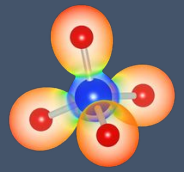
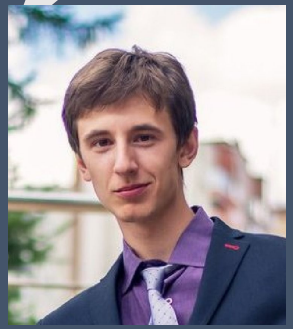
Crystallography and Crystal Chemistry
VIII International School-Conference of Young Scientists 2023



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



Dr. **Anton** O. **Boev**

PhD in **Physics, Research Scientist**

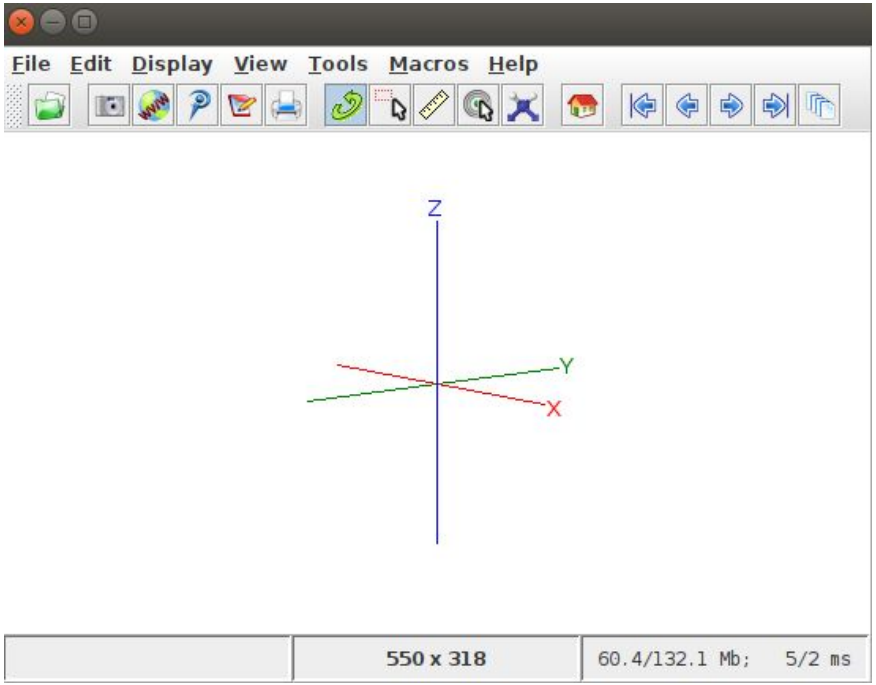
Center for **Energy Science** and **Technology**

Skoltech, Moscow, Russian Federation

November 10th, 2023


Jmol

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



http://jmol.sourceforge.net/ web_version

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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
```

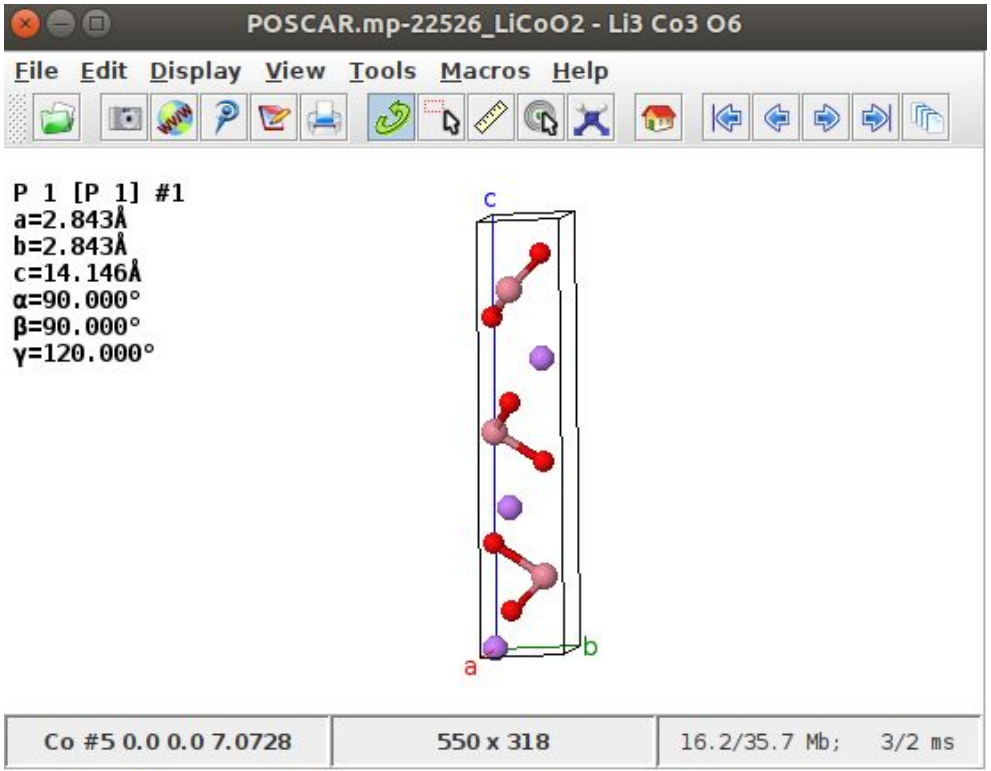
```
# generated using pymatgen
data_LiCoO2
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   2.84289827
_cell_length_b   2.84289827
_cell_length_c   14.14561550
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   120.00000000
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Li  Li0  1  0.00000000  0.00000000  0.00000000  1.0
  Li  Li1  1  0.66666667  0.33333333  0.33333333  1.0
  Li  Li2  1  0.33333333  0.66666667  0.66666667  1.0
  Co  Co3  1  0.33333333  0.66666667  0.16666667  1.0
  Co  Co4  1  0.00000000  0.00000000  0.50000000  1.0
  Co  Co5  1  0.66666667  0.33333333  0.83333333  1.0
  O  O6  1  0.00000000  0.00000000  0.23958700  1.0
  O  O7  1  0.66666667  0.33333333  0.09374633  1.0
  O  O8  1  0.66666667  0.33333333  0.57292033  1.0
  O  O9  1  0.33333333  0.66666667  0.42707967  1.0
  O  O10  1  0.33333333  0.66666667  0.90625367  1.0
  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



