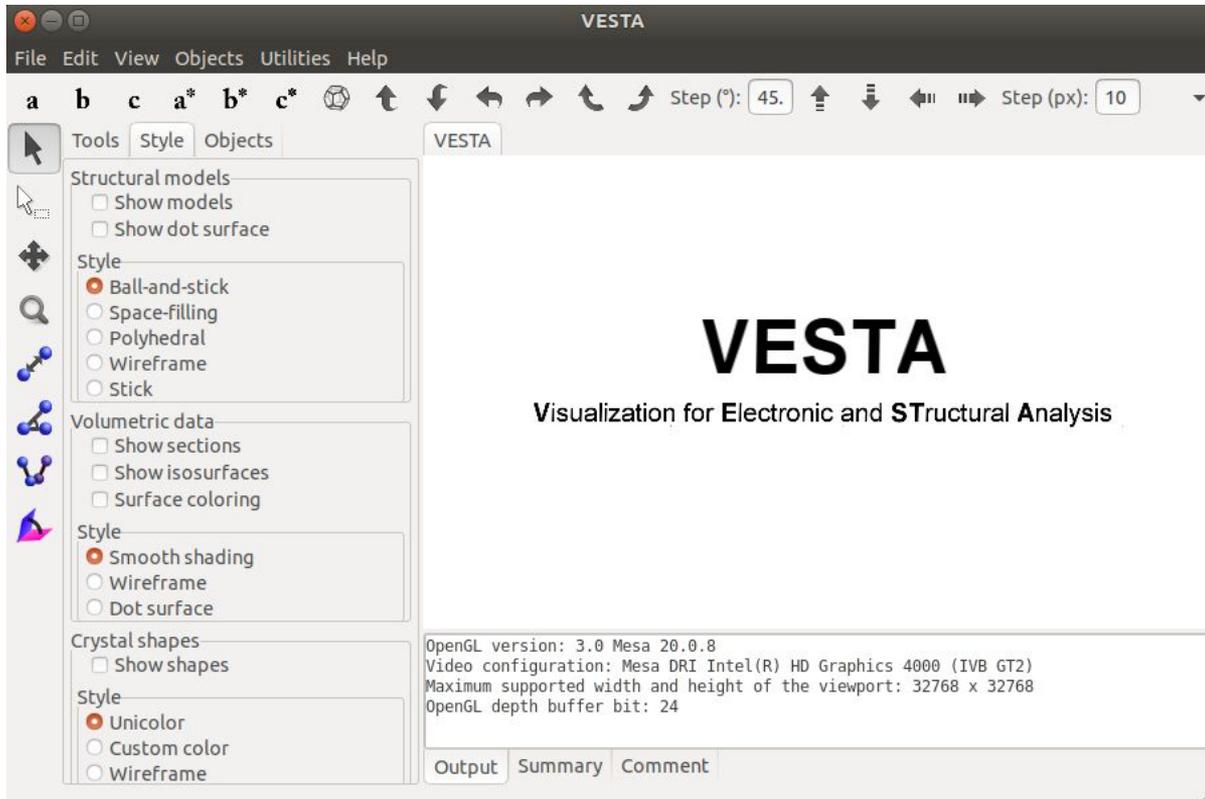


# VESTA

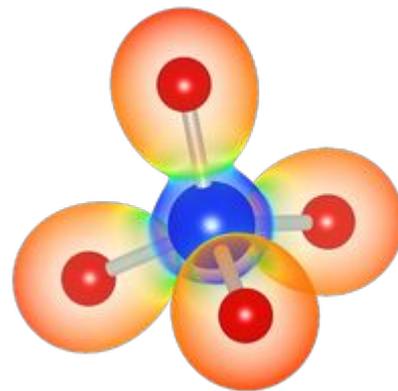
Visualization for Electronic and Structural Analysis



