

# **CRYSTAL Tutorial**

## **University of Michigan**

**Yanbing Zhou 05/19/2022**

# Outline

- Crystal Structure Informations
  - where to find them
- How to run *crystal*
  - Parameter file setup
  - Basis sets library
  - ECP
  - AFM
- How to run *properties*
  - Band structure plot generation

# Crystal Structure Information

## ICSD: Inorganic Crystal Structure Database

umich login:

[https://icsd-fiz-karlsruhe-  
de.proxy.lib.umich.edu/search/  
basic.xhtml;jsessionid=1701C7A256A9  
2AA6E023A9498D99BA40](https://icsd-fiz-karlsruhe-de.proxy.lib.umich.edu/search/basic.xhtml;jsessionid=1701C7A256A92AA6E023A9498D99BA40)

Welcome to ICSD Web. IP authenticated (141.211.4.224). Univ of Michigan

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Change Password | Close session

**Search Action**

**Search Summary**  
Basic Search: -

**Query History**  
Number of queries: 0

**ICSD**

**Login**  
LoginId:   
Password:   
  
Lost password?

**Basic Search & Retrieve**

**Free Text Search**  
General Attributes

**Bibliography**  
Authors   
Title of Journal   
Title of Article   
Year of Publication

**Content Selection** ?  
 Experim. inorganic structures  
 Experim. metal-organic str.  
 Theoretical structures

**Navigation**

**Chemistry**  
Composition  Periodic Table  
Number of Elements

**Cell**  
Cell Parameters   
Cell Volume  Tolerance +/-  %

**Symmetry**  
Space Group Symbol  Space Group Number   
Crystal System  Centering

**Exp. Info. & Ref. Data**  
New Data Only   
PDF Number  Temperature  K  
ICSD Collection Code  Pressure  MPa

# Options for Different Searches

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**Basic Search & Retrieve**

**Free Text Search**

General Attributes

**Bibliography**

Authors Year of Publication

Title of Journal

Title of Article

DOI

**Chemistry**

Composition Periodic Table

Number of Elements

**Cell**

Cell Parameters

Cell Volume

Tolerance +/- %

**Symmetry**

Space Group Symbol

Space Group Number

Crystal System Centering

**Expt. Info. & Ref. Data**

Data Only

Pressure Temperature

Pressure MPa

ICSD Collection

**Clear Basic Search** **Count Basic Search**

**Navigation**

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography**
- Cell**
- Chemistry**
- Symmetry**
- Crystal Chemistry**
- Structure Type**
- Experimental Information**
- DB Info**
- Expert Search**
- Query Management**
- Manage Queries**
- List Combined Queries**
- Create Combined Query**
- ICSD links**
- ICSD News**

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Version 4.8.0 (build 20220419-1910) - Data Release 2022.1  
Buildnumber 2a6817d652a4a2067b1d66e404f43557d784e976

- Navigation**
- Basic search & retrieve
  - Advanced search & retrieve**
  - Bibliography**
  - Cell**
  - Chemistry**
  - Symmetry**
  - Crystal Chemistry**
  - Structure Type**
  - Experimental Information**
  - DB Info**
  - Expert Search**
  - Query Management**
  - Manage Queries**
  - List Combined Queries**
  - Create Combined Query**
  - ICSD links**
  - ICSD News**

# Search Example: Diamond

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**Chemistry Search**

Composition	<input type="text" value="C"/> <a href="#">Periodic Table</a>	Number of Elements	<input type="text" value="1"/>
e.g. Na Cl			
Structural Formula	<input type="text" value="e.g. Pb (W O4)"/>		
Chemical Name	<input type="text" value="Mineral Name IMA"/>		
Mineral Name	<input type="text" value="diamond"/> <a href="#">e.g Adamite</a>	Mineral Name IMA	<input type="text" value="e.g Halamishite"/>
Mineral Group	<input type="text" value="e.g. Pyroxene"/>		
ANX Formula	<input type="text" value="Number of Formula Units"/>		
AB Formula	<input type="text" value=""/>		
Formula Weight	<input type="text" value=""/>		

[Clear Chemistry Search](#) [Count Chemistry Search](#)

**Search Action**

[Run Query](#) [Clear Query](#)

**Search Summary**

Bibliography:	-
Cell:	-
Chemistry:	0
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
<b>Combined Results:</b>	0

**Query History**

Number of queries:	2
<a href="#">Clear Query History</a>	
2022-05-19T03:09	7
2022-05-19T03:09	60

# Eliminating Options



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Results: List View

# of Hits: 7

	HMS	Struct. Form.	Struct. Type	Cell Parameter	Cell Volume	Temperature	Publication Year	Filter
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56669(5) 3.56669 3.5666	45.37	283.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56672(19) 3.56672(19) 3.	45.37	293.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56678(4) 3.56678 3.5667	45.38	303.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56684(4) 3.56684 3.5668	45.38	313.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56690(4) 3.5669 3.5669	45.38	323.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56686(2) 3.56686(2) 3.56	45.38	293.00	1951	
<input type="checkbox"/>	<input type="checkbox"/>	F d -3 m S	C	Diamond#C(cF8)#a-Sn 3.56694(3) 3.56694(3) 3.56	45.38	293.00	1951	

(1 of 1)

1 2 3 4 5 6 7 8 9 10

# Eliminating Options

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Results: List View

Back to Query Show Detailed View Export Data Print Compare Structures Compare Powder Pattern Column Selection Filter

HMS	Struct. Form.	Struct. Type	Cell Parameter	Cell Volume	Temperature	Publication Year
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56669(5) 3.56669 3.5666 45.37	283.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56672(19) 3.56672(19) 3. 45.37	293.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56678(4) 3.56678 3.5667 45.38	303.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56684(4) 3.56684 3.5668 45.38	313.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56690(4) 3.5669 3.5669 ! 45.38	323.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56686(2) 3.56686(2) 3.56 45.38	293.00	1951	
F d -3 m S	C	Diamond#C(cF8)#a-Sn	3.56694(3) 3.56694(3) 3.56 45.38	293.00	1951	

(1 of 1) 1 10

Column Selection Filter

**Quality Filter**

All Data   
 High Quality Data only  
 Standard Quality Data only

**Radiation Type**  
X-Ray, Electrons, Neutrons, Synchotron

**Sample Type**  
Single Crystal, Powder

**R-value**  
Any R-value

**Experimental Conditions**  
Any condition

Reset Filter

# Eliminating Options

		HMS	Struct. Form.	Struct. Type	Cell Parameter	Cell Volume	Temperature	Publication Year	Star	More
<input type="checkbox"/>		F m -3 m	Ni O	NaCl	4.178(1) 4.178(1) 4.178(1)	72.93	293.00	1979		
<input type="checkbox"/>		F m -3 m	Ni O	Yb7+xSe8	8.3532(1) 8.3532(1) 8.3532	582.85	293.00	1998		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9517(2) 2.9517(2) 7.2170	54.45	10.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9518(2) 2.9518(2) 7.2167	54.46	50.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9520(2) 2.9520(2) 7.2179	54.47	100.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9523(2) 2.9523(2) 7.2205	54.50	150.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9532(2) 2.9532(2) 7.2227	54.55	200.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9541(2) 2.9541(2) 7.2273	54.62	250.00	2000		
<input type="checkbox"/>		R -3 m H	Ni O	NiO	2.9549(5) 2.9549(5) 7.2320	54.69	295.00	2000		
<input type="checkbox"/>		F m -3 m	Ni O	NaCl	4.1718(2) 4.1718(2) 4.1718	70.61	293.00	2021		

# Eliminating Options

HMS		Struct. Form.	Struct. Type	Cell Parameter		Cell Volume	Temperature	Publication Year	Operations
<input type="checkbox"/>	<input checked="" type="checkbox"/>	F m -3 m	Ni O	NaCl	4.178(1) 4.178(1) 4.178(1)	72.93	293.00	1979	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	F m -3 m	Ni O	Yb7+xSe8	8.3532(1) 8.3532(1) 8.3532	582.85	293.00	1998	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9517(2) 2.9517(2) 7.2170	54.45	10.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9518(2) 2.9518(2) 7.2167	54.46	50.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9520(2) 2.9520(2) 7.2179	54.47	100.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9523(2) 2.9523(2) 7.2205	54.50	150.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9532(2) 2.9532(2) 7.2227	54.55	200.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9541(2) 2.9541(2) 7.2273	54.62	250.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	R -3 m H	Ni O	NiO	2.9549(5) 2.9549(5) 7.2320	54.69	295.00	2000	
<input type="checkbox"/>	<input checked="" type="checkbox"/>	F m -3 m	Ni O	NaCl	4.1718(9) 4.1718(9) 4.1718	72.61	293.00	2021	

# Hermann-Mauguin notation (HNM) & Struct Type

HMS	Struct. Form	Struct. Type	Cell Parameter	Cell Volume	Temperature	Publication Year	Star	Download					
F m -3 m	Ni O	NaCl	4.1718(9) 4.1718(9) 4.1718	72.61	293.00	2021							
F m -3 m	Ni O	NaCl	4.17 4.17 4.17 90. 90. 90.	72.51	293.00	2021							
F m -3 m	Ni O	NaCl	4.170(3) 4.170(3) 4.170(3)	72.51	293.00	2020							
F m -3 m	Ni O	NaCl	4.17824 4.17824 4.17824	72.94	293.00	2019							
F m -3 m	Ni O	NaCl	4.198 4.198 4.198 90. 90.	73.98	293.00	2019							
F m -3 m	Ni O	NaCl	4.4145(1) 4.4145(1) 4.4145	86.02	293.00	2016							
F m -3 m	Ni O	NaCl	4.1910 4.1910 4.1910 90.	73.61	293.00	2016							
F m -3 m	Ni O	NaCl	4.173 4.173 4.173 90. 90.	72.67	293.00	2016							
F m -3 m	Ni O	NaCl	4.184724 4.184724 4.1847	73.28	293.00	2016							
F m -3 m	Ni O	NaCl	4.179 4.179 4.179 90. 90.	72.98	293.00	2012							
(1	f 5)												

Detailed View

Entry 1 of 1

[Back to Query](#)[Back to List](#)[CCDC](#)[Export Cif](#)[Print](#)[Feedback to Editor](#)

## Summary

Collection Code 112324

Struct. formula

Ni O

Cell parameter

4.1718(9) 4.1718(9) 4.1718(9) 90. 90. 90.

Cell volume

72.61 [Å<sup>3</sup>]

Temperature

room temperature

Data quality

High quality

Author

Singh, Jay; Lee, Seulgi; Kim, Sungjin; Singh, Satendra Pal; Kim, Jaekook; Rai, Alok Kumar

Reference

Journal of Alloys and Compounds (2021) 850, Article ID 156755 (p. null-null)

Structure type

NaCl

Space group

F m -3 m (225)

Z

4

Pressure

atmospheric

R-value

0.0334

Title

Fabrication of TD mesoporous NiO nano-rods as high capacity and long-life anode material for lithium ion batteries

DOI

10.1016/j.jallcom.2020.156755

## Details

Visualization

Chemistry

Sum. formula

Ni<sub>1</sub> O<sub>1</sub>

Molecular weight

74.7090 [u]

ANX formula

AX

Chemical name

Nickel oxide

Struct. formula

Ni O

Z

4

AB formula

AB

Published Crystal Structure Data

Standardized Crystal Structure Data

Distances and Angles

Bibliography

Experimental information

Additional information

# Crystal Structure Data

## Published Crystal Structure Data

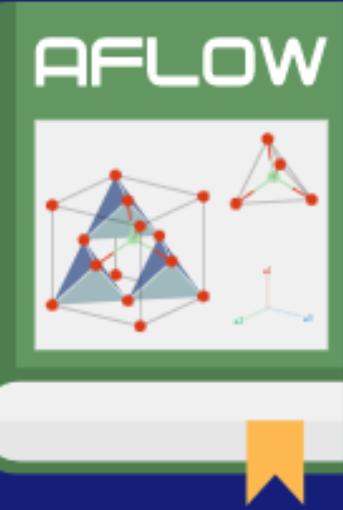
Cell parameter	4.1718(9) 4.1718(9) 4.1718(9) 90. 90. 90.
Cell volume	72.61 Å <sup>3</sup>
Crystal system	cubic
Laue class	m-3m
Structure type	NaCl
Pearson symbol	cF8
Wyckoff sequence	b a
Calc. density	6.83 [g/cm <sup>3</sup> ]

Space group	F m -3 m (225)		
Z	4		
Crystal class	m-3m		
Axis ratios	a/b	b/c	c/a
	1.0000	1.0000	1.0000

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	B
Ni	1	+2.00	4 a	0	0	0	1	1.46(9)
O	1	-2.00	4 b	0.5	0.5	0.5	1	1.3(1)

# Crystal Structure information

<http://www.aflowlib.org/prototype-encyclopedia/>

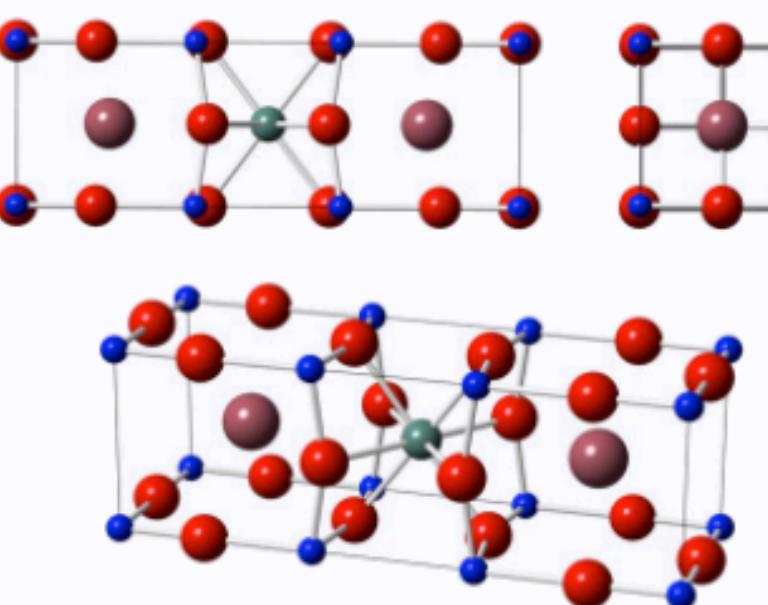


## ENCYCLOPEDIA OF CRYSTALLOGRAPHIC PROTOTYPES

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes: Part 1, Comp. Mat. Sci. 136, S1-S828 (2017). (doi=10.1016/j.commatsci.2017.01.017)

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes: Part 2, Comp. Mat. Sci. 161, S1-S1011 (2019). (doi=10.1016/j.commatsci.2018.10.043)

D. Hicks, M.J. Mehl, M. Esters, C. Osse, O. Levy, G.L.W. Hart, C. Toher, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes: Part 3, Comp. Mat. Sci. 199, 110450 (2021). (doi=10.1016/j.commatsci.2021.110450)



Search by common name or composition...

search

The AFLOW standard encyclopedia of crystallographic prototypes provides a complete description of each structure, including formulas for the primitive vectors, basis vectors, and AFLOW commands to generate the standardized cells.