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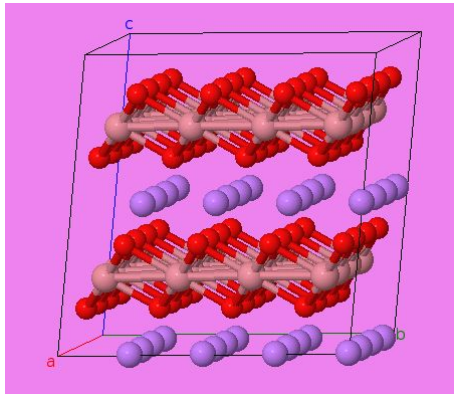
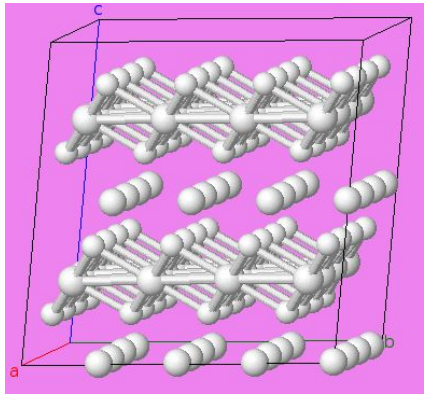
Some useful tools in Jmol

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

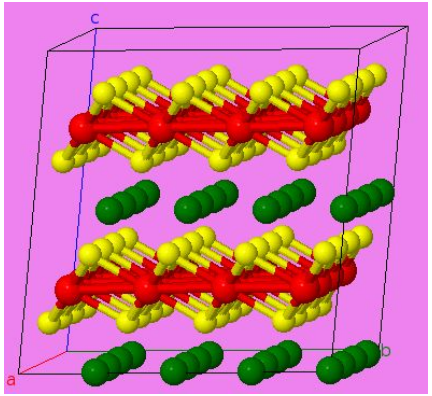
```
$ color background violet
```



```
$ color atoms white
```



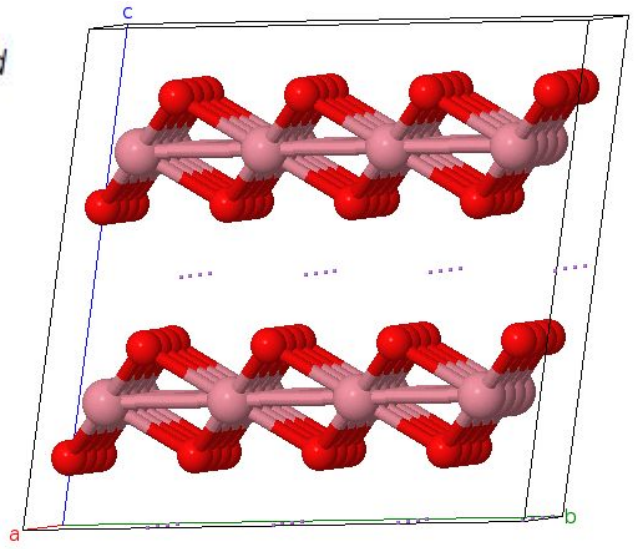
```
$ select li
32 atoms selected
$ color green
$ select co
32 atoms selected
$ color red
$ select o
64 atoms selected
$ color yellow
```



