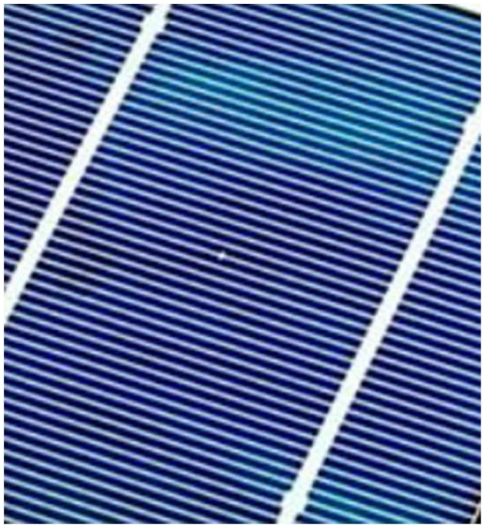
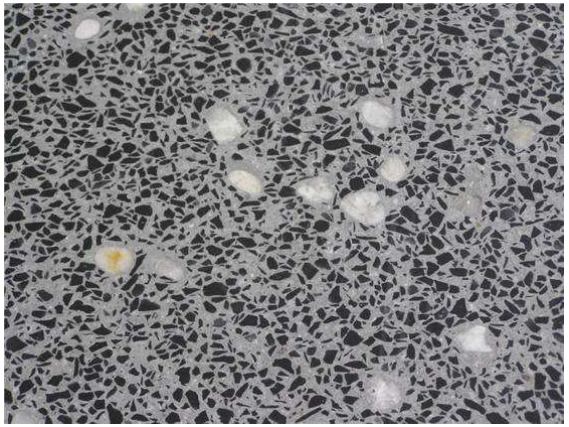
Introduction to Solid State Physics