Electronic structure geometry files are available to download in both CIF and POSCAR formats.

Number of prototypes in the encyclopedia: **1100**

**Search prototypes via space group, Pearson symbol, Strukturbericht designation, and chemical symbols.**

Space Group

Pearson Symbol

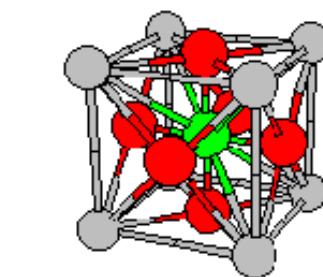
Strukturbericht

Chemical Symbols

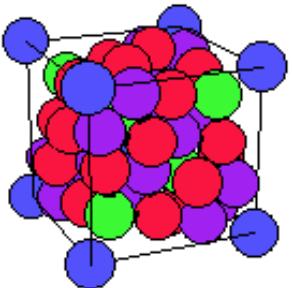
Prototype Index

AFLOW-XtalFinder

# Crystal Structure Information



Crystal Lattice\*<sup>\*</sup>-Structures



Indexed by	
<a href="#">Strukturbericht Designation</a>	<a href="#">Pearson Symbol</a>
<a href="#">Space Group</a>	<a href="#">Prototype</a>
<a href="#">Structures of Intermetallic Alloy Phases</a>	

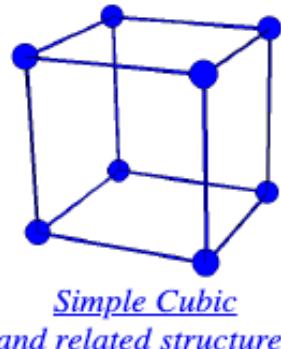
lattices can be obtained by clicking on the desired structure below.

This page currently contains links to 286 structures in 98 of the 230 space groups.

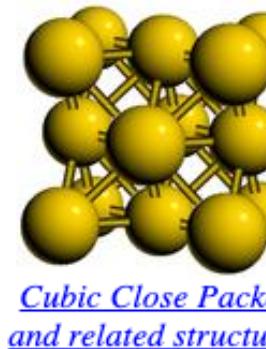
[Matlockite \(PbFCI\)](#)

[β-V<sub>2</sub>N](#)

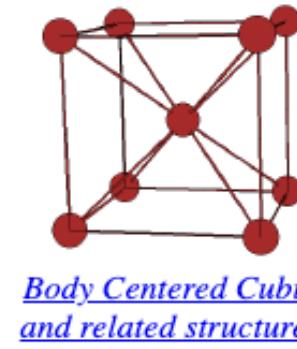
<https://www.atomic-scale-physics.de/lattice/index.html>



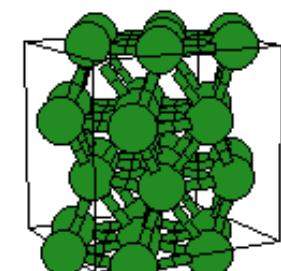
[Simple Cubic  
and related structures](#)



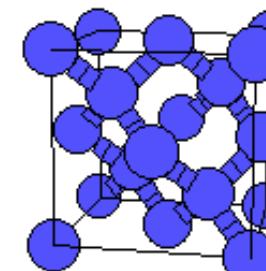
[Cubic Close Packed  
and related structures](#)



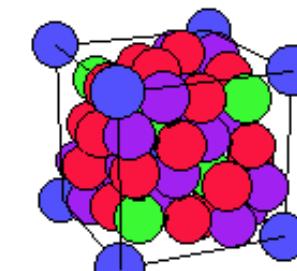
[Body Centered Cubic  
and related structures](#)



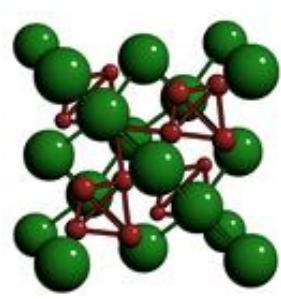
[Hexagonal Close Packed  
and related structures](#)



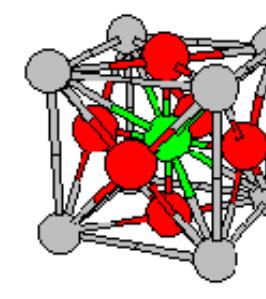
[Carbon  
and Related Structures](#)



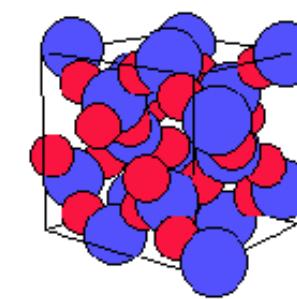
[Manganese Structures](#)



[The Laves Phases](#)



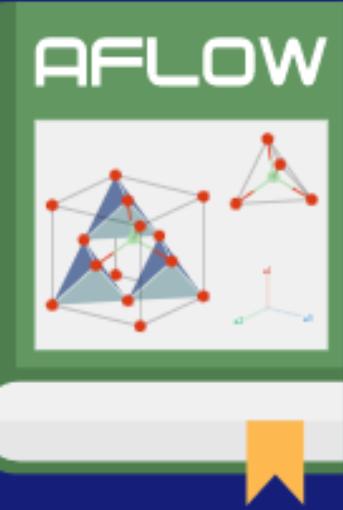
[Perovskite  
and Related Structures](#)



[Quartz \(SiO<sub>2</sub>\)  
and Related Structures](#)

# Crystal Structure information

<http://www.aflowlib.org/prototype-encyclopedia/>

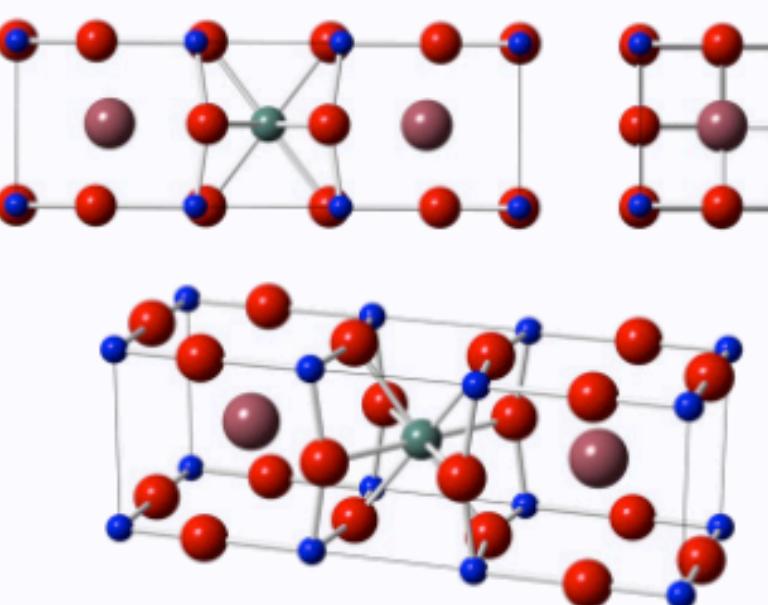


## ENCYCLOPEDIA OF CRYSTALLOGRAPHIC PROTOTYPES

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D. Hicks, M.J. Mehl, M. Esters, C. Osse, O. Levy, G.L.W. Hart, C. Toher, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes: Part 3, Comp. Mat. Sci. 199, 110450 (2021). (doi=10.1016/j.commatsci.2021.110450)



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Search by common name or composition...

**search**

**Search prototypes via space group, Pearson symbol, Strukturbericht designation, and chemical symbols.**

**Space Group**

**Pearson Symbol**

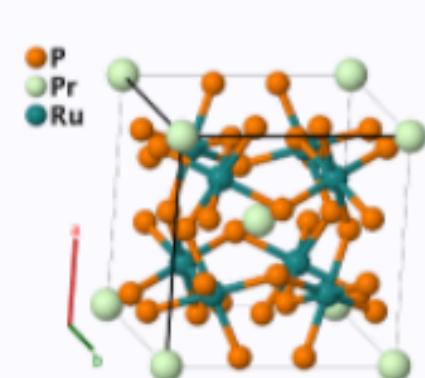
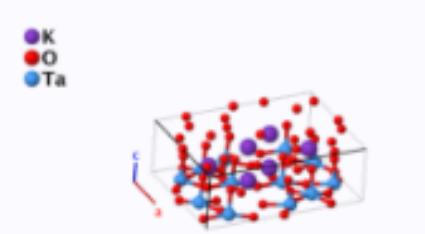
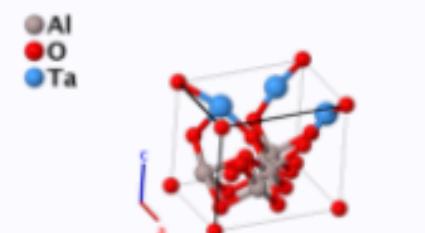
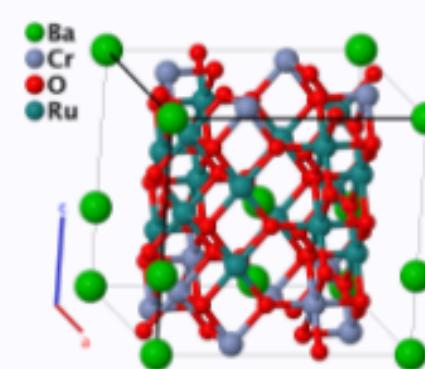
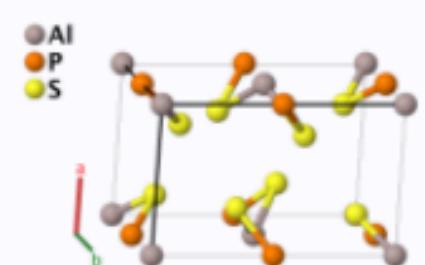
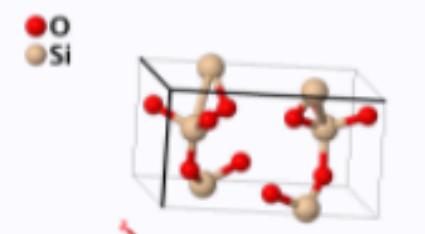
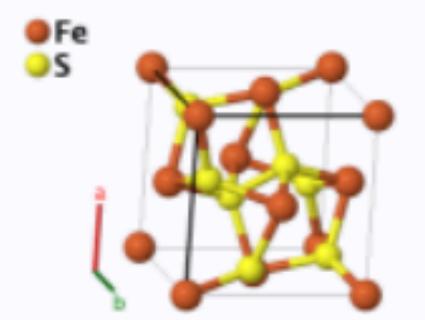
**Strukturbericht**