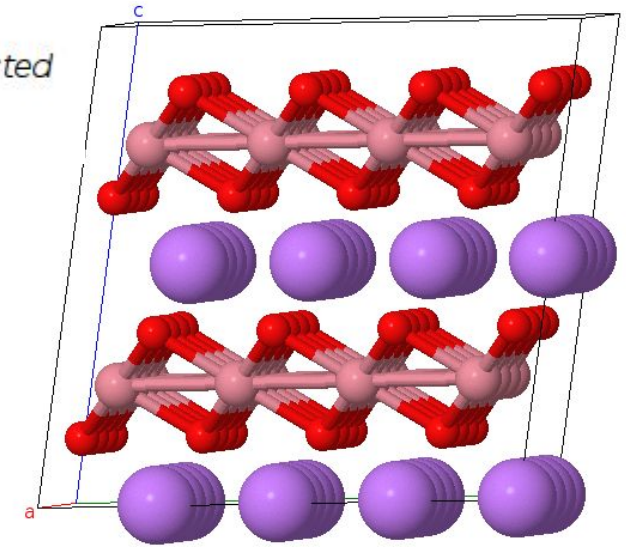
Some useful tools in Jmol

Using console you can manage the atomic size

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




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



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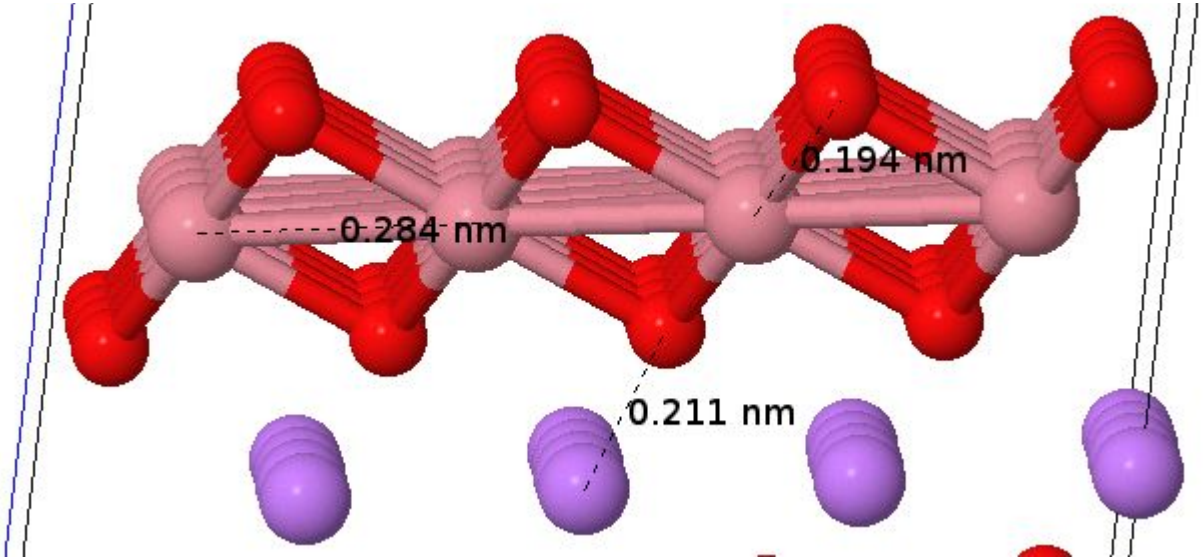
Some useful tools in Jmol

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



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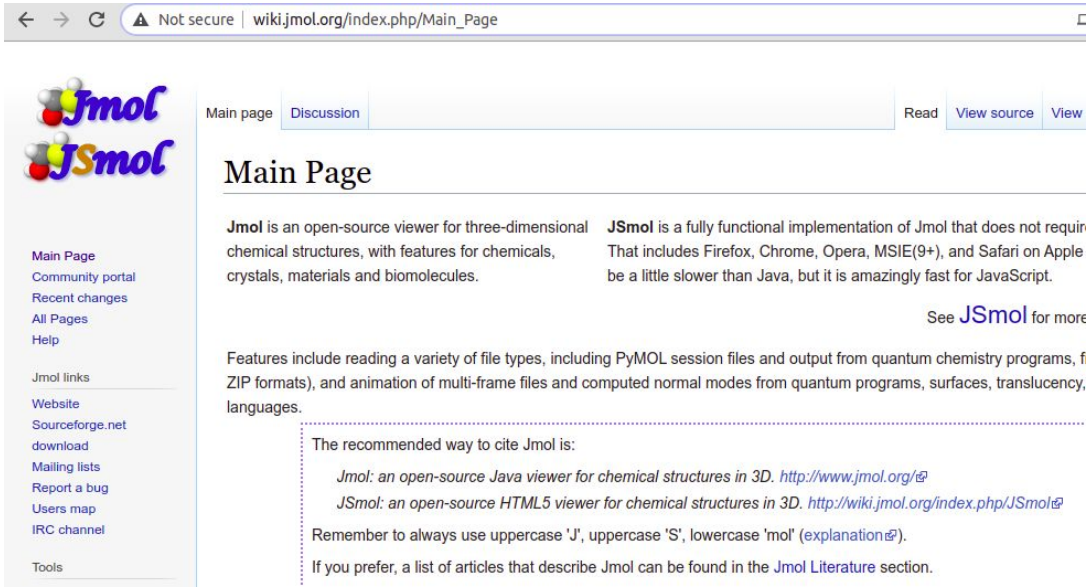
Some useful tools in Jmol