# VESTA



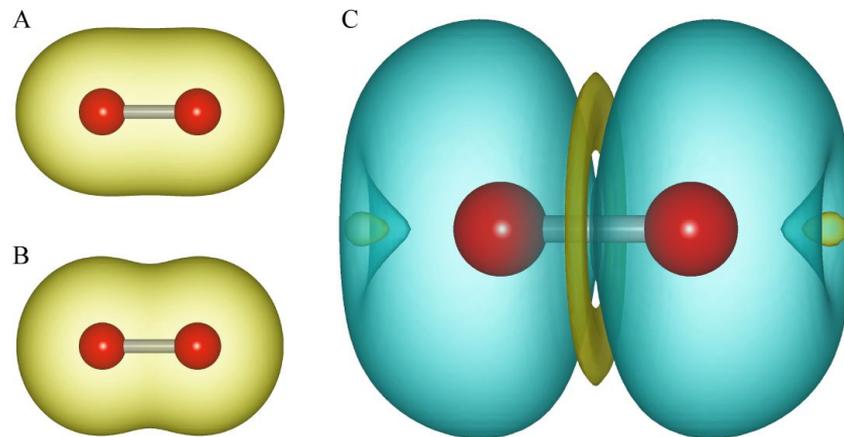
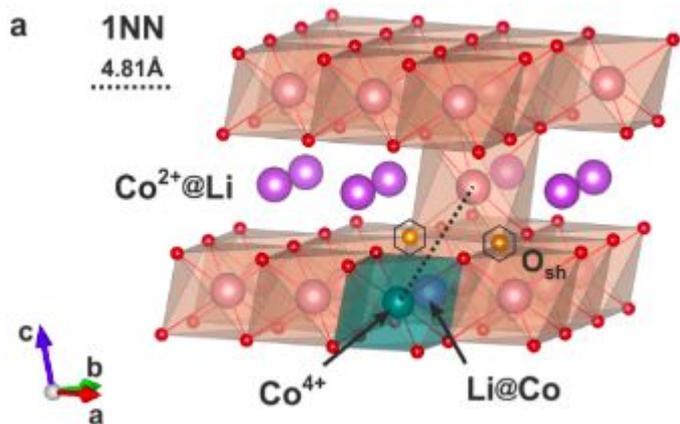
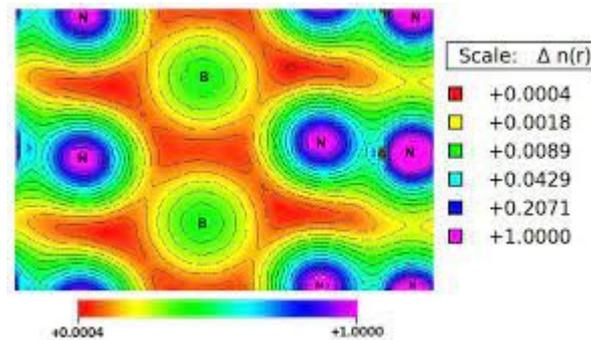
VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies.



<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

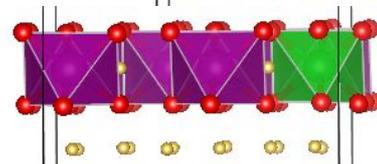
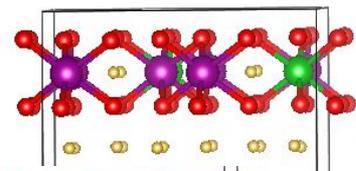
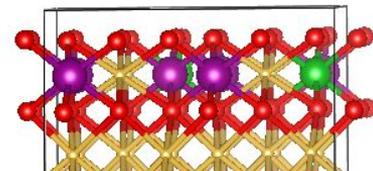
2) Bonds: you can change bond color, thickness and even switch off some of them