**Chemical Symbols**

**Prototype Index**

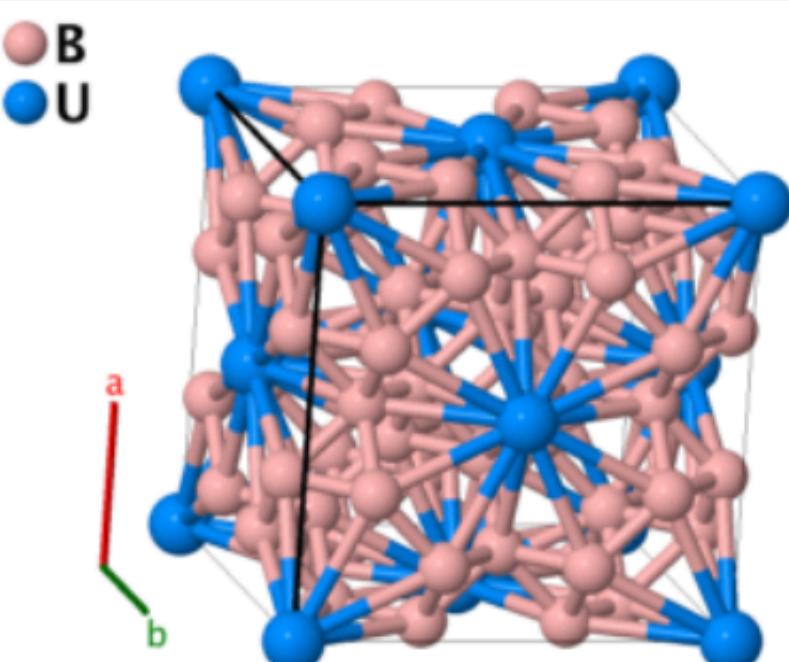
**AFLOW-XtalFinder**

## Space Groups

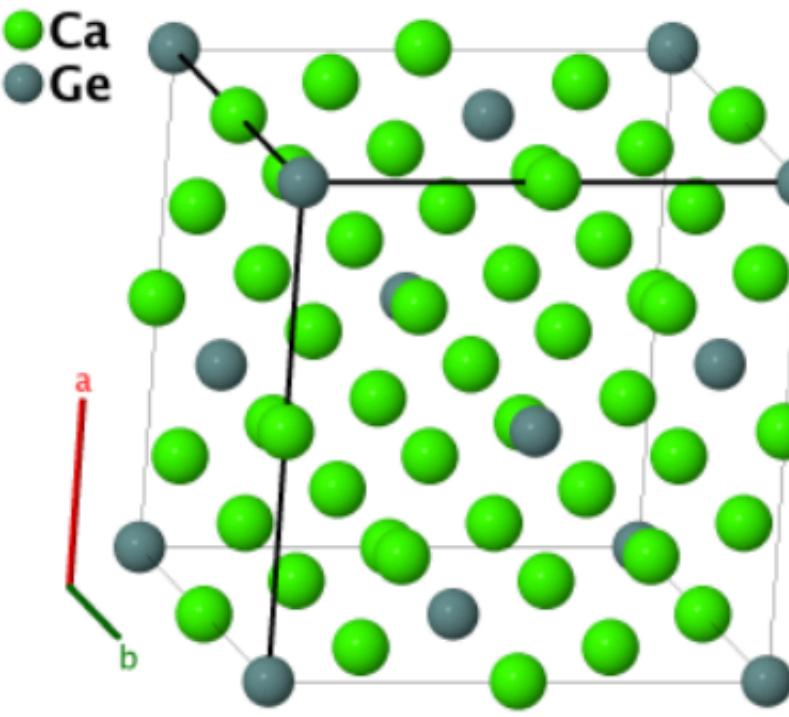


## Fm $\bar{3}$ m (#225)

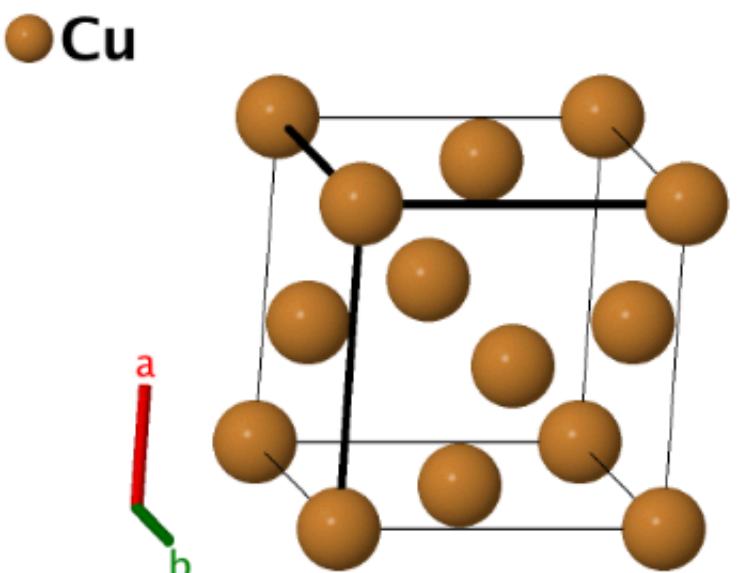
UB<sub>12</sub> ( $D2_f$ ) Structure: A12B\_cF52\_225\_i\_a



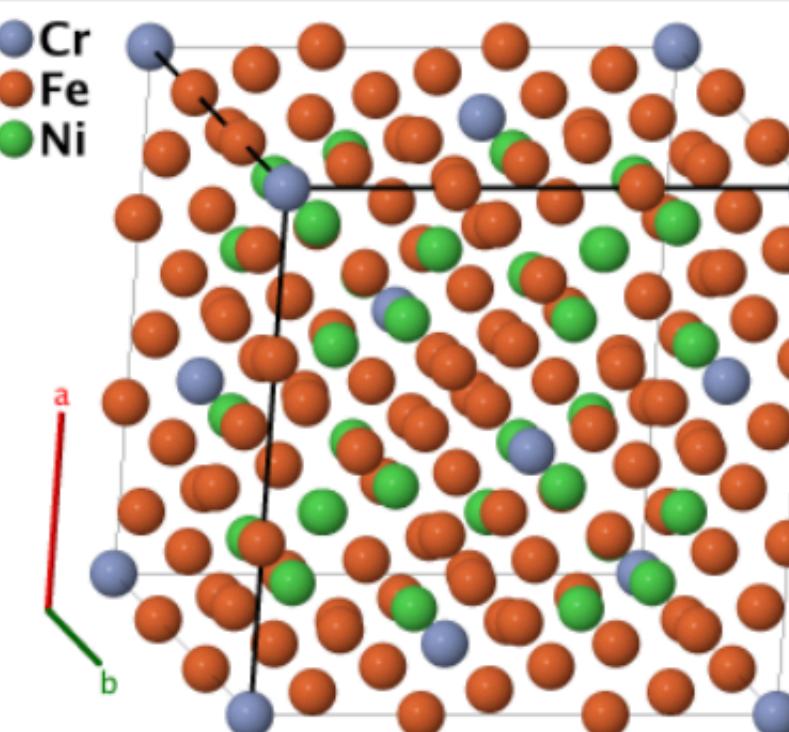
Ca<sub>7</sub>Ge Structure: A7B\_cF32\_225\_bd\_a



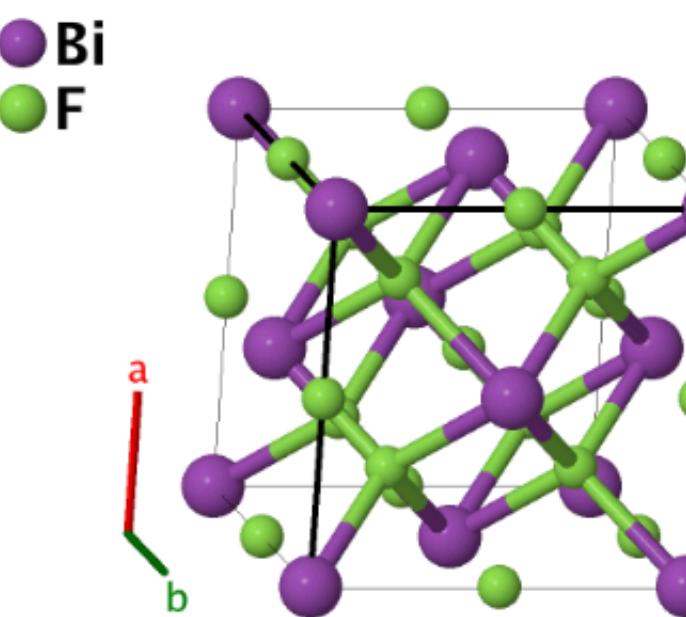
Face-Centered Cubic (Cu, A1, fcc) Structure: ...



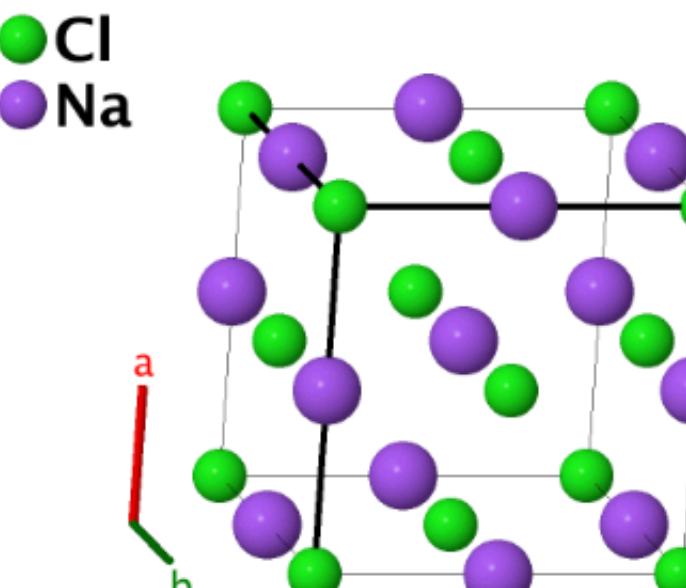
Model of Austenite Structure (cF108): AB18C...



BiF<sub>3</sub> ( $D0_3$ ) Structure: AB<sub>3</sub>\_cF16\_225\_a\_bc



Rock Salt (NaCl, B1) Structure: AB\_cF8\_225...



Prototype	:	NaCl
AFLOW prototype label	:	AB_cF8_225_a_b
Strukturbericht designation	:	B1
Pearson symbol	:	cF8
Space group number	:	225
Space group symbol	:	Fm $\bar{3}$ m
AFLOW prototype command	:	aflow --proto=AB_cF8_225_a_b --params=a

[View the structure from several different perspectives](#)

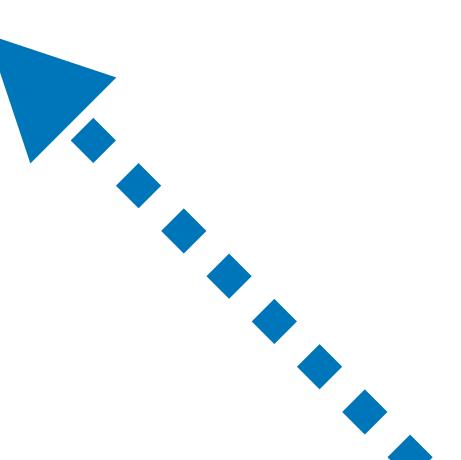
[View the primitive and conventional cell](#)

#### Other compounds with this structure

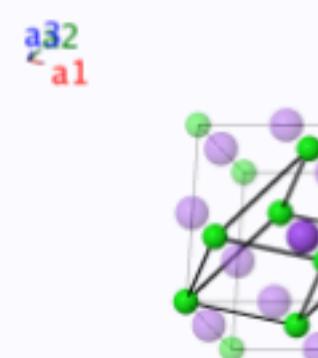
- AgCl, BaS, CaO, CeSe, DyAs, GdN, KBr, LaP, LiCl, LiF, MgO, NaBr, NaF, NiO, PrBi, PuC, RbF, ScN, SrO, TbTe, UC, YN, YbO, ZrO

#### Face-centered Cubic primitive vectors:

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	B
Ni	1	+2.00	4 a	0	0	0	1	1.46(9)
O	1	-2.00	4 b	0.5	0.5	0.5	1	1.3(1)



$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}\end{aligned}$$



#### Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$= 0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(4a)	Cl
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(4b)	Na

# Running Crystal on Pauli

```
/home/egull/software/crystal17_v1_0_2/bin/Linux-ifort14_XE_emt64/std/crystal < diamond.d12 > diamond.out
```