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



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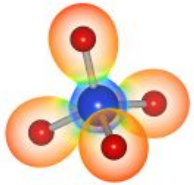
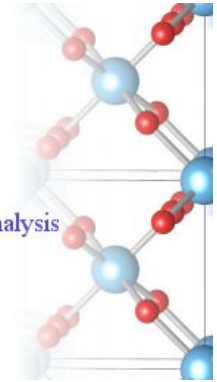
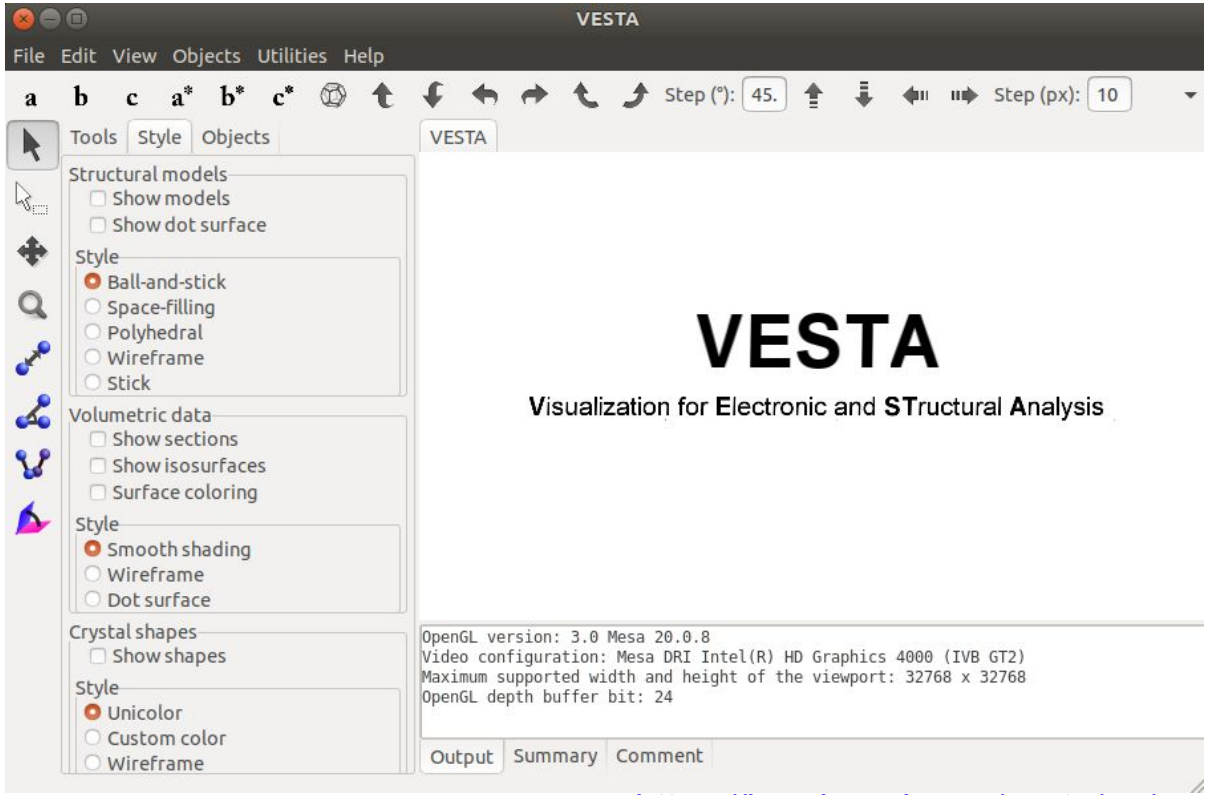