Peter Hadley

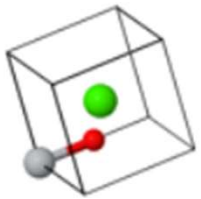
Solid materials

Metals and alloys
Plastics
Ceramics
Biological materials
Composite materials

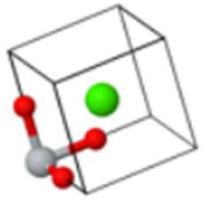




Crystals

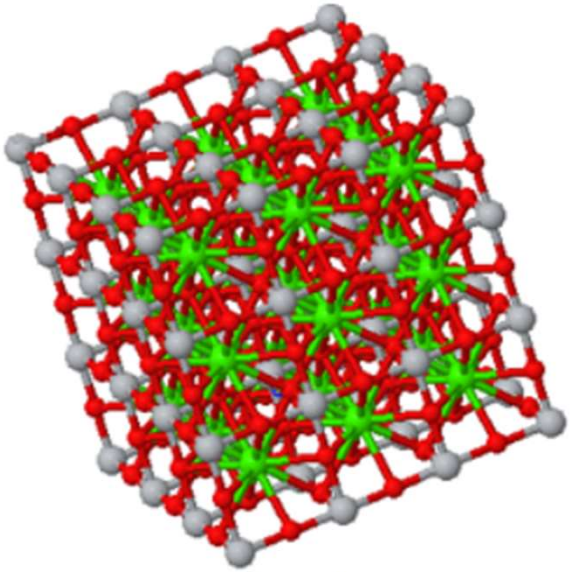


Asymmetric unit



Primitive unit cell

Conventional unit cell

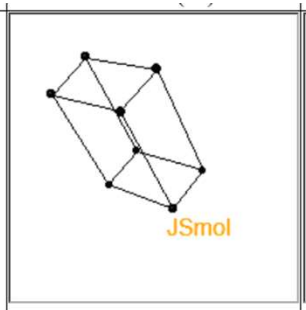
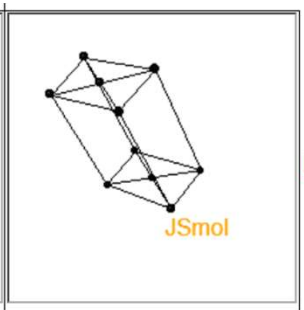
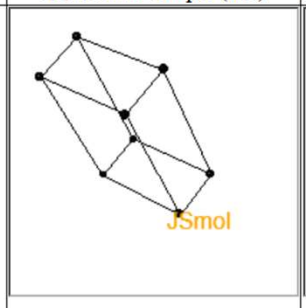
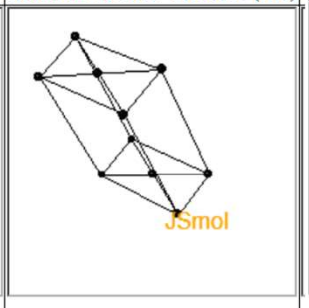
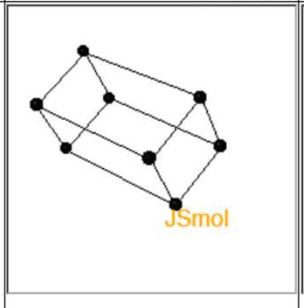
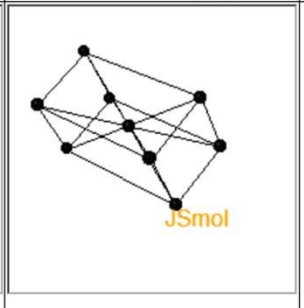
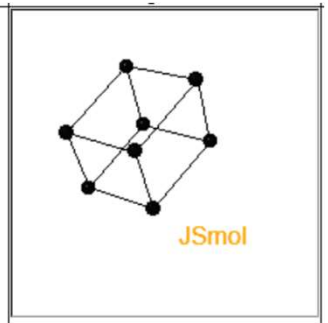


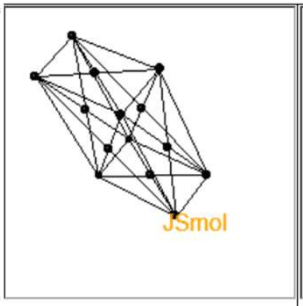
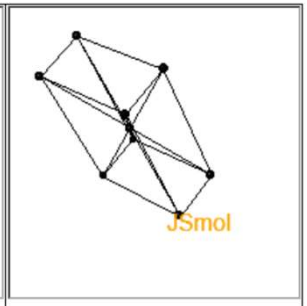
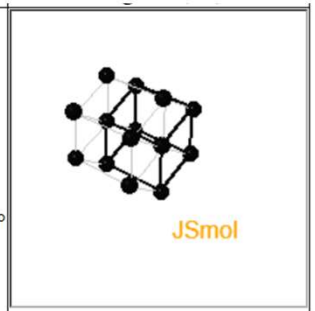
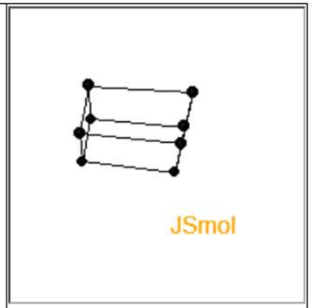
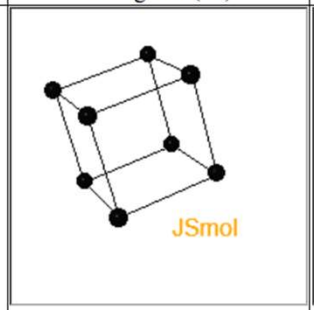
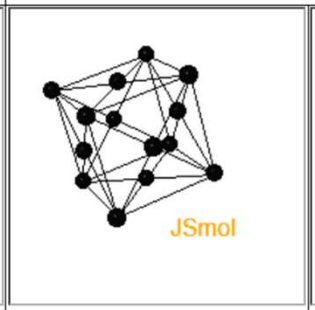
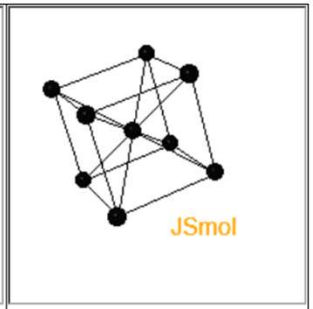
Crystal

14 Bravais lattices

Points of a Bravais lattice do not necessarily represent atoms.