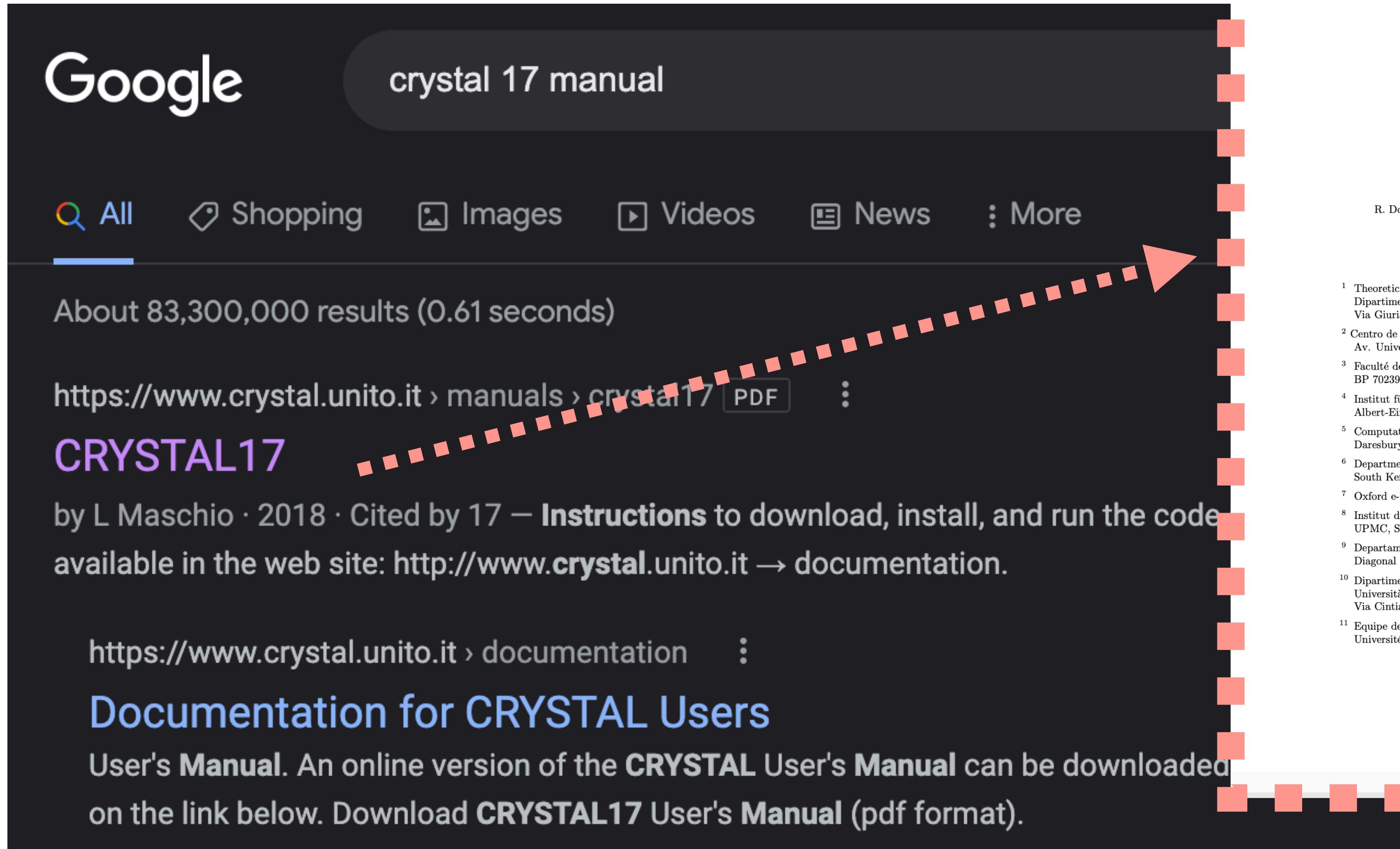
```
1 C - Diamond
2 CRYSTAL
3 0 0 0
4 227
5 3.567
6 1
7 6 0.125 0.125 0.125
8 BASISSET
9 CARBON
10 DFT
11 EXCHANGE
12 LDA
13 CORRELAT
14 VWN
15 XLGRID
16 END
17 TOLINTEG
18 8 8 8 8 16
19 SHRINK
20 8 8
21 FMIXING
22 30
23 NODIIS
```

**diamond.d12**

```
1 #BASIS
2 CARBON
3 6 5
4 0 0 6 2. 1.
5 4563.24000 0.196665000E-02
6 682.024000 0.152306000E-01
7 154.973000 0.761269000E-01
8 44.4553000 0.260801000
9 13.0290000 0.616462000
10 1.82773000 0.221006000
11 0 1 3 4. 1.
12 20.9642000 0.114660000 0.402487000E-01
13 4.80331000 0.919999000 0.237594000
14 1.45933000 -0.303068000E-02 0.815854000
15 0 1 1 0. 1.
16 0.483456000 1.000000000 1.000000000
17 0 1 1 0. 1.
18 0.185000 1.000000000 1.000000000
19 0 3 1 0. 1.
20 0.850000 1.000000000
21 99 0
```

**BASISSETS.DAT**

# Crystal User Manual



Google search results for "crystal 17 manual". The results page shows a dark-themed interface with a search bar containing "crystal 17 manual". Below the search bar are filters for "All", "Shopping", "Images", "Videos", "News", and "More". A message indicates "About 83,300,000 results (0.61 seconds)". The first result is a link to the CRYSTAL17 User's Manual PDF, which is titled "CRYSTAL17" and describes it as "by L Maschio · 2018 · Cited by 17 – Instructions to download, install, and run the code available in the web site: http://www.crystal.unito.it → documentation." The second result is a link to the Documentation for CRYSTAL Users, which also mentions the User's Manual PDF.

crystal 17 manual

All Shopping Images Videos News More

About 83,300,000 results (0.61 seconds)

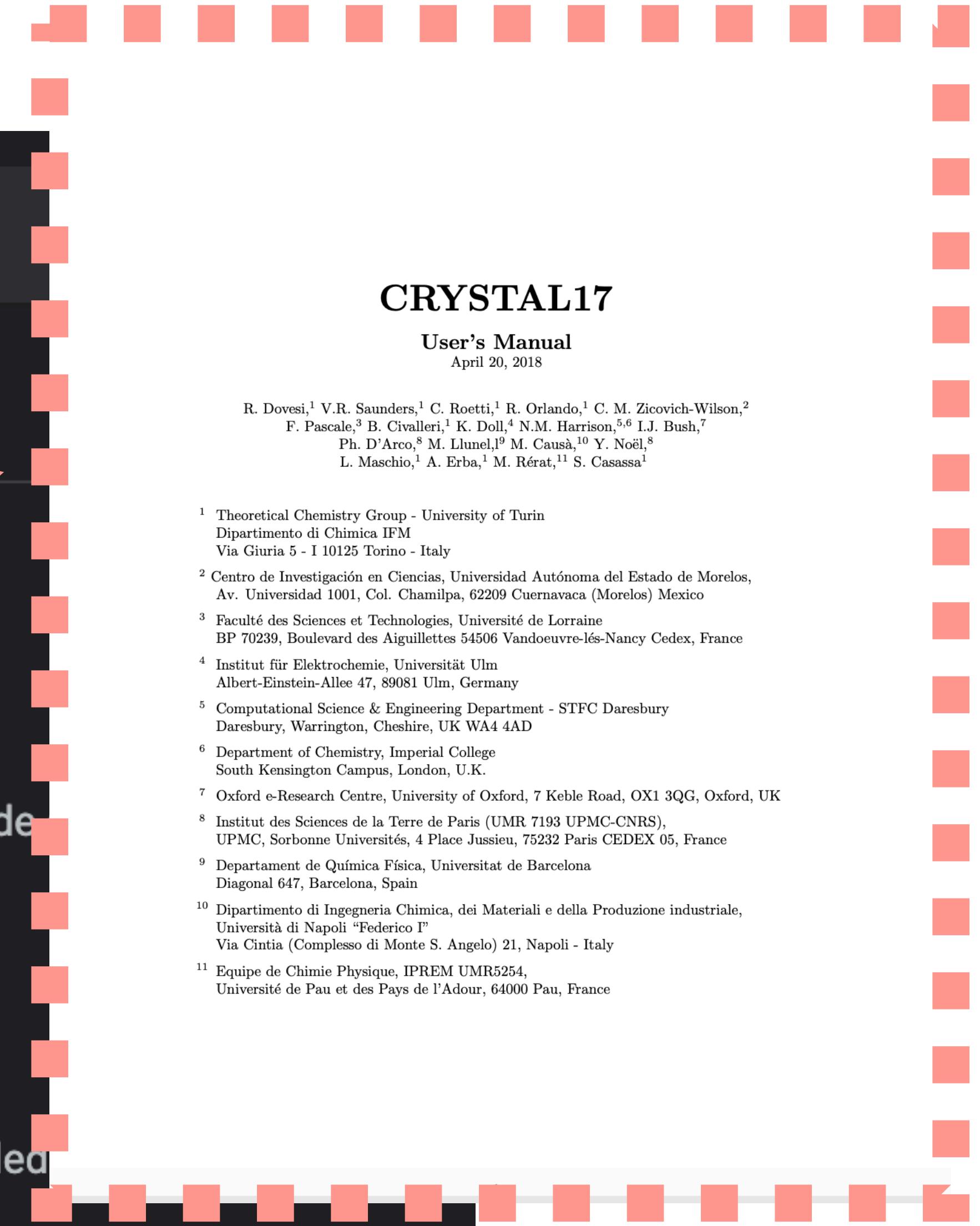
<https://www.crystal.unito.it › manuals › crystal17> PDF

CRYSTAL17  
by L Maschio · 2018 · Cited by 17 – Instructions to download, install, and run the code available in the web site: <http://www.crystal.unito.it> → documentation.

<https://www.crystal.unito.it › documentation>

Documentation for CRYSTAL Users

User's Manual. An online version of the CRYSTAL User's Manual can be downloaded on the link below. Download CRYSTAL17 User's Manual (pdf format).



# Running Crystal on Pauli

```
/home/egull/software/crystal17_v1_0_2/bin/Linux-ifort14_XE_emt64/std/crystal < diamond.d12 > diamond.out
```

```
1 C - Diamond
2 CRYSTAL
3 0 0 0
4 227
5 3.567
6 1
7 6 0.125 0.125 0.125
8 BASISSET
9 CARBON
10 DFT
11 EXCHANGE
12 LDA
13 CORRELAT
14 VWN
15 XLGRID
16 END
17 TOLINTEG
18 8 8 8 8 16
19 SHRINK
20 8 8
21 FMIXING
22 30
23 NODIIS
```

**diamond.d12**

```
1 #BASIS
2 CARBON
3 6 5
4 0 0 6 2. 1.
5 4563.24000 0.196665000E-02
6 682.024000 0.152306000E-01
7 154.973000 0.761269000E-01
8 44.4553000 0.260801000
9 13.0290000 0.616462000
10 1.82773000 0.221006000
11 0 1 3 4. 1.
12 20.9642000 0.114660000 0.402487000E-01
13 4.80331000 0.919999000 0.237594000
14 1.45933000 -0.303068000E-02 0.815854000
15 0 1 1 0. 1.
16 0.483456000 1.000000000 1.000000000
17 0 1 1 0. 1.
18 0.185000 1.000000000 1.000000000
19 0 3 1 0. 1.
20 0.850000 1.000000000
21 99 0
```

**BASISSETS.DAT**

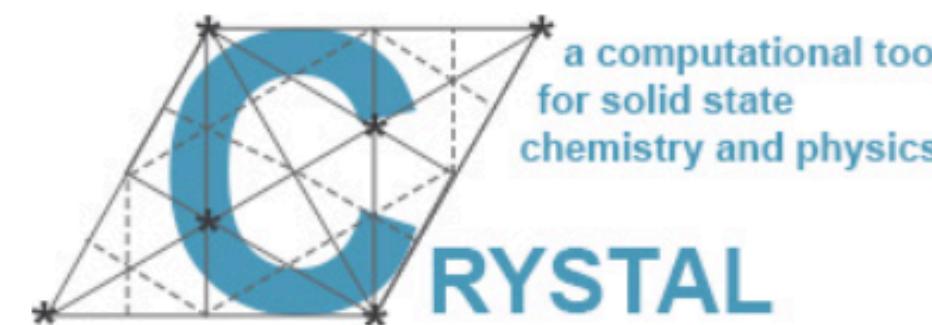
# Crystal Basis Set Format

```
#BASIS CARBON
6 5
0 0 6 2. 1.
1535.21000 0.19000000E-02
682.024000 0.152306000E-01
154.973000 0.761269000E-01
44.4553000 0.260801000
13.0290000 0.616462000
1.82773000 0.221006000
0 1 3 4. 1.
20.9642000 0.114660000
4.80331000 0.919999000
1.45933000 -0.303068000E-02
0 1 1 0. 1.
SP shell
0 1 1 0. 1.
0.185000 1.000000000
0 3 1 0. 1.
0.850000 1.000000000
99 0
```

0	0	6	2	1
---	---	---	---	---

- Yellow: type of basis set to be used
- Green: shell type.
  - 0: s, 1: sp, 2: p, 3: d, ...
- Cyan: number of Gaussian primitives in shell
- Pink: electron charge in shell
- Red: scale factor

# Crystal Basis Set Library



[Home](#) [News](#) [Events](#) [FAQ](#) [Contacts](#)

CRYSTAL - Basis Sets Library

**<https://www.crystal.unito.it/basis-sets.php>**

CRYSTAL

- Features
  - Theoretical background
  - How to cite
  - CRYSTAL User's Manual

CRYSPLOT

SOFTWARE

- How to get a copy
  - License fee
  - Platforms

DOCS & SETS

- Documentation
  - Encoded Packages
    - CRYSCOR  
(only CRYSTAL14)
    - TOPOND

The table is regularly updated. CRYSTAL users are kindly requested to supply new basis sets optimized for their research.