VESTA

Visualization for Electronic and STructural Analysis

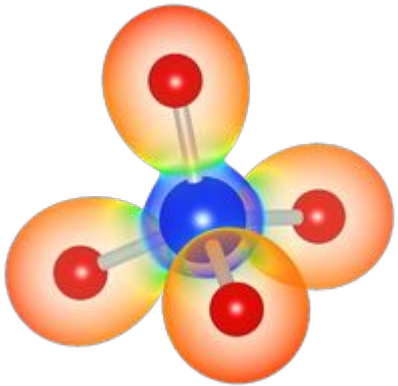


VESTA



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

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



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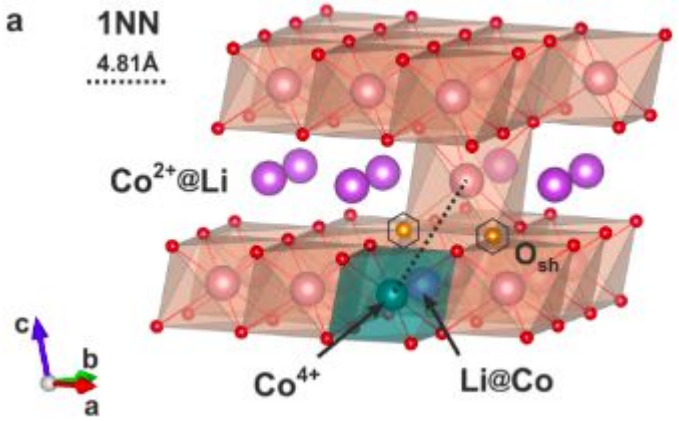
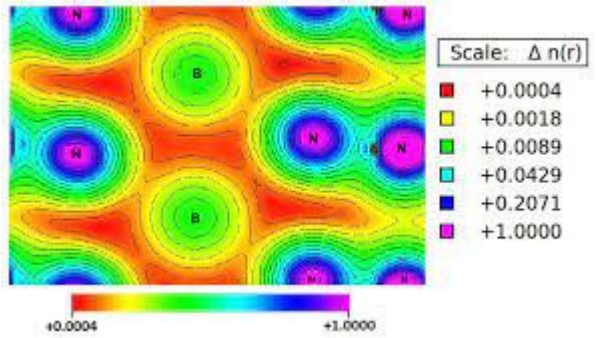
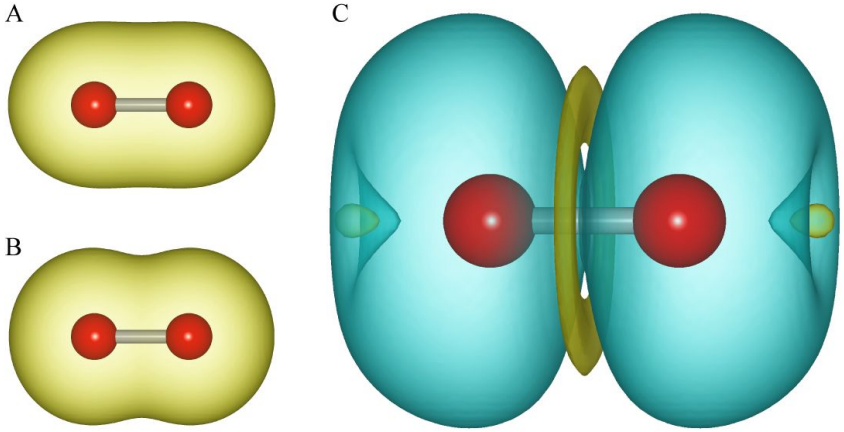
VESTA's advantageous

- 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.

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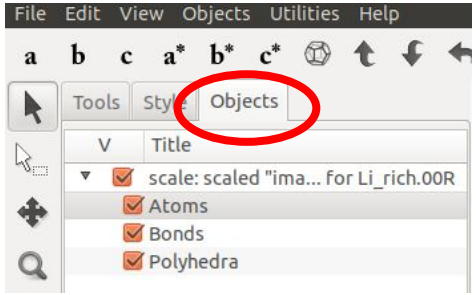
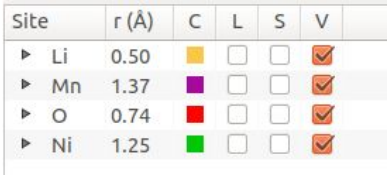
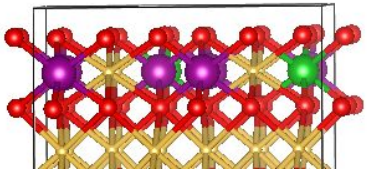
VESTA: style options



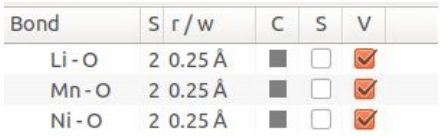
Objects tab allows us to manage style

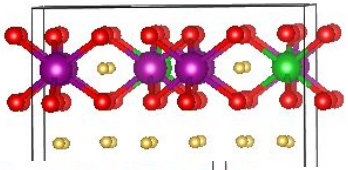
1) Atoms: you can change atomic radii and colors



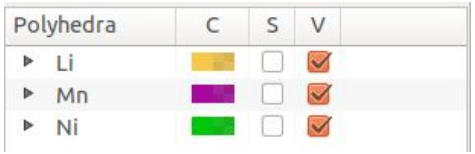


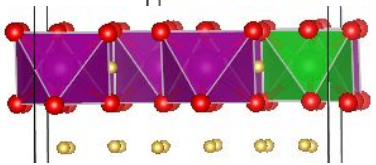
2) Bonds: you can change bond color, thickness and even switch off some of them





