# Crystallography PHY312

## Insulators (high bandgap)



Rocksalt  $E_g = 3.1 \text{ eV}$ 



Gypsum E<sub>g</sub> = 5-7 eV



Calcite Magnesite

 $E_g = 6 \text{ eV}$ 

 $E_g = 5.4 \text{ eV}$ 



**Diamond** 

 $E_{g} = 5.47 \text{ eV}$ 

## Insulators (lower bandgap)















 $E_{g} = 2.3 \text{ eV}$ 

## Metals



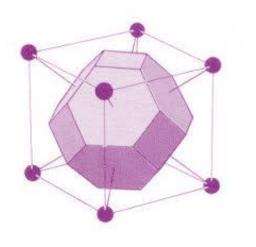
#### **Semiconductors**



GaP, 2.26 eV



Silicon, 1.1 eV

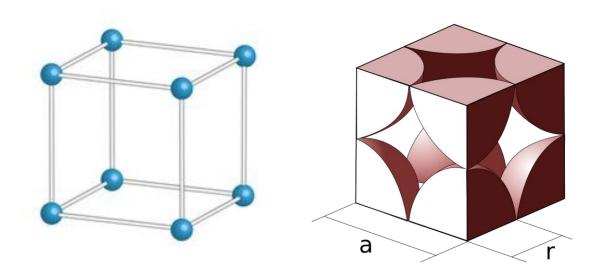


### Wigner seitz cell (3D)

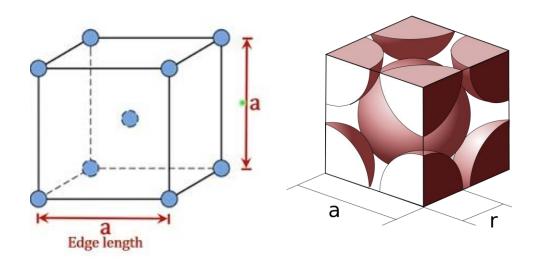
## **Crystal System Table**

| System       | Axial length | Axial Angle                               | Unit Cell Geometry |
|--------------|--------------|---|--------------------|
| Cubic        | a = b = c    | $\alpha = \beta = \gamma = 90^{\circ}$    |                    |
| Tetragonal   | a = b ≠ c    | $\alpha = \beta = \gamma = 90^{\circ}$    |                    |
| Orthorhombic | a≠b≠c        | $\alpha = \beta = \gamma = 90^{\circ}$    |                    |
| Rhombohedral | a = b = c    | $\alpha = \beta = \gamma \neq 90^{\circ}$ |                    |
| Hexagonal    | a = b ≠ c    | α = β = 90°,<br>γ=120°                    |                    |
| Monoclinic   | a≠b≠c        | α = γ = 90°,<br>β≠90°                     |                    |
| Triclinic    | a≠b≠c        | α≠β≠γ                                     |                    |