H																				He	
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				

Lanthanides	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Actinides	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

# CRYSTAL Geometry Examples

## List of CRYSTAL geometry input examples

SYSTEM	Features	Keywords	Input	Output	Tutorial
Covalent systems	Fullerene crystal	TESTGEOM	buck.d12	buck.out	Basic tutorials "Geometry"
Covalent systems	Fullerene crystal with inclusion of He atoms	TESTGEOM	buck_he.d12	buck_he.out	Basic tutorials "Geometry"
Covalent systems	Diamond crystal	TESTGEOM	diamond.d12	diamond.out	Basic tutorials "Geometry"
Covalent systems	Diamond - from 3D to 2D - (100) slab - 9 atomic	TESTGEOM	diam_100a.d12	diam_100a.out	Basic tutorials "Geometry"
Covalent systems	Diamond - from 3D to 2D - (100) slab - 10 atomic	TESTGEOM	diam_100b.d12	diam_100b.out	Basic tutorials "Geometry"
Covalent systems	Slab (2D) parallel to (100) plane - 9 atomic layers	TESTGEOM	diam_sl100a.d12	diam_sl100a.out	Basic tutorials "Geometry"
Covalent systems	Slab (2D) parallel to (100) plane - 10 atomic layers	TESTGEOM	diam_sl100b.d12	diam_sl100b.out	Basic tutorials "Geometry"
Covalent systems	Graphite crystal - hexagonal form	TESTGEOM	gra_hexa.d12	gra_hexa.out	Basic tutorials "Geometry"
Covalent systems	Graphite crystal - rhombohedral form	TESTGEOM	gra_rhom.d12	gra_rhom.out	Basic tutorials "Geometry"
Covalent systems	Graphite crystal - hexagonal form - from 3D to 2D - (001) monolayer	TESTGEOM	gra_h001.d12	gra_h001.out	Basic tutorials "Geometry"
Covalent systems	Graphite 2D monolayer	TESTGEOM	gra_ml.d12	gra_ml.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Alumina- hexagonal form	TESTGEOM	al2o3_h.d12	al2o3_h.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Alumina- rhombohedral form	TESTGEOM	al2o3_r.d12	al2o3_r.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Alumina- hexagonal form - (001) slab - 6 atomic layers	TESTGEOM	al2o3_001.d12	al2o3_001.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Alumina- hexagonal form - (110) slab - 10 atomic layers	TESTGEOM	al2o3_110.d12	al2o3_110.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Slab parallel to (001) plane - 6 atomic layers	TESTGEOM	al2o3_sl001.d12	al2o3_sl001.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Slab parallel to (110) plane - 10 atomic layers	TESTGEOM	al2o3_sl110.d12	al2o3_sl110.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk	TESTGEOM	mgo_bulk.d12	mgo_bulk.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk - use of ROTATE keyword - (100) plane	TESTGEOM	mgo_rot100.d12	mgo_rot100.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk - (100) slab - 3 atomic layers	TESTGEOM	mgo_100.d12	mgo_100.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk - (103) slab - 5 atomic layers	TESTGEOM	mgo_103.d12	mgo_103.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk - (110) slab - 3 atomic layers	TESTGEOM	mgo_110.d12	mgo_110.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	MgO bulk - (111) slab - 4 atomic layers starting from	TESTGEOM	mgo_111.d12	mgo_111.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Slab parallel to (110) plane - 2 atomic layers	TESTGEOM	mgo_sl110a.d12	mgo_sl110a.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Slab parallel to (110) plane - 3 atomic layers	TESTGEOM	mgo_sl110b.d12	mgo_sl110b.out	Basic tutorials "Geometry"
Ionic and semi-ionic systems	Step of MgO on a MgO (100) monolayer	TESTGEOM	mgo_100ad.d12	mgo_100ad.out	Basic tutorials "Geometry"

<http://tutorials.crystalsolutions.eu/tutorial.html?td=geometry&tf=list>

# ECP

1 BiVO<sub>3</sub> A-AFM  
2 CRYSTAL  
3 0 1 1  
4 221  
5 3.935  
6 5  
7 283 0.0 0.0 0.0  
8 23 0.5 0.5 0.5  
9 8 0.0 0.5 0.5  
10 8 0.5 0.0 0.5  
11 8 0.5 0.5 0.0  
12 SUPERCEL  
13 1. 0. 0.  
14 0. 1. 0.  
15 0. 0. 2.  
16 END

17 283 10

18 INPUT

19 23. 0 2 4 4 2 2  
20 13.043090 283.264227 0  
21 8.221682 62.471959 0  
22 10.467777 72.001499 0  
23 9.118901 144.002277 0  
24 6.754791 5.007945 0  
25 6.252592 9.991550 0  
26 8.081474 36.396259 0  
27 7.890595 54.597664 0  
28 4.955556 9.984294 0  
29 4.704559 14.981485 0  
30 4.214546 13.713383 0

31 4.133400 18.194308 0  
32 6.205709 -10.247443 0  
33 6.227782 12.055712 0  
34 0 0 4 2.0 1.  
35 39.591887390 0.024348865  
36 23.850320013 -0.199547887  
37 15.258171924 0.546090  
38 6.998651071 -0.874929634  
39 0 0 4 2.0 1.  
40 9.443573268 0.031000642  
41 5.880514498 -0.225962949  
42 1.836879895 0.908924  
43 0.965752700 0.501350163  
44 0 0 1 0.0 1.  
45 0.300010454 1.0  
46 0 0 1 0.0 1.  
47 0.108980371 1.0  
48 0 2 4 6.0 1.  
49 10.735903661 -0.058659373  
50 7.471032027 0.139083  
51 2.093017780 -0.196743961  
52 0.953500458 -0.153805526  
53 0 2 1 3.0 1.  
54 0.258082627 1.0  
55 0 2 1 0.0 1.  
56 0.078070203 1.0  
57 0 3 4 10.0 1.  
58 16.646819570 0.007825015  
59 7.017131289 -0.068321586  
60 2.349573912 0.339864061  
61 1 143638506 0 485831

# Running Crystal on Pauli

```
/home/egull/software/crystal17_v1_0_2/bin/Linux-ifort14_XE_emt64/std/crystal < diamond.d12 > diamond.out
```

```
1 C - Diamond
2 CRYSTAL
3 0 0 0
4 227
5 3.567
6 1
7 6 0.125 0.125 0.125
8 BASISSET
9 CARBON
10 DFT
11 EXCHANGE
12 LDA
13 CORRELAT
14 VWN
15 XLGRID
```

**diamond.d12**

```
16 END
17 TOLINTEG
18 8 8 8 8 16
19 SHRINK
20 8 8
21 FMIXING
22 30
23 NODIIS
```

```
1 #BASIS
2 CARBON
3 6 5
4 0 0 6 2. 1.
5 4563.24000 0.196665000E-02
6 682.024000 0.152306000E-01
7 154.973000 0.761269000E-01
8 44.4553000 0.260801000
9 13.0290000 0.616462000
10 1.82773000 0.221006000
11 0 1 3 4. 1.
12 20.9642000 0.114660000 0.402487000E-01
13 4.80331000 0.919999000 0.237594000
14 1.45933000 -0.303068000E-02 0.815854000
15 0 1 1 0. 1.
16 0.483456000 1.000000000 1.000000000
17 0 1 1 0. 1.
18 0.185000 1.000000000 1.000000000
19 0 3 1 0. 1.
20 0.850000 1.000000000
21 99 0
```

**BASISSETS.DAT**

# SCF Convergence Tools

## SCF Convergence Tools

L. Maschio

### Summary

- Introduction
- First thing to check: the starting geometry and atomic charges
- A first case study: the diamond crystal using a cc-pVDZ basis set
- A second case study: single-walled carbon nanotube
- The DIIS convergence accelerator
- Summary

### Introduction

A proper convergence of the Hartree-Fock or DFT Self-Consistent Field (SCF) iterations is by far the most important aspect of any quantum chemistry program, as it conveys the system's total energy and wavefunction and is the starting point for the calculation of any property. While in most cases such convergence is achieved in a few cycles, a number of critical situations exist. Such ill-behaved calculations can experience an excessively high number of SCF cycles, convergence to a wrong result or could even not be able to reach a final convergence.

Such critical convergence can be specially experienced in the case of:

- Presence of diffuse functions in the basis set for a densely packed system
- Open-shell systems containing transition metal atoms with partly filled d- or f- orbitals
- Metallic systems

Several tools are available in the CRYSTAL code to the user who wants to improve convergence in the SCF

- Fock mixing (damping) percentage
- Shifting of virtual levels
- Spin Locking and single level shifting for open-shell systems
- Tuning of direct space integral thresholds
- Tuning of reciprocal space sampling mesh
- Convergence Accelerators (DIIS, Broyden, Anderson).

In the following we will see examples on how some of these tools can be used in connection with specific causes for convergence problems. Away from the claim to be comprehensive of the (very many) situations that can happen in "real life" problems, we will focus on two systems, a 3D diamond crystal and a 1D carbon nanotube, to highlight some of the most common convergence problems.

More advanced tools to help convergence in open-shell and spin polarized cases (magnetic systems, metallic systems) are discussed in the respective tutorials.

### First thing to check: the starting geometry and atomic charges

As trivial as it may seem, the most general and widespread causes of convergence issues are user mistakes in the input. If you see your SCF is not converging, as a first check we suggest to :

- Check carefully the crystal geometry, specially if in the input some geometry manipulation is performed.
- Think about the chemistry of your system, and adapt atomic charges in input to resemble the expected final charges of the individual ions

### A first case study: the diamond crystal using a cc-pVDZ basis set

Since any crystal is an infinite system, integral screenings must be adopted in order to truncate direct space summations to a finite value.

Too severe truncations, although making the calculation faster, can however lead to a number of numerical inaccuracies and issues, such as non-idempotency of the density matrix and non-convergence of the Fourier series.

The practical effect of the above occurrence is the appearance of unphysical states in the solution. If the numerical inaccuracies are small, such states lie in the virtual manifold and never enter the density matrix, hence the ground state solution. But when they do, they have negative effects on the SCF procedures, even leading to convergence at a wrong state or causing huge oscillations in energy from one cycle to another.

Let us consider this case of a simple diamond crystal ([diamond.pbe.1.d12](#)) with a cc-pVDZ basis set and PBE functional. Diamond is usually a simple system as regards SCF convergence, but the use of such a molecular

# Supercell and Spin

```
1 BiVO3 A-AFM
2 CRYSTAL
3 0 1 1
4 221
5 3.935
6 5
7 283  0.0 0.0 0.0
8 23   0.5 0.5 0.5
9 8    0.0 0.5 0.5
10 8   0.5 0.0 0.5
11 8   0.5 0.5 0.0
12 SUPERCEL
13 1. 0. 0.
14 0. 1. 0.
15 0. 0. 2.
16 END
128 DFT
129 SPIN
130 PBE0
131 XLGRID
132 END
133 TOLINTEG
134 7 7 7 7 14
135 SHRINK
136 8 8
137 LEVSHIFT
138 3 1
139 MAXCYCLE
140 300
141 SPINLOCK
142 0 15
143 ATOMSPIN
144 2
145 1 1 2 -1
146 END
```

## How to run CRYSTAL17

# Run CRYSTAL17

- Download the executables: [full license \(serial and parallel versions\)](#) (max 10000 atoms/cell)/ [demo license \(serial version\)](#) (max 10 atoms/cell)
- Download the [scripts](#) to run the programs
- Download the graphical package [Crgra2006](#) (check your postscript viewer)  
Alternatively, use [CRYSPLOT](#) the new web-based graphical interface to plot computed properties
- Install the package following the [instructions](#)

The CRYSTAL package consists of 2 programs:

- *crystal* compute wave function - optimize geometry, if requested
- *properties* compute one electron properties

Two scripts are supplied to control the execution:

- *runcry17* compute wave function (and properties, if input data exist)
- *runprop17* wave function analysis and one electron properties

For visualizing full information on usage modes, type the script name without parameters.

File name extension are interpreted by the scripts according to the following rules:

.d12	wave function calculation input (program <i>crystal</i> )
.out	wf calculation printed output file (it may be modified by setting environment variable \$OUTFILE)
.d3	properties calculation input (program <i>properties</i> )
.outp	properties calculation output file (it may be modified by setting environment variable)
.ps	postscript file - written by one of the programs of the package <a href="#">Crgra2006</a>
.maps	maps06 control file (see <a href="#">Crgra2006</a> )
.band	band06 control file (see <a href="#">Crgra2006</a> )
.doss	doss06 control file (see <a href="#">Crgra2006</a> )

# Band Structure Calculation

The screenshot shows a research article from the journal "Computational Materials Science". The title of the article is "High-throughput electronic band structure calculations: Challenges and tools". The authors listed are Wahyu Setyawan <sup>a</sup>, Stefano Curtarolo <sup>a, b</sup>. The article was published in Volume 49, Issue 2, August 2010, Pages 299-312. The Elsevier logo is visible at the top left. Below the article summary, there are links to "Add to Mendeley", "Share", and "Cite", along with the DOI link: <https://doi.org/10.1016/j.commatsci.2010.05.010>.

<https://doi.org/10.1016/j.commatsci.2010.05.010>

## Appendix:

### A.2. Face-centered cubic (FCC, cF)

(See Fig. 2 and Table 3.)