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

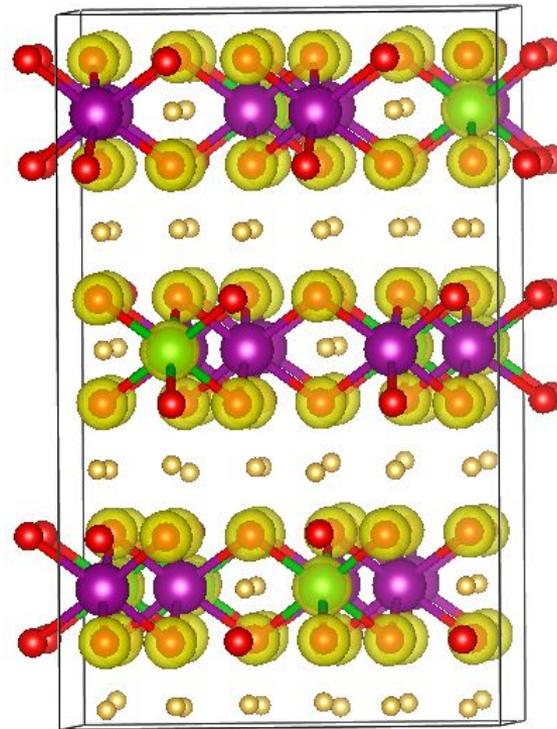
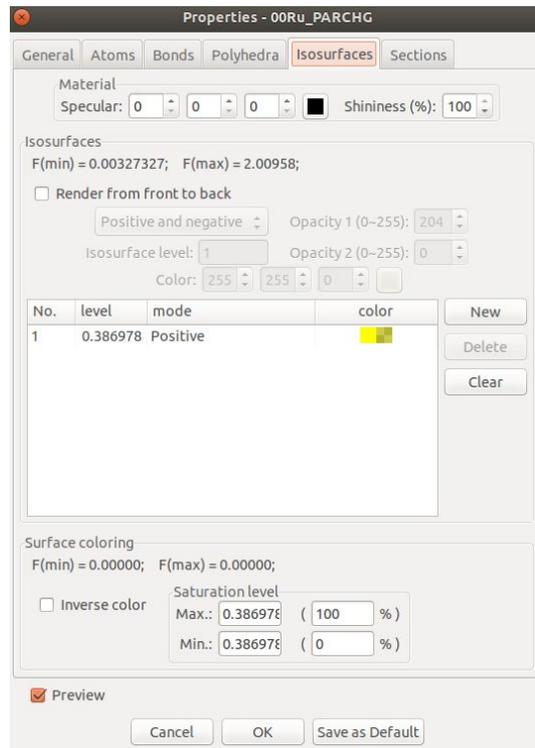
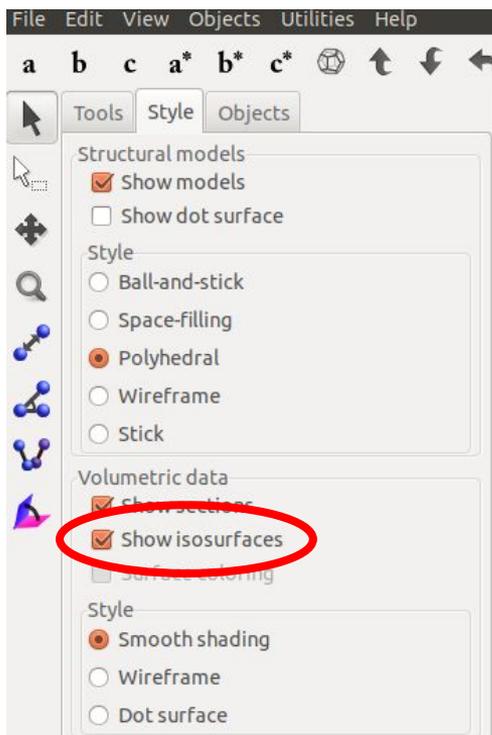
Site	r (Å)	C	L	S	V
▶ Li	0.50		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ Mn	1.37		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
▶ O	0.74		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>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



# How can we get structure files?



Take info about structure from papers and create the file yourself



Take geometry file from structure database

# Crystal structure databases

**Avito** Авто Недвижимость Работа Услуги ещё...

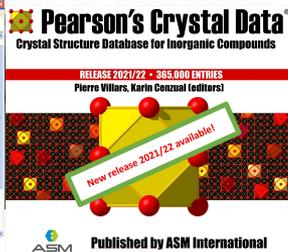
Любая категория ▾ **crystallography database** По всей России ▾ Найти

только в названиях  только с фото

Все объявления в России 59 534 913

Личные вещи 24 244 956    Хобби и отдых 4 675 282    Работа 2 247 359    Для бизнеса 520 449  
Транспорт 12 262 268    Бытовая электроника 4 615 909    Услуги 1 644 450  
Для дома и дачи 6 141 648    Недвижимость 2 634 303    Животные 548 289

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- Доставка**  
Проверка при получении и возможность бесплатно вернуть товар
- Автотека**  
Отчёт с историей авто: пробег, владельцы, сведения о залоге, ДТП и ремонтах

# Materials Project

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Search for materials information by chemistry, composition, or property

Explore Materials [Advanced Search Syntax](#)

by Elements  search

1	H																	2	He																		
3	Li	4	Be																	5	B	6	C	7	N	8	O	9	F	10	Ne						
11	Na	12	Mg																	13	Al	14	Si	15	P	16	S	17	Cl	18	Ar						
19	K	20	Ca	21	Sc	22	Ti	23	V	24	Cr	25	Mn	26	Fe	27	Co	28	Ni	29	Cu	30	Zn	31	Ga	32	Ge	33	As	34	Se	35	Br	36	Kr		
37	Rb	38	Sr	39	Y	40	Zr	41	Nb	42	Mo	43	Tc	44	Ru	45	Rh	46	Pd	47	Ag	48	Cd	49	In	50	Sn	51	Sb	52	Te	53	I	54	Xe		
55	Cs	56	Ba	57-71	La-Lu	72	Hf	73	Ta	74	W	75	Re	76	Os	77	Ir	78	Pt	79	Au	80	Hg	81	Tl	82	Pb	83	Bi	84	Po	85	At	86	Rn		
87	Fr	88	Ra	89-103	Ac-Lr	104	Rf	105	Db	106	Sg	107	Bh	108	Hs	109	Mt	110	Ds	111	Rg	112	Cn														
		57	La	58	Ce	59	Pr	60	Nd	61	Pm	62	Sm	63	Eu	64	Gd	65	Tb	66	Dy	67	Ho	68	Er	69	Tm	70	Yb	71	Lu						
		89	Ac	90	Th	91	Pa	92	U	93	Np	94	Pu	95	Am	96	Cm	97	Bk	98	Cf	99	Es	100	Fm	101	Md	102	No	103	Lr						