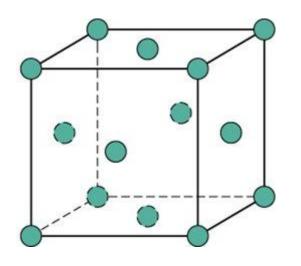
## Simple cubic

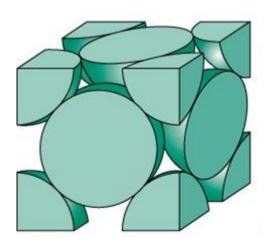


## **Body centered cubic**

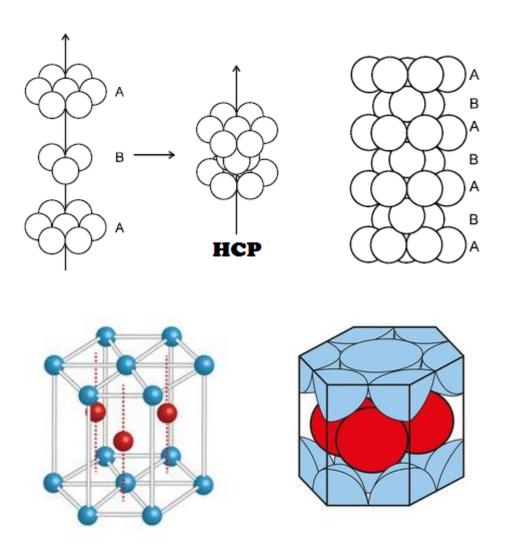


#### Face centered cubic

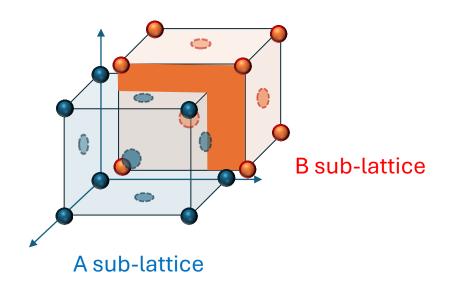




### Hexagonal closed pack structure



#### Interpenetrating FCC structure

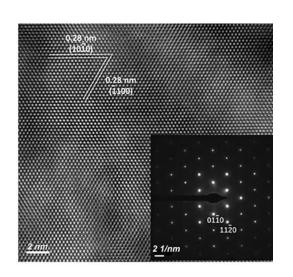


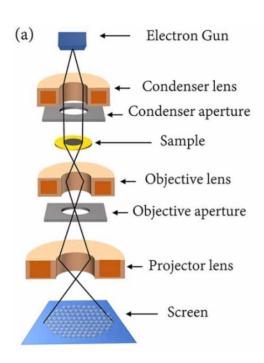
#### **Co-ordinates**

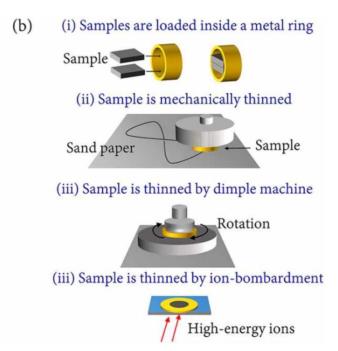
A-sublattice (0 0 0) B-Sublattice (¼ ¼ ¼)

A = B, Diamond structure A ≠ B, Zinc-Blende (ZnS) structure

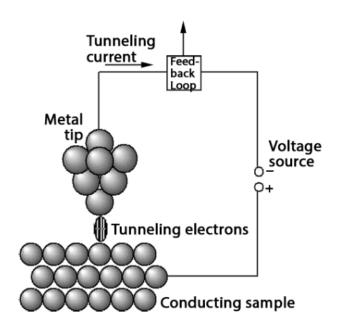
#### **Transmission electron microscopy**