Conventional lattice

$$\mathbf{a}_1 = (a, 0, 0)$$

$$\mathbf{a}_2 = (0, a, 0)$$

$$\mathbf{a}_3 = (0, 0, a)$$

Primitive lattice

$$\mathbf{a}_1 = (0, a/2, a/2)$$

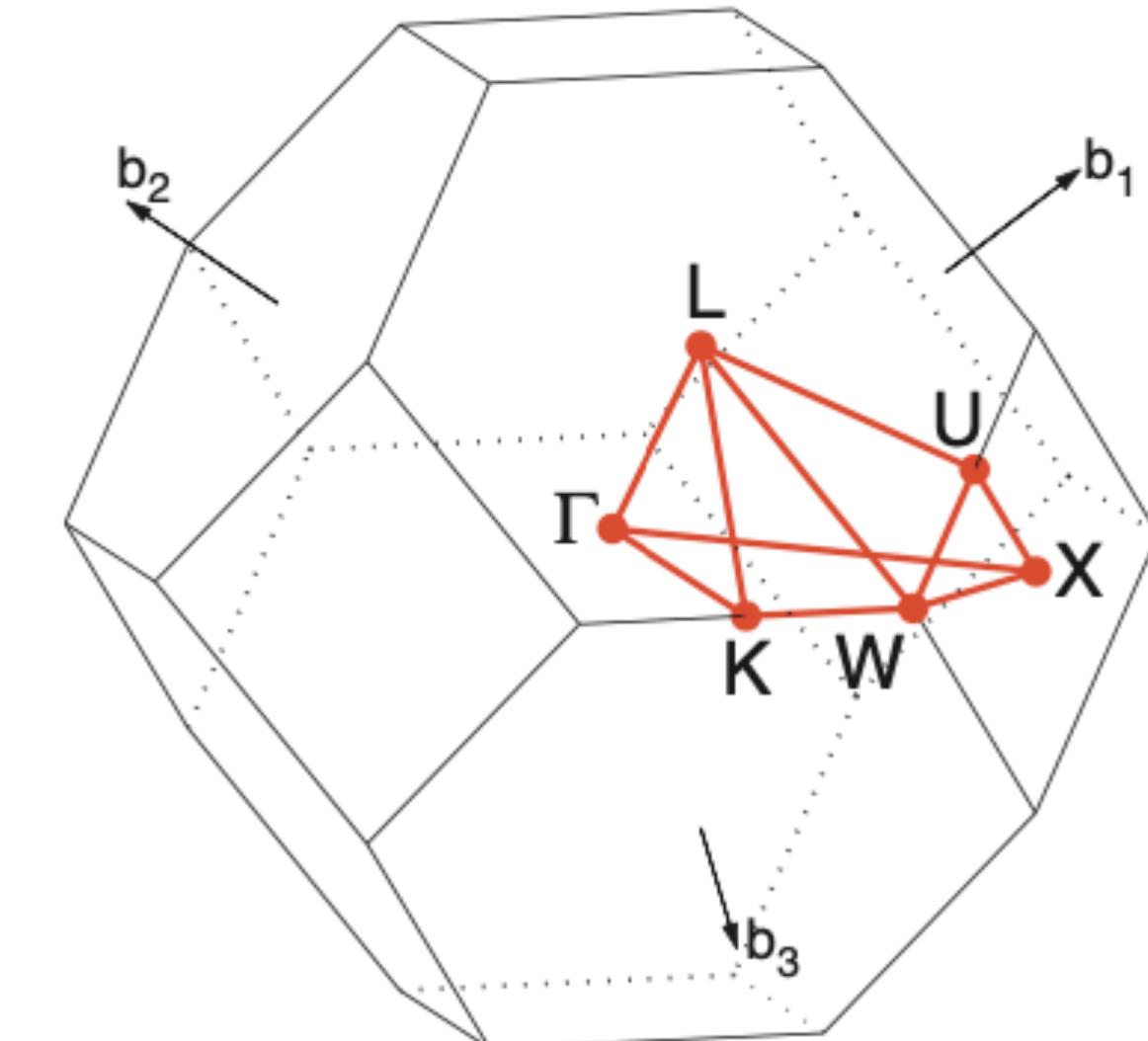
$$\mathbf{a}_2 = (a/2, 0, a/2)$$

$$\mathbf{a}_3 = (a/2, a/2, 0)$$

**Table 2**

Symmetry  $\mathbf{k}$ -points of CUB lattice.

$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$	$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$
0 1/2	0 1/2	0 0	$\Gamma$ $M$	1/2 0	1/2 1/2 0 $R$ $X$



**Fig. 2.** Brillouin zone of FCC lattice. Path:  $\Gamma$ -X-W-K- $\Gamma$ -L-U-W-L-K|U-X. An example of band structure using this path is given in Fig. 27.

# Crystal Structure Data:

## Pearson Symbol

Prototype	:	NaCl
AFLOW prototype label	:	AB_cF8_225_a_b
Strukturbericht designation	:	B1
Pearson symbol	:	cF8
Space group number	:	225
Space group symbol	:	Fm $\bar{3}m$
AFLOW prototype command	:	aflow --proto=AB_cF8_225_a_b --params=a

[View the structure from several different perspectives](#)

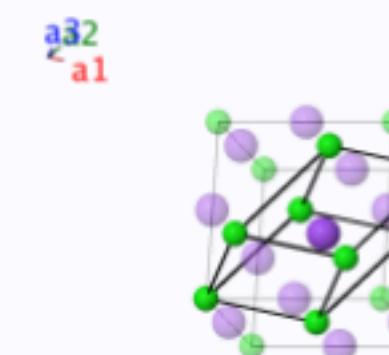
[View the primitive and conventional cell](#)

### Other compounds with this structure

- AgCl, BaS, CaO, CeSe, DyAs, GdN, KBr, LaP, LiCl, LiF, MgO, NaBr, NaF, NiO, PrBi, PuC, RbF, ScN, SrO, TbTe, UC, YN, YbO, ZrO

### Face-centered Cubic primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}\end{aligned}$$



### Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$= 0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(4a)	Cl
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(4b)	Na

# Band Structure Calculation

The screenshot shows a research article from the journal "Computational Materials Science". The title of the article is "High-throughput electronic band structure calculations: Challenges and tools". The authors listed are Wahyu Setyawan <sup>a</sup>, Stefano Curtarolo <sup>a, b</sup>. The article was published in Volume 49, Issue 2, August 2010, Pages 299-312. The article is freely available at <https://doi.org/10.1016/j.commatsci.2010.05.010>.

## Appendix:

### A.2. Face-centered cubic (FCC, cF)

(See Fig. 2 and Table 3.)

Conventional lattice

$$\mathbf{a}_1 = (a, 0, 0)$$

$$\mathbf{a}_2 = (0, a, 0)$$

$$\mathbf{a}_3 = (0, 0, a)$$

Primitive lattice

$$\mathbf{a}_1 = (0, a/2, a/2)$$

$$\mathbf{a}_2 = (a/2, 0, a/2)$$

$$\mathbf{a}_3 = (a/2, a/2, 0)$$

Symmetry  $\mathbf{k}$ -points of CUB lattice.

$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$	$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$
0	0	0	$\Gamma$	1/2	1/2
1/2	1/2	0	$M$	0	1/2

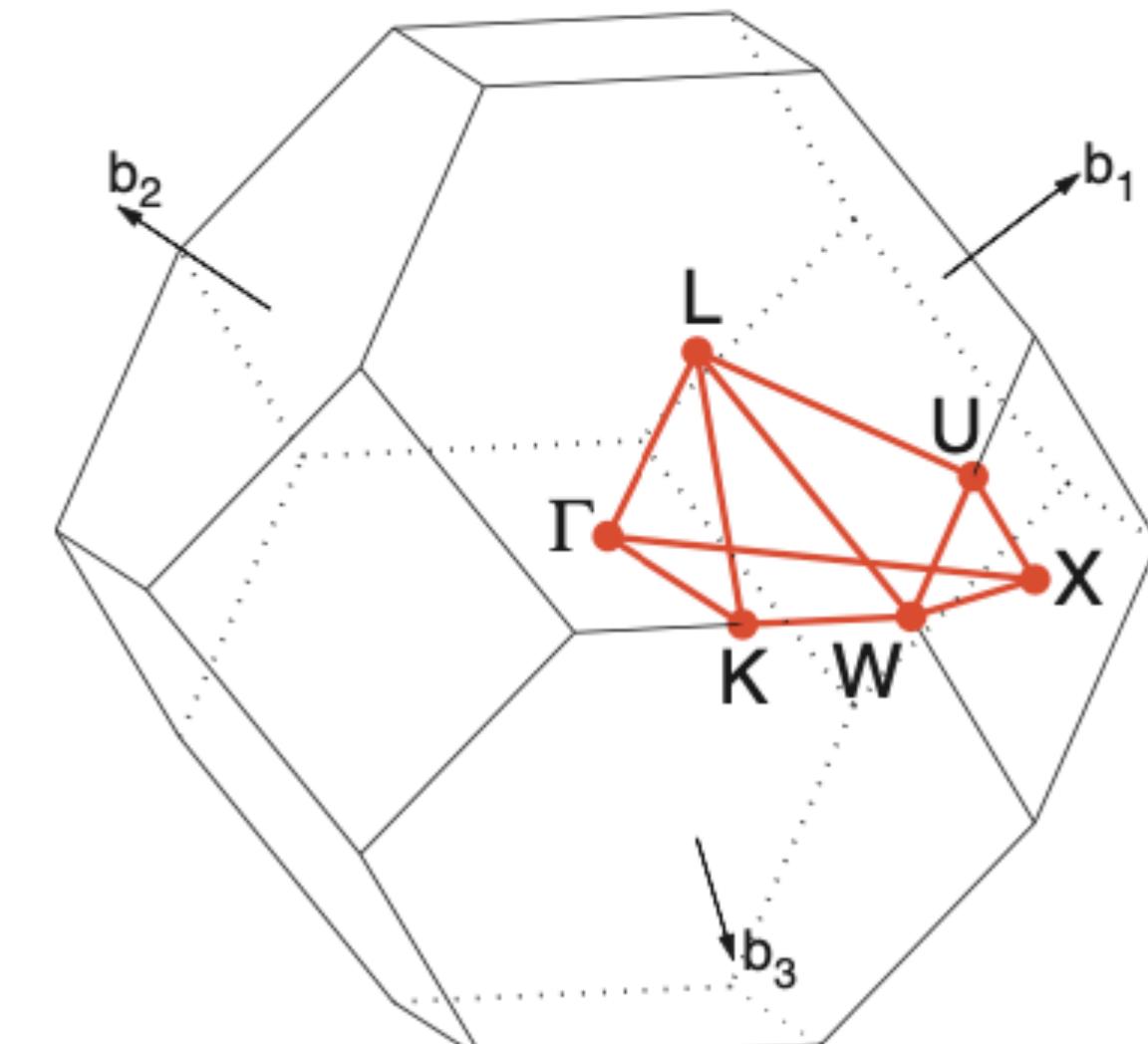


Fig. 2. Brillouin zone of FCC lattice. Path:  $\Gamma-X-W-K-\Gamma-L-U-W-L-K|\bar{U}-X$ . An example of band structure using this path is given in Fig. 27.

# Crystal Input File Example: BN

```
/home/egull/software/crystal17_v1_0_2/bin/Linux-ifort14_XE_emt64/std/properties < bn.band.d3 > bn.band.out
```

Prototype	:	BN
AFLOW prototype label	:	AB_hP4_194_c_d
Strukturbericht designation	:	B <sub>4</sub>
Pearson symbol	:	hp4
Space group number	:	194
Space group symbol	:	P6 <sub>3</sub> /mmc
AFLOW prototype command	:	aflow --proto=AB_--params=a,c/a

## A.10. Hexagonal (HEX, hP)

Lattice (see Fig. 13 and Table 13)

$$\mathbf{a}_1 = \left( a/2, -\left(a\sqrt{3}\right)/2, 0 \right)$$

$$\mathbf{a}_2 = \left( a/2, \left(a\sqrt{3}\right)/2, 0 \right)$$

$$\mathbf{a}_3 = (0, 0, c)$$

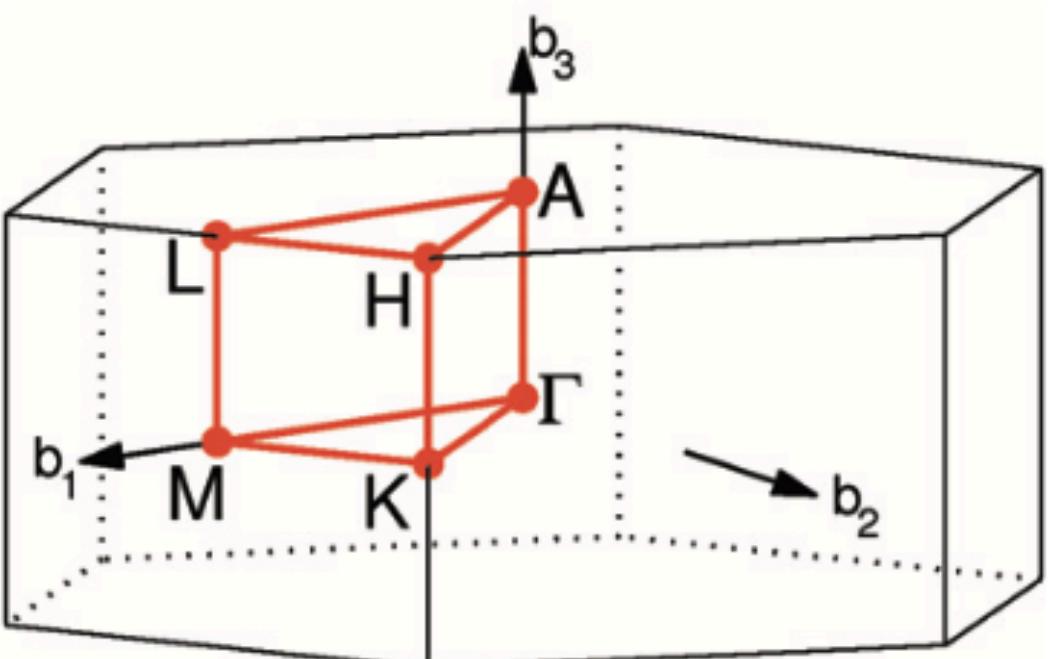


Fig. 13. Brillouin zone of HEX lattice. Path:  $\Gamma$ -M-K- $\Gamma$ -A-L-H-A|L-M|K-H. An example of band structure using this path is given in Fig. 28.