P … primitive
I … body centered
F … face centered
A,C … centered
R … Rhombohedral

Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$ $\beta = \gamma = 90°$	 Monoclinic simple (mP)	 Monoclinic Base centered (mS)
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	 Orthorhombic simple (oP)	 Base centered (oS)
Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90°$	 Simple (tP)	 Body centered (tI)
Trigonal $a = b = c$ $\alpha = \beta = \gamma \neq 90°$	 Trigonal (hR)	

 Face centered (oF)	 Body centered (oI)	
Hexagonal $a = b \neq c$ $\alpha = 120°, \beta = \gamma = 90°$	 Hexagonal (hP)	
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	 Triclinic (aP)	
Cubic $a = b = c$ $\alpha = \beta = \gamma = 90°$	 Simple (cP)	 Face centered (cF)
 Body centered (cI)		

CIF files and programs to visualize crystal structures

Crystal structure data is often stored in a CIF file. This is a text file that contains the asymmetric unit of the crystal, the symmetries of the space group, and a reference to the source where the data was first published. It is important to check the publication to see the conditions used during the experiment. Some experiments are performed at high temperatures or high pressures where the crystal structure can be different than at room temperature and ambient pressure. The links below will display a crystal structure and it's corresponding CIF file.

Simple Cubic, Polonium Po $Pm\bar{3}m$ #221
Face-centered Cubic (fcc) $Fm\bar{3}m$ #225
Body-centered Cubic (bcc) $Im\bar{3}m$ #229
Hexagonal, Boron nitride BN #194
Hexagonal Close Packed (hcp) P63/mmc #194
Perovskite, Calcium titanate $CaTiO_3$ (perovskite) $Pm\bar{3}m$ #221
Caesium chloride CsCl $Pm\bar{3}m$ #221
Rocksalt NaCl $Fm\bar{3}m$ #225
Zincblende #216
Wurtzite #186
Diamond (C) #227
β-Sn #141
Graphite C P63mc #186

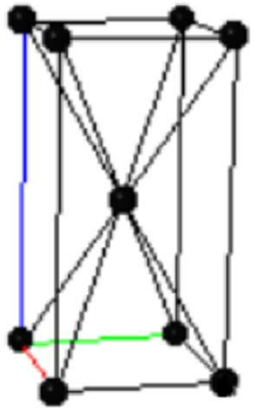
Sucrose P21 #4
Magnetite Fe_3O_4 Fd3m #227
Cementite Fe_3C #62
Copper oxide CO (Tenorite) #15
Pyrite FeS_2 #205
Rutile TiO_2 #136
Spinel $MgAl_2O_4$ #227
$Sr_2FeMoO6_6$ (double perovskite) I4/mmm #139
$YBa_2Cu_3O_7$ #47
ZIF8 #1
Zinc oxide ZnO (wurtzite) P63mc #186
ZnS (wurtzite) #186

Prototypes | Periodic Table | Semiconductors | Ceramics

MAS.020 Introduction to Solid State Physics
04.10.2024

Problem 2

The element Sn is a metal above 13° C and a semiconductor below 13° C.



(a) The metallic phase has a body centered tetragonal Bravais lattice with two atoms in the primitive unit cell. The conventional unit cell of the metallic phase is shown on the right where the black points are the Bravais lattice points. How many atoms are there in the conventional unit cells? Explain your reasoning.

(b) The semiconducting phase has an fcc Bravais lattice with two atoms in the primitive unit cell. The Miller indices are given in terms of the simple cubic conventional unit cell. Give the Miller indices of a direction that points from one Bravais lattice point to a nearest neighbor Bravais lattice point.