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





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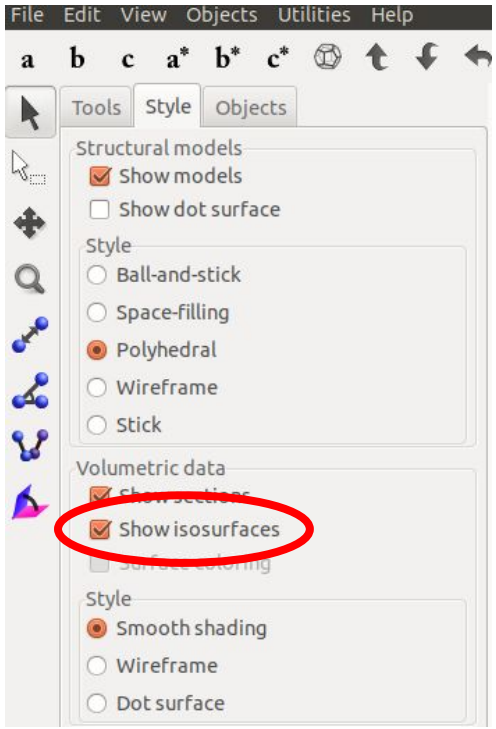
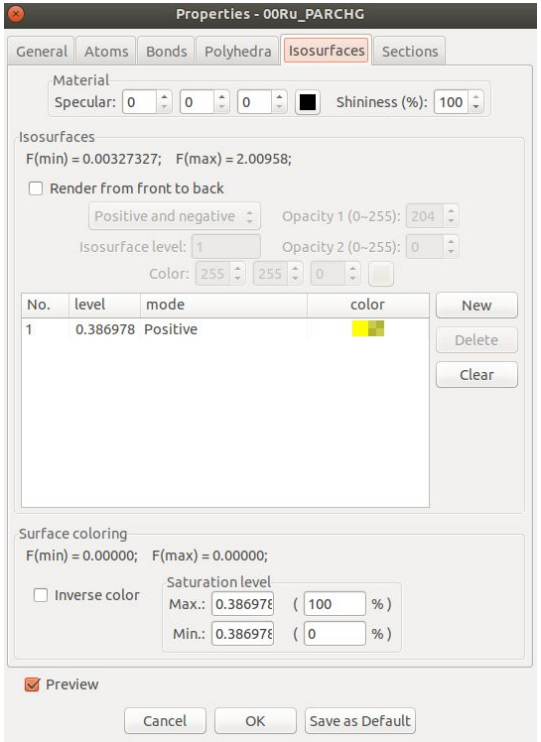
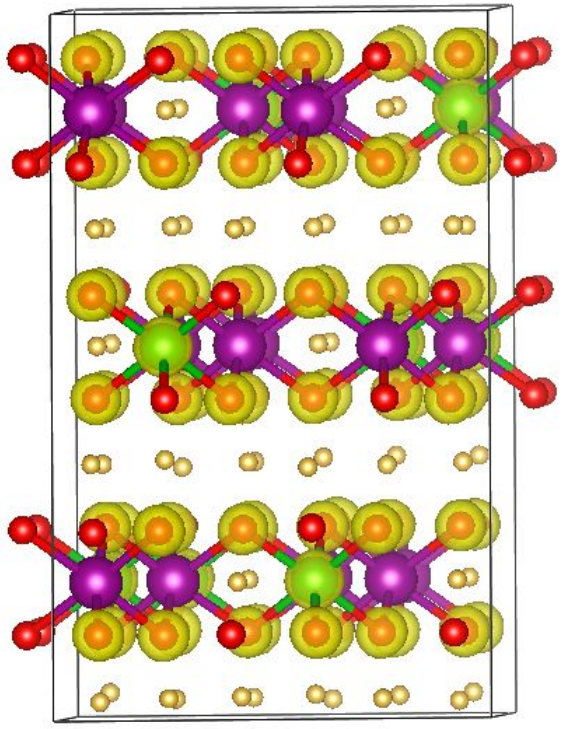
VESTA: Charge isosurface visualization







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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

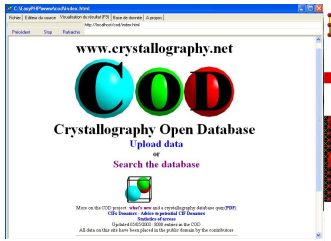
Все объявления в России 59 534 913

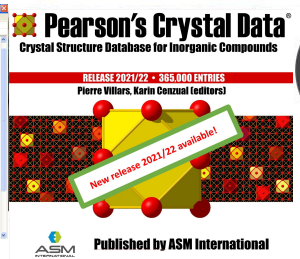
Личные вещи 24 244 956 | Хобби и отдых 4 675 282 | Работа 2 247 359 | Для бизнеса 520 449

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

Рекомендации для вас

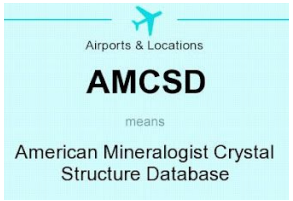




Сервисы и услуги Авито

Доставка
Проверка при получении и возможность бесплатно вернуть товар

Автотека
Отчёт с историей авто: пробег, владельцы, сведения о залоге, ДТП и ремонтах