Table 13  
Symmetry k-points of HEX

$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$	$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$
0	0	0	$\Gamma$	1/3	1/3
0	0	1/2	A	1/2	0
1/3	1/3	1/2	H	1/2	0

```

1      NEWK
2      8   8
3      1   0
4      BAND
5      bn
6      7   12  150  1   20  1   0
7      0   0   0     6   0   0     G   M
8      6   0   0     4   4   0     M   K
9      4   4   0     0   0   0     K   G
10     0   0   0     0   0   6     G   A
11     0   0   6     6   0   6     A   L
12     6   0   6     4   4   6     L   H
13     4   4   6     0   0   6     H   A
14
15      END
      END

```

# Plot Generation

```
BAND.DAT
1 # NKPT      150 NBND      20 NSPIN      1
2 # NPANEL     3
3 #      1   A
4 #      56  A
5 #     119 A
6 #     150 A
```

```
20 @ XAXIS TICK SPEC
21 @ XAXIS TICK      0,
22 @ XAXIS TICKLABEL
23 @ XAXIS TICK      1,
24 @ XAXIS TICKLABEL
25 @ XAXIS TICK      2,
26 @ XAXIS TICKLABEL
27 @ XAXIS TICK      3,
28 @ XAXIS TICKLABEL
```

4	0.00000
0,"A	"
0.76663	
1,"A	"
1.65186	
2,"A	"
2.09447	
3,"A	"

# Plot Generation

## ‘BAND.DAT’

30	@VIEW	0.00000E+00	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.51876E+00	-0.51570E+00	-0.32630E+00	-0.32453E+00	-0.15597E+00	-0.15392E+00	-0.54071E-01	-0.16772E-01	0.17600E+00	0.20996E+00	0.37828E+00	0.38533E+00	0.65129E+00	0.68021E+00	0.79761E+00	0.79806E+00
31	0.13939E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.51899E+00	-0.51586E+00	-0.32603E+00	-0.32423E+00	-0.15591E+00	-0.15386E+00	-0.54418E-01	-0.16933E-01	0.17633E+00	0.21030E+00	0.37828E+00	0.38536E+00	0.65117E+00	0.68005E+00	0.79713E+00	0.79762E+00	
32	0.27877E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.51966E+00	-0.51633E+00	-0.32520E+00	-0.32334E+00	-0.15571E+00	-0.15367E+00	-0.55447E-01	-0.17419E-01	0.17732E+00	0.21133E+00	0.37831E+00	0.38547E+00	0.65082E+00	0.67957E+00	0.79573E+00	0.79631E+00	
33	0.41816E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.52075E+00	-0.51713E+00	-0.32383E+00	-0.32188E+00	-0.15540E+00	-0.15336E+00	-0.57124E-01	-0.18237E-01	0.17896E+00	0.21302E+00	0.37835E+00	0.38565E+00	0.65021E+00	0.67877E+00	0.79341E+00	0.79412E+00	
34	0.55755E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.52222E+00	-0.51824E+00	-0.32193E+00	-0.31987E+00	-0.15495E+00	-0.15291E+00	-0.59398E-01	-0.19394E-01	0.18124E+00	0.21534E+00	0.37842E+00	0.38590E+00	0.64936E+00	0.67766E+00	0.79023E+00	0.79108E+00	
35	0.69694E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.52404E+00	-0.51967E+00	-0.31952E+00	-0.31733E+00	-0.15438E+00	-0.15235E+00	-0.62207E-01	-0.20895E-01	0.18414E+00	0.21825E+00	0.37852E+00	0.38621E+00	0.64824E+00	0.67623E+00	0.78623E+00	0.78722E+00	
36	0.83632E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.52617E+00	-0.52139E+00	-0.31661E+00	-0.31431E+00	-0.15369E+00	-0.15166E+00	-0.65484E-01	-0.22736E-01	0.18762E+00	0.22170E+00	0.37866E+00	0.38657E+00	0.64683E+00	0.67449E+00	0.78144E+00	0.78258E+00	
37	0.97571E-01	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.52857E+00	-0.52337E+00	-0.31324E+00	-0.31083E+00	-0.15287E+00	-0.15084E+00	-0.69164E-01	-0.24909E-01	0.19166E+00	0.22565E+00	0.37884E+00	0.38699E+00	0.64514E+00	0.67245E+00	0.77592E+00	0.77722E+00	
38	0.11151E+00	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.53121E+00	-0.52561E+00	-0.30944E+00	-0.30693E+00	-0.15193E+00	-0.14991E+00	-0.73184E-01	-0.27396E-01	0.19623E+00	0.23005E+00	0.37907E+00	0.38747E+00	0.64314E+00	0.67011E+00	0.76974E+00	0.77118E+00	
39	0.12545E+00	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.53406E+00	-0.52806E+00	-0.30523E+00	-0.30264E+00	-0.15086E+00	-0.14885E+00	-0.77486E-01	-0.30173E-01	0.20127E+00	0.23485E+00	0.37935E+00	0.38799E+00	0.64083E+00	0.66749E+00	0.76293E+00	0.76451E+00	
40	0.13939E+00	-0.13630E+02	-0.62437E+01	-0.62437E+01	-0.53707E+00	-0.53070E+00	-0.30066E+00	-0.29800E+00	-0.14968E+00	-0.14767E+00	-0.82017E-01	-0.33213E-01	0.20676E+00	0.24000E+00	0.37970E+00	0.38856E+00	0.63820E+00	0.66459E+00	0.75557E+00	0.75729E+00	
41	0.15333E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.54023E+00	-0.53350E+00	-0.29574E+00	-0.29303E+00	-0.14837E+00	-0.14637E+00	-0.86732E-01	-0.36485E-01	0.21265E+00	0.24547E+00	0.38011E+00	0.38917E+00	0.63524E+00	0.66144E+00	0.74771E+00	0.74956E+00	
42	0.16726E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.54351E+00	-0.53644E+00	-0.29051E+00	-0.28776E+00	-0.14695E+00	-0.14496E+00	-0.91588E-01	-0.39958E-01	0.21889E+00	0.25120E+00	0.38058E+00	0.38983E+00	0.63197E+00	0.65803E+00	0.73941E+00	0.74138E+00	
43	0.18120E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.54688E+00	-0.53948E+00	-0.28499E+00	-0.28223E+00	-0.14541E+00	-0.14343E+00	-0.96551E-01	-0.43601E-01	0.22546E+00	0.25716E+00	0.38112E+00	0.39054E+00	0.62838E+00	0.65440E+00	0.73072E+00	0.73280E+00	
44	0.19514E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.55031E+00	-0.54261E+00	-0.27922E+00	-0.27645E+00	-0.14376E+00	-0.14179E+00	-0.10159E+00	-0.47384E-01	0.23231E+00	0.26332E+00	0.38173E+00	0.39128E+00	0.62448E+00	0.65054E+00	0.72168E+00	0.72388E+00	
45	0.20908E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.55380E+00	-0.54581E+00	-0.27322E+00	-0.27045E+00	-0.14200E+00	-0.14004E+00	-0.10667E+00	-0.51279E-01	0.23940E+00	0.26964E+00	0.38242E+00	0.39207E+00	0.62028E+00	0.64649E+00	0.71236E+00	0.71466E+00	
46	0.22302E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.55731E+00	-0.54906E+00	-0.26701E+00	-0.26426E+00	-0.14014E+00	-0.13819E+00	-0.11178E+00	-0.55259E-01	0.24672E+00	0.27610E+00	0.38317E+00	0.39290E+00	0.61581E+00	0.64224E+00	0.70279E+00	0.70518E+00	
47	0.23696E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.56084E+00	-0.55233E+00	-0.26061E+00	-0.25789E+00	-0.13816E+00	-0.13622E+00	-0.11689E+00	-0.59301E-01	0.25421E+00	0.28267E+00	0.38400E+00	0.39377E+00	0.61107E+00	0.63781E+00	0.69301E+00	0.69550E+00	
48	0.25090E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.56437E+00	-0.55562E+00	-0.25404E+00	-0.25135E+00	-0.13609E+00	-0.13416E+00	-0.12198E+00	-0.63383E-01	0.26186E+00	0.28933E+00	0.38490E+00	0.39468E+00	0.60609E+00	0.63322E+00	0.68307E+00	0.68564E+00	
49	0.26484E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.56789E+00	-0.55891E+00	-0.24732E+00	-0.24468E+00	-0.13391E+00	-0.13200E+00	-0.12704E+00	-0.67485E-01	0.26963E+00	0.29604E+00	0.38587E+00	0.39563E+00	0.60090E+00	0.62848E+00	0.67300E+00	0.67565E+00	
50	0.27877E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.57139E+00	-0.56218E+00	-0.24047E+00	-0.23788E+00	-0.13205E+00	-0.13165E+00	-0.12975E+00	-0.71590E-01	0.27751E+00	0.30279E+00	0.38691E+00	0.39662E+00	0.59550E+00	0.62360E+00	0.66284E+00	0.66556E+00	
51	0.29271E+00	-0.13630E+02	-0.62438E+01	-0.62438E+01	-0.57485E+00	-0.56544E+00	-0.23351E+00	-0.23098E+00	-0.13700E+00	-0.12740E+00	-0.12740E+00	-0.75681E-01</									

# Plot Generation

## ‘BAND.DAT’

<http://crysplot.crystalsolutions.eu/#>

The screenshot shows the CRYSPLOT website. At the top, there is a navigation bar with links for "What is", "Sample files", "Documentation", and "Contacts". A red box highlights the "Make a plot" button. Below the navigation bar is a large banner with the CRYSPLOT logo and a blue background featuring a wavy pattern. The banner text reads: "CRYSPLOT" and "A modern and easy to use visualization environment for plotting properties of crystalline solids as computed by means of the CRYSTAL code." A "Learn more!" button is located in the bottom left corner of the banner. Below the banner, there are three main sections: "What is CRYSPLOT?", "Why use CRYSPLOT?", and "How CRYSPLOT is made?". Each section contains a brief description of its purpose.

**CRYSPLOT**

A modern and easy to use visualization environment for plotting properties of crystalline solids as computed by means of the CRYSTAL code.

Learn more!

**What is CRYSPLOT?**

CRYSPLOT is an online web-oriented tool to visualize computed properties of periodic systems. It is targeted for plotting properties of crystalline solids computed with CRYSTAL code and in particular, one can represent band structure and density of states, among many others.

**Why use CRYSPLOT?**

CRYSPLOT is a modern and flexible online tool that make CRYSTAL more users friendly. CRYSPLOT is also totally free and easy to use. It permits the modification and customization of plots to meet the standards required for scientific graphics.

**How CRYSPLOT is made?**

CRYSPLOT has been designed with advanced and freely available graphical javascript libraries, namely: [Plotly](#). CRYSPLOT allows users to read information from CRYSTAL output files and automatically generate charts for a given property.