Exam 21 November 2024

Space Group → Bravais Lattice, Point Group

The space group of a crystal uniquely determines the Bravais lattice and the point group. The point group does not uniquely determine the Bravais lattice.

Space Group	Bravais lattice	Point group International	Point group Schoenflies
1 P1	Triclinic	1	C_1
2 $P\bar{1}$	Triclinic	$\bar{1}$	$S_2 = C_i$
3 P2	Simple Monoclinic	2	C_2
4 $P2_1$	Simple Monoclinic	2	C_2
5 C2	Base-Centered Monoclinic	2	C_2
6 Pm	Simple Monoclinic	m	$C_{1h} = C_s$
7 Pc	Simple Monoclinic	m	$C_{1h} = C_s$
8 Cm	Base-Centered Monoclinic	m	$C_{1h} = C_s$
9 Cc	Base-Centered Monoclinic	m	$C_{1h} = C_s$
10 P2/m	Simple Monoclinic	$\frac{2}{m}$	C_{2h}
11 $P2_1/m$	Simple Monoclinic	$\frac{2}{m}$	C_{2h}
12 C2/m	Base-Centered Monoclinic	$\frac{2}{m}$	C_{2h}
13 P2/c	Simple Monoclinic	$\frac{2}{m}$	C_{2h}
14 $P2_1/c$	Simple Monoclinic	$\frac{2}{m}$	C_{2h}
15 C2/c	Base-Centered Monoclinic	$\frac{2}{m}$	C_{2h}
16 P222	Simple Orthorhombic	222	$V = D_2$
17 $P222_1$	Simple Orthorhombic	222	$V = D_2$
18 $P2_12_12$	Simple Orthorhombic	222	$V = D_2$
19 $P2_12_12_1$	Simple Orthorhombic	222	$V = D_2$
20 $C222_1$	Base-Centered Orthorhombic	222	$V = D_2$
21 C222	Base-Centered Orthorhombic	222	$V = D_2$
22 F222	Face-Centered Orthorhombic	222	$V = D_2$
23 I222	Body-Centered Orthorhombic	222	$V = D_2$
24 $I2_12_12_1$	Body-Centered Orthorhombic	222	$V = D_2$

The Materials Project

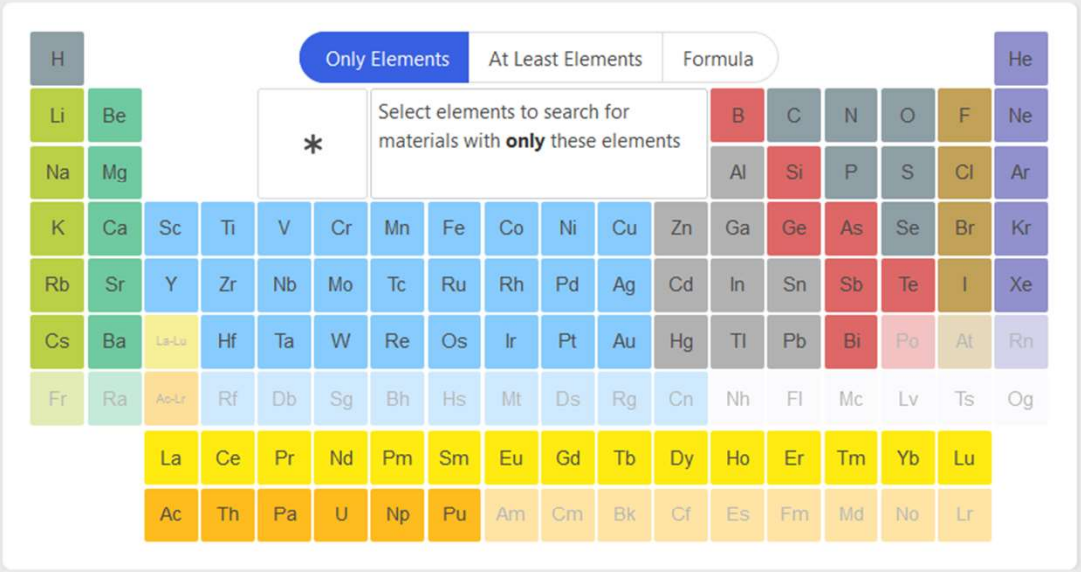
Home / Apps / Materials Explorer

Materials Explorer

References | Documentation

Search for materials information by chemistry, composition, or property.