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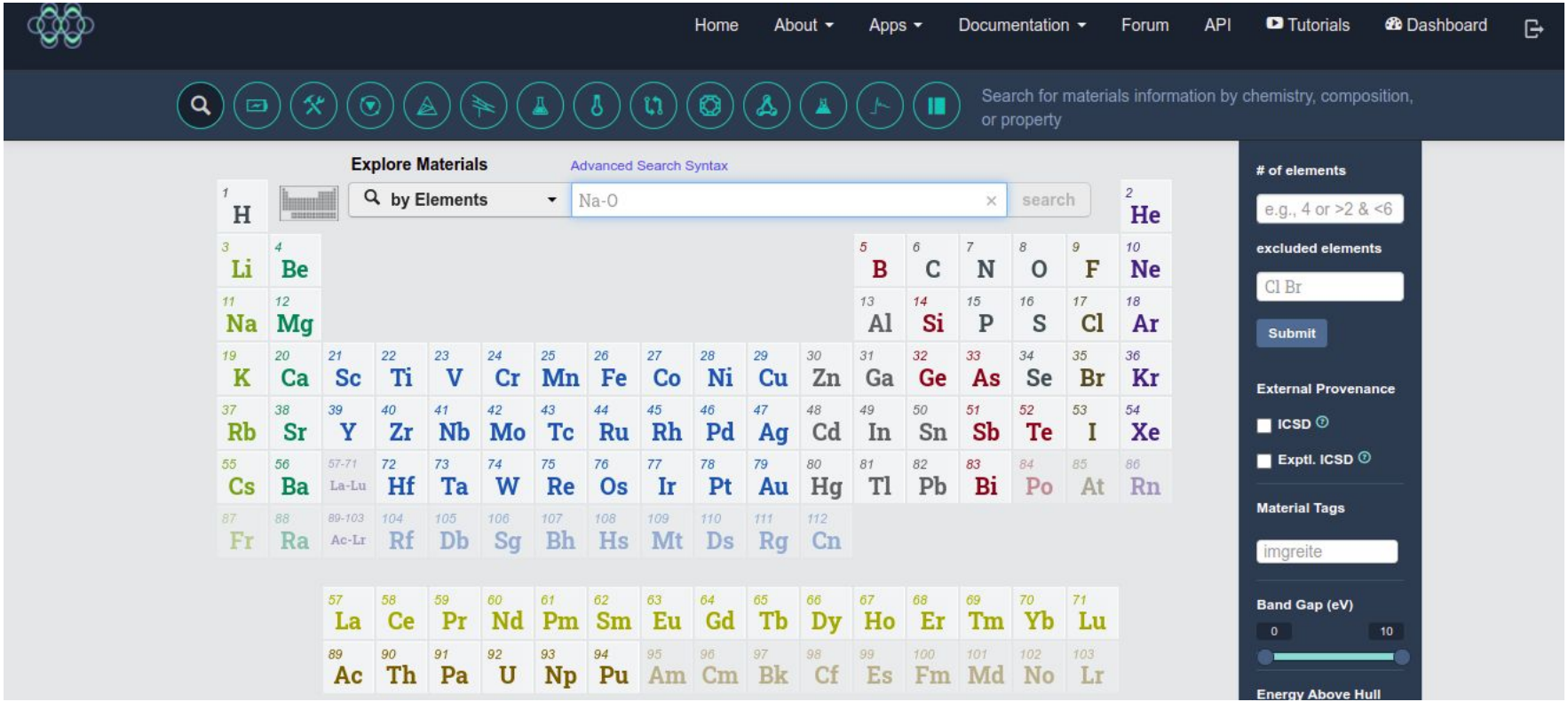
Materials Project



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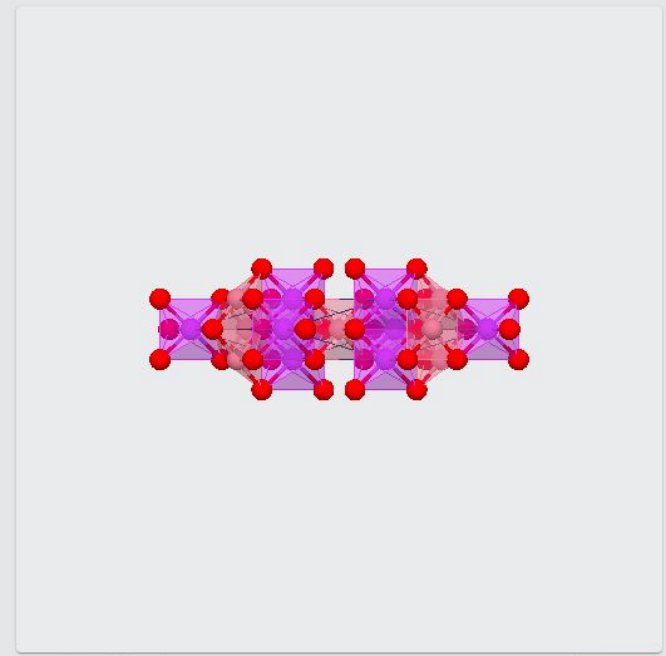
Materials Project database: $LiCoO_2$