# Plot Generation

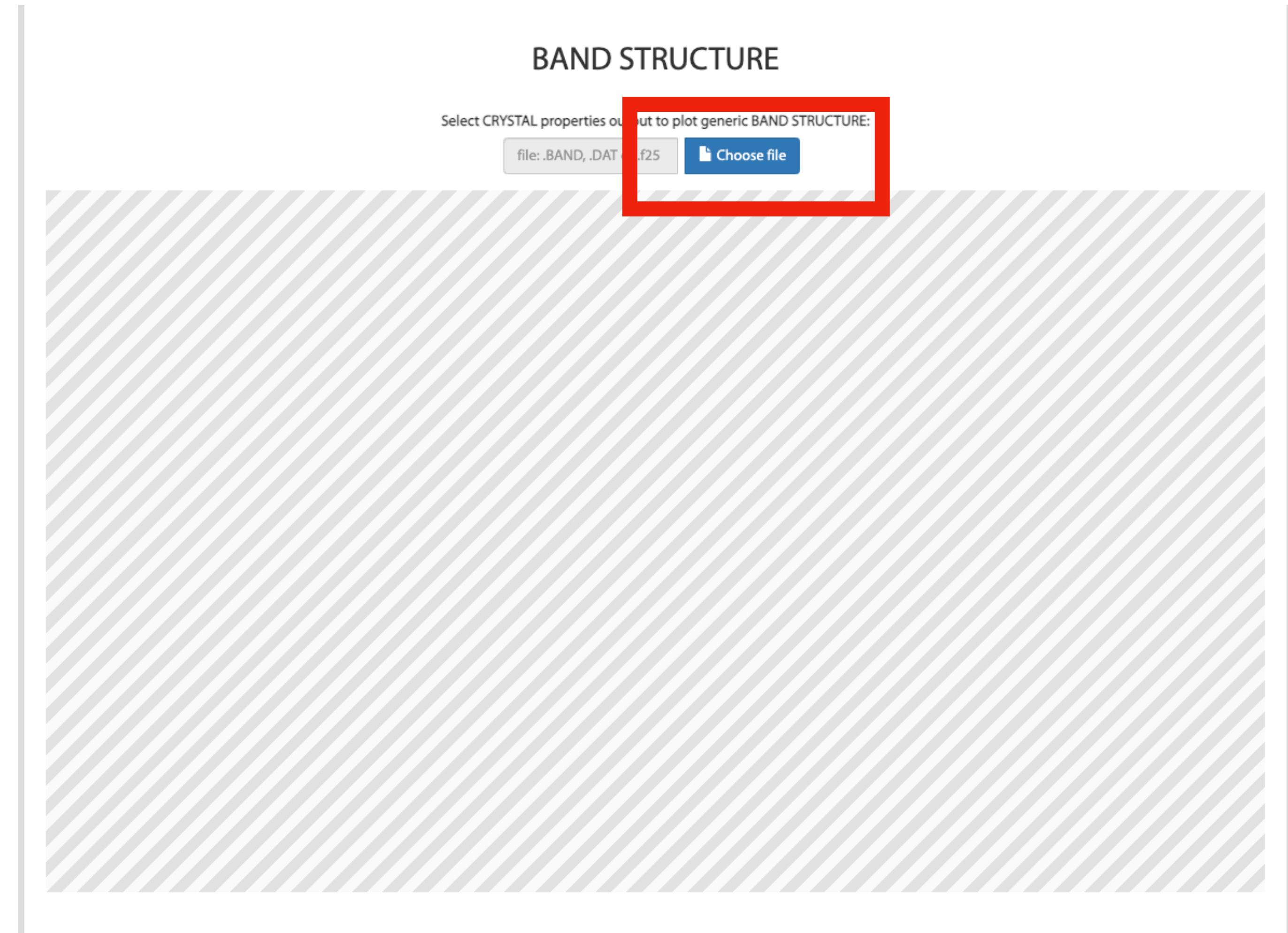
## ‘BAND.DAT’

The screenshot shows the Crysplot software interface. At the top right, there is a logo for "CRYSPLOT" and a blue button labeled "Make a plot ▾". The main menu is organized into several categories:

- Band structure** (highlighted with a red box):
  - Band structure plot
- Density of states**:
  - Density of states plot
  - Crystal orbital overlap population
  - Crystal orbital Hamiltonian population
- Unified plot of band structure and density of states**
- Vibrational spectra & animations**
- Electron charge density and Electrostatic potential**:
  - Electrostatic potential map
  - Electron charge density map
  - Difference map from a single file
  - Difference map from multiple files
  - Electron charge density profile
- Electron momentum density**:
  - Compton profiles
  - Autocorrelation function
- Elastic properties**
- Vibrational spectra**:
  - Infrared spectra
  - Infrared spectra comparison
  - Raman spectra
  - Raman spectra comparison
  - Raman and infrared spectra
  - Reflectance spectra
  - Complex dielectric function
- Phonon dispersion**:
  - Phonon band structure
  - Phonon density of states
- Volumetric data**
- Transport properties**:
  - Electron conductivity
  - Seebeck coefficient
  - Electron thermal conductivity
  - Seebeck  $\sigma$
- TOPOND**:
  - Topological analysis map
  - Topological analysis difference map
- Geometry optimization**
- Geometry structure**
- Pair correlation function**

# Plot Generation

## ‘BAND.DAT’



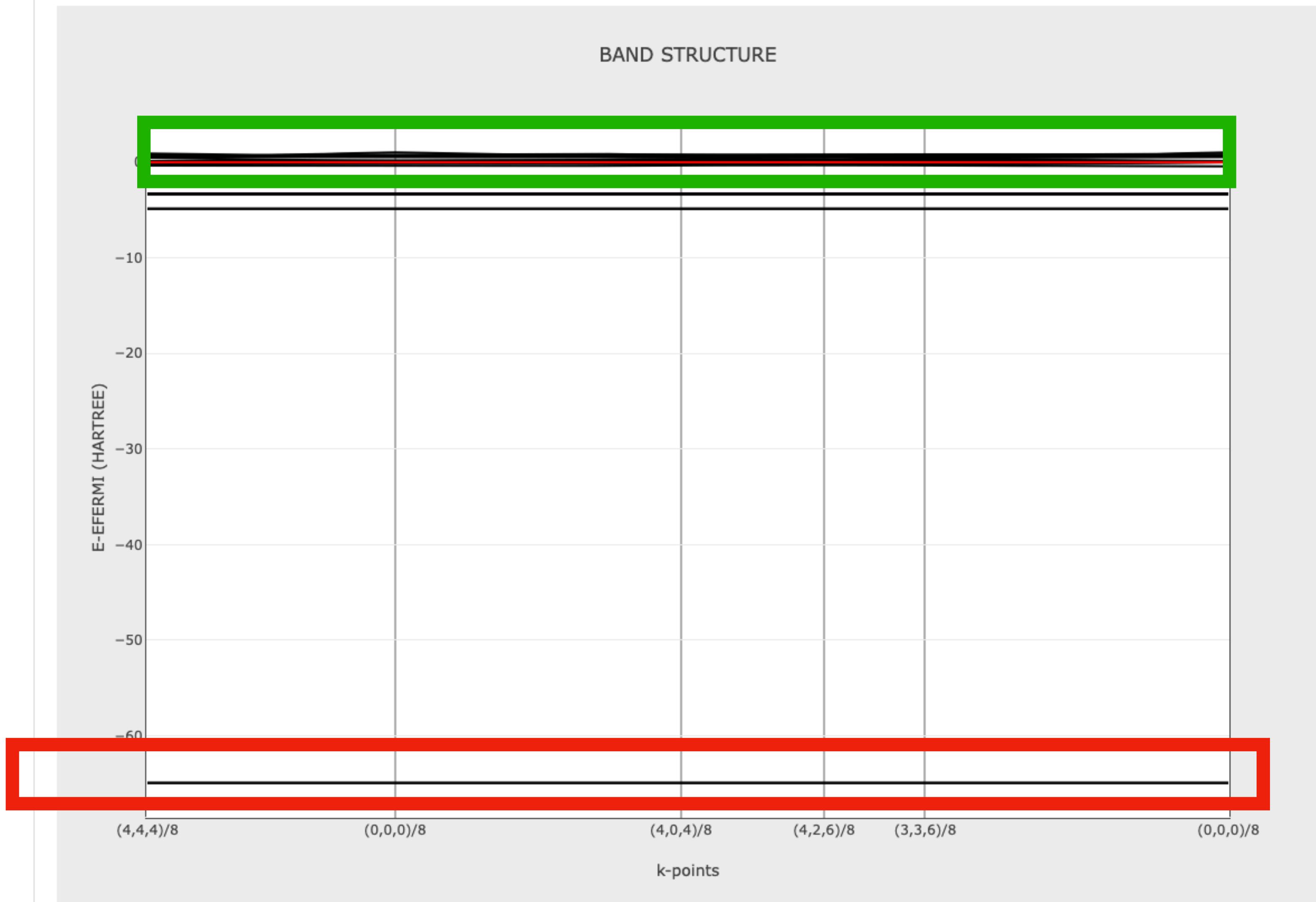
# Plot Generation ‘BAND.DAT’

## BAND STRUCTURE

Select CRYSTAL properties output to plot generic BAND STRUCTURE:

BAND.pop.DAT

 Choose file



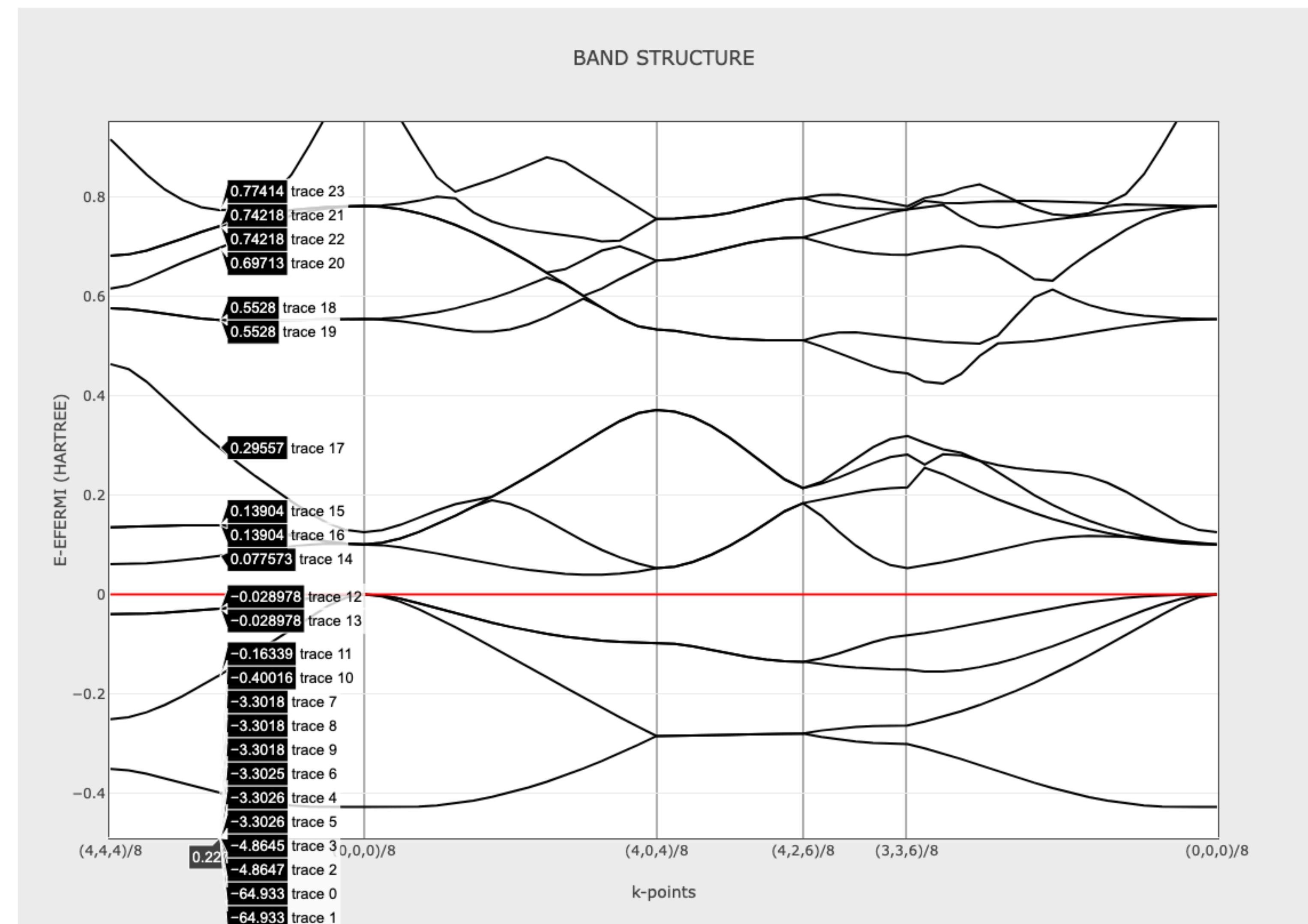
# Plot Generation ‘BAND.DAT’

BAND STRUCTURE

Select CRYSTAL properties output to plot generic BAND STRUCTURE:

BAND.pop.DAT

Choose file



# **properties: Example Inputs**

## List of available input decks and output files

Here a list of the available input decks is reported. In some cases the corresponding output files are also available.

Directory	Input	Output	Description
mgo	mgo.d12	mgo.out	Magnesium oxide single point calculation (HF)
	mgo-band.d3	mgo-band.out	Magnesium oxide band structure calculation
	mgo-doss.d3	mgo-doss.out	Magnesium oxide density of states calculation
	mgo-echg.d3	mgo-echg.out	Magnesium oxide electron charge density calculation
	mgo_coop.d3	mgo_coop.out	Magnesium oxide COOP calculation
	mgo_cohp.d3	mgo_cohp.out	Magnesium oxide COHP calculation
si	si.d12	si.out	Silicon single point calculation (HF)
	si-band.d3	si-band.out	Silicon band structure calculation
	si-doss.d3	si-doss.out	Silicon density of states calculation
	si-echg.d3	si-echg.out	Silicon electron charge density calculation
	si_coop_cohp.d3	si_coop_cohp.out	Silicon COOP/COHP calculation
be	be.d12	be.out	Berillium single point calculation (HF)
	be-band.d3	be-band.out	Berillium band structure calculation
	be-doss.d3	be-doss.out	Berillium density of states calculation
	be-echg.d3	be-echg.out	Berillium electron charge density calculation
	be_coop_cohp.d3	be_coop_cohp.out	Berillium COOP/COHP calculation
urea	urea.d12	urea.out	Urea single point calculation (HF)
	urea-band.d3	urea-band.out	Urea band structure calculation
	urea-doss.d3	urea-doss.out	Urea density of states calculation
	urea-echg.d3	urea-echg.out	Urea electron charge density calculation
	urea_coop_cohp.d3	urea_coop_cohp.out	Urea COOP/COHP calculation