Materials | e.g. Li-Fe or Li,Fe or Li3Fe or mp-19017 | Search



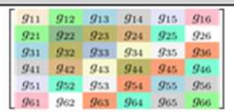
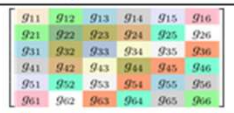
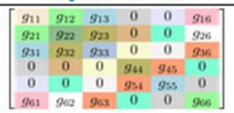
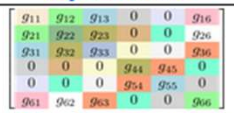
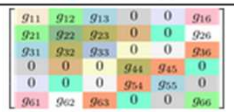
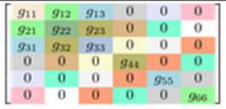
Filters | Reset

▸ Composition

All **153,235 materials**
Showing 1-15

Columns | Export Table

Material ID	Formula	Crystal System	Space Group Symbol	Sites	Energy Above Hull (eV/atom)	Band Gap (eV)

rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric
$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{12} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & g_{15} & 0 \\ 0 & 0 & 0 & g_{24} & g_{25} & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ 0 & 0 & 0 & g_{34} & g_{35} & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric
rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
	$\begin{bmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	 reduced, symmetric, asymmetric

http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html

Symmetric Tensors

$$\chi^E_{ij} = \frac{\partial P_i}{\partial E_j} = -\frac{\partial^2 G}{\partial E_i \partial E_j} = \frac{\partial P_j}{\partial E_i} = \chi^E_{ji}$$

$$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$$

Tensor notation

We need a way to represent 3rd and 4th rank tensors in 2-d.

$$1\,1 \rightarrow 1 \quad 1\,2 \rightarrow 6 \quad 1\,3 \rightarrow 5$$
$$2\,2 \rightarrow 2 \quad 2\,3 \rightarrow 4$$
$$3\,3 \rightarrow 3$$

rank 3

$$g_{36} \rightarrow g_{312}$$

rank 4

$$g_{14} \rightarrow g_{1123}$$

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Cu

mp-30

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  - Equations of State
  - X-ray Absorption Spectra

Elastic Constants

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$$

Data | Methods | API

Stiffness Tensor (GPa)

$$\begin{bmatrix} 159 & 129 & 129 & 0 & 0 & 0 \\ 129 & 159 & 129 & 0 & 0 & 0 \\ 129 & 129 & 159 & 0 & 0 & 0 \\ 0 & 0 & 0 & 79 & 0 & 0 \\ 0 & 0 & 0 & 0 & 79 & 0 \\ 0 & 0 & 0 & 0 & 0 & 79 \end{bmatrix}$$

Compliance Tensor (TPa^{-1})

$$\begin{bmatrix} 23.2 & -10.4 & -10.4 & 0 & 0 & 0 \\ -10.4 & 23.2 & -10.4 & 0 & 0 & 0 \\ -10.4 & -10.4 & 23.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12.7 \end{bmatrix}$$

$$\begin{bmatrix} g_{11} & g_{12} & g_{12} & 0 & 0 & 0 \\ g_{12} & g_{11} & g_{12} & 0 & 0 & 0 \\ g_{12} & g_{12} & g_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{44} \end{bmatrix}$$

Elastic Constants

Bulk Modulus, Voigt	139 GPa
Bulk Modulus, Reuss	139 GPa
Bulk Modulus, Voigt-Reuss-Hill	139 GPa
Shear Modulus, Voigt	53 GPa
Shear Modulus, Reuss	29 GPa
Shear Modulus, Voigt-Reuss-Hill	41 GPa
Poisson's Ratio	0.37
Universal Anisotropy	4.17