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	$LiCoO_2$	$R\bar{3}m$	-1.752	0	0.733	33.003	4	4.924	☐
mp-849273	$LiCoO_2$	$Fd\bar{3}m$	-1.72	0.032	0.000	138.634	16	4.689	☐
mp-853240	$LiCoO_2$	Imma	-1.715	0.037	1.884	138.594	16	4.691	☐
mp-1097885	$LiCoO_2$	C2/m	-1.708	0.043	2.013	138.978	16	4.678	☐
mp-867664	$LiCoO_2$	$P\bar{1}$	-1.666	0.085	0.442	167.512	20	4.851	☐
mp-753473	$LiCoO_2$	$P6_3mc$	-1.659	0.093	0.896	73.734	8	4.408	☐
mp-1222334	$LiCoO_2$	P4/mmm	-1.541	0.211	0.000	34.567	4	4.702	☐

Materials Project database: $LiCoO_2$ (R-3m) card



Material Details

Final Magnetic Moment
0.000 μ_B

Magnetic Ordering
NM

Formation Energy / Atom
-1.752 eV

Energy Above Hull / Atom
0.000 eV

Density
4.92 g/cm^3

Decomposes To
Stable

Band Gap
0.733 eV

Space Group

Lattice Parameters

a	4.993 Å	α	33.082°
b	4.993 Å	β	33.082°
c	4.993 Å	γ	33.082°

Volume 33.003 Å^3

Final Structure
Fractional Coordinates
CIF

Li

a	b	c
0	0	0

Co

a	b	c
0.5	0.5	0.5

O

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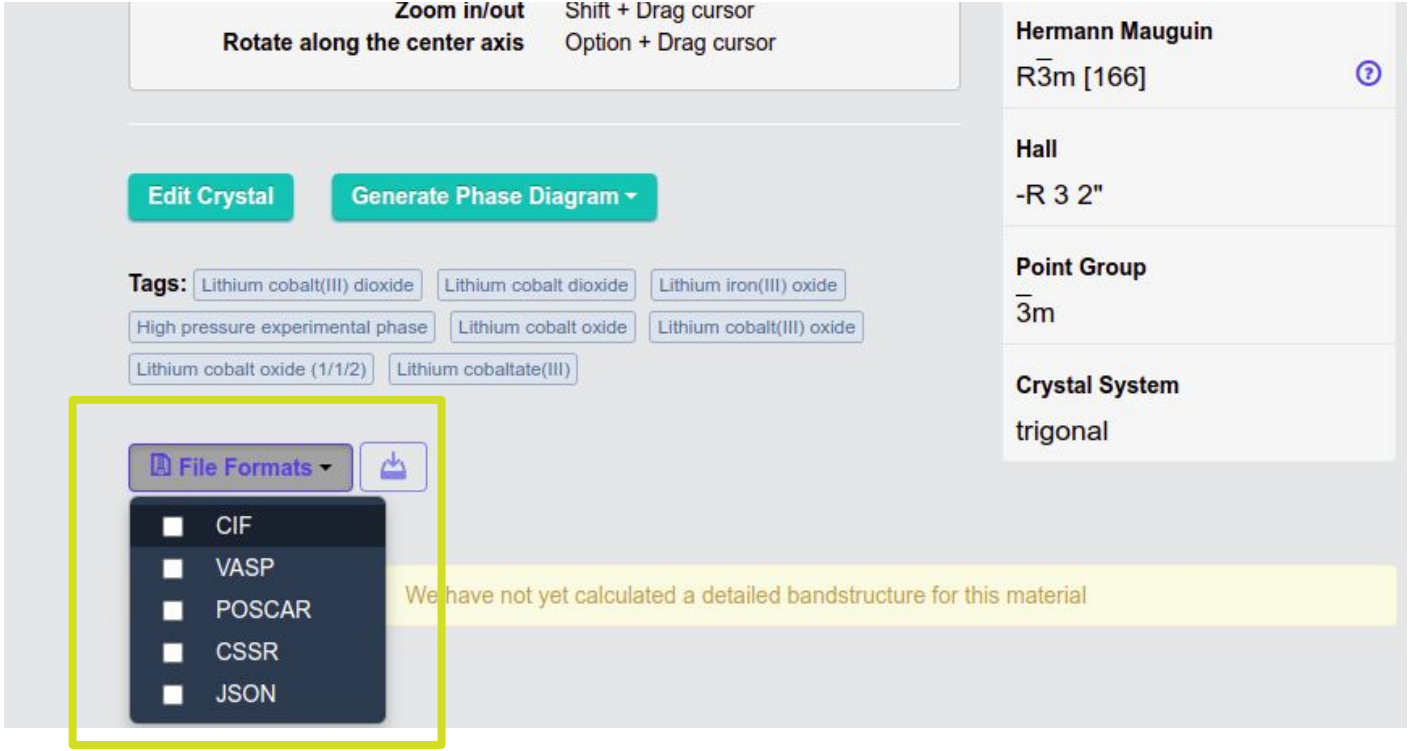
Materials Project database: $LiCoO_2$ (R-3m) get a geometry file



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Thx!