# of elements

excluded elements

Submit

External Provenance  
 ICSD   
 Exptl. ICSD

Material Tags

Band Gap (eV)

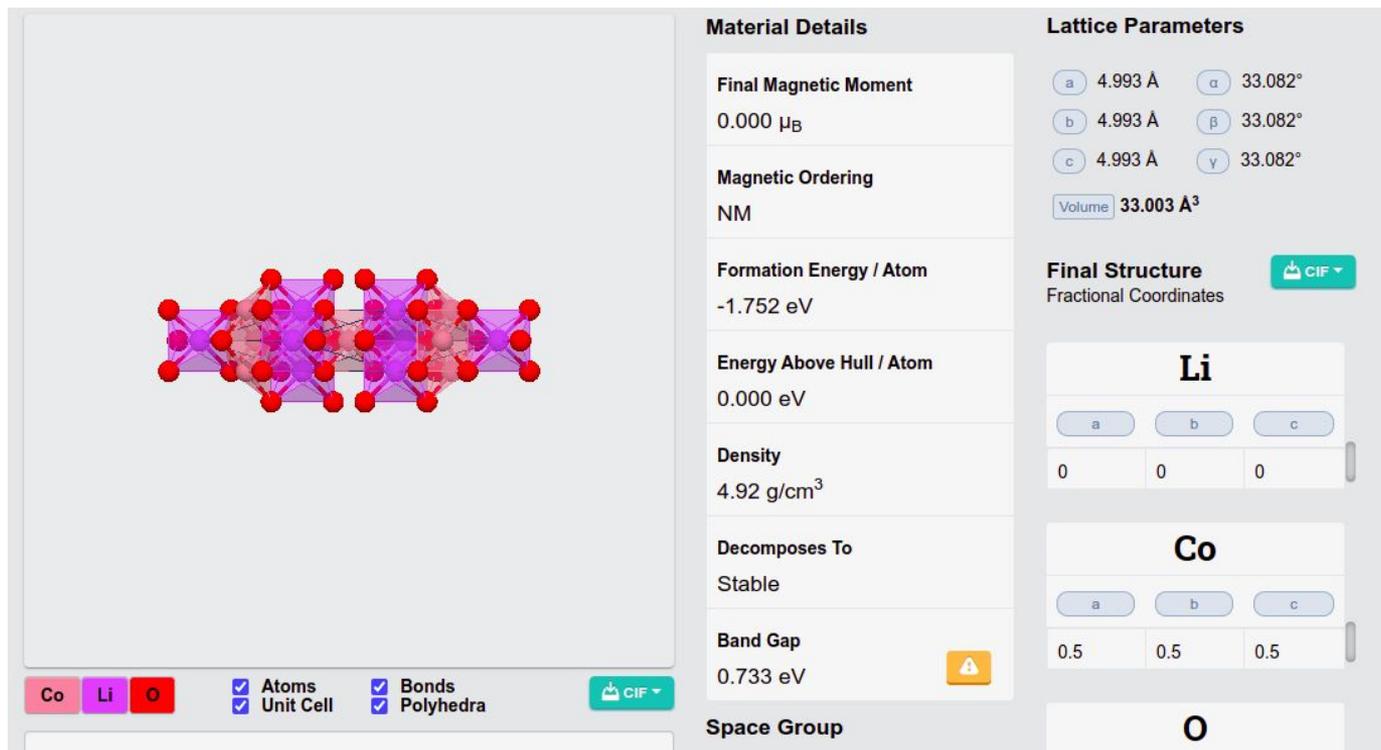
Energy Above Hull

# 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-3m) card



# Materials Project database: $\text{LiCoO}_2$ (R-3m) get a geometry file

Zoom in/out  
Rotate along the center axis

Shift + Drag cursor  
Option + Drag cursor

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

Hall  
-R 3 2"

Point Group  
 $\bar{3}m$

Crystal System  
trigonal

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)

File Formats

- CIF
- VASP
- POSCAR
- CSSR
- JSON

We have not yet calculated a detailed bandstructure for this material

**Thx**