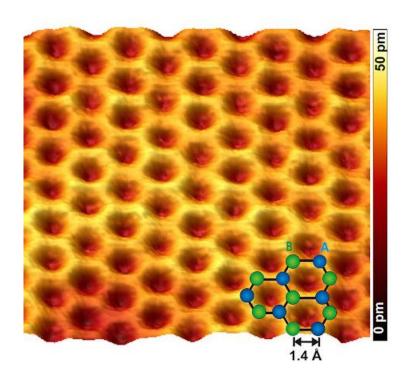




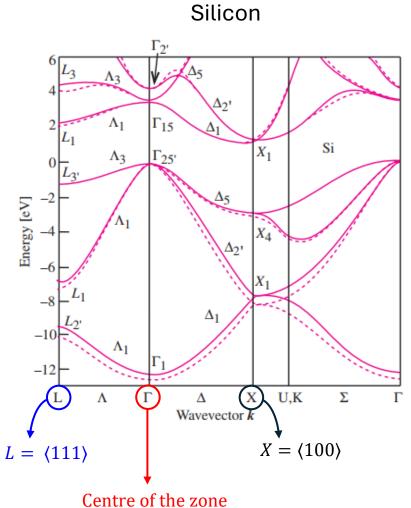


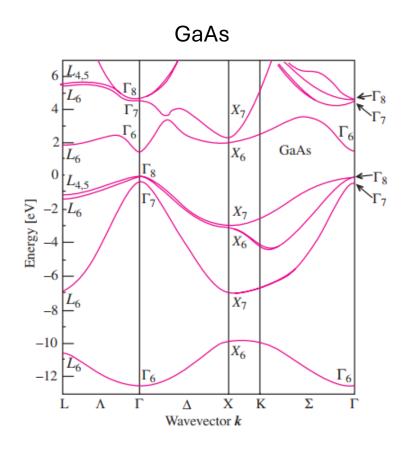
#### **Scanning Tunnelling Microscopy**



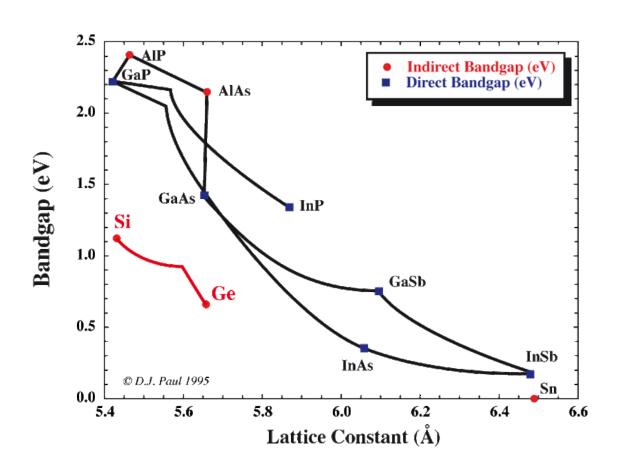


#### **Bandstructure:**





#### **Bandgap for different semiconductors:**



| 1<br>IA<br>1                                   |  |   |   |  |  |  |   |  |  |   |  |  |  |  |  |   | 18<br>VIIIA<br>2                                 |
|--|--|---|---|--|--|--|---|--|--|---|--|--|--|--|--|---|--|
| Hydrogen<br>1.008                              | 2<br>IIA   |   |   |  |  |  |   |  |  |   |  | 13<br>IIIA   | 14<br>IVA                                      | 15<br>VA   | 16<br>VIA  | 17<br>VIIA  | Helium<br>4.0026                                 |
| 3<br>Li<br>Lithium                             | 4<br>Be<br>Beryllium   | Subcategory metals  Alkali metals                 |   |  |  |  | s, nonmetals, and metalloids  Metalloids  Lanthanides |  |  |   |  | B<br>Boron   | 6<br>C<br>Carbon                               | 7<br>N<br>Nitrogen                                   | 8<br>Oxygen                                      | 9<br>Fluorine   | Ne Neon  |
| 6.94<br>2-1<br><b>11</b>                       | 9.013<br>2-1<br>12   |   |   | Alkaline   | earth metals                                     | Acti   | inides  |  | Reactive non<br>Noble gases                                | metals  |  | 10.81<br>2-3<br>13   | 12.011<br>2-4<br>14                            | 14.007<br>2-5<br><b>15</b>                           | 15.999<br>2-6<br>16                              | 18.998<br>2-7<br>17                                   | 20.18<br>2-8<br>18                               |
| Na<br>Sodium<br>22.98<br>2-8-1                 | Magnesium<br>24.32<br>2-8-2                                  | 3<br>1111B  | 4<br>IVB  | Transiti 5 VB  | on metals  6  VIB                                | 7<br>VIIB  | t transition n  8  VIIIB                              | oetais<br>9<br>VIIIB   | Unknown pro<br>10<br>VIIIB                                 | 11  | 12<br>IIB  | Aluminium<br>26.98<br>2-8-3  | Si<br>Silicon<br>28.085<br>2-8-4               | Phosphorus<br>30.97<br>2-8-5                         | Sulfur<br>32.06<br>2-8-6                         | Cl<br>Chlorine<br>35.45<br>2-8-7                      | Argon<br>39.95<br>2-8-8                          |
| 19<br>K  | 20<br>Ca   | 21<br>Sc  | 22<br><b>Ti</b>   | $\overset{23}{\mathbf{V}}$                             | cr   | 25<br>Mn   | 26 <b>Fe</b>  | 27<br><b>Co</b>  | 28<br><b>Ni</b>  | 29<br>Cu  | 30<br>Zn   | 31<br>Ga   | Ge   | 33<br><b>As</b>                                      | 34<br>Se   | 35<br>Br  | 36<br><b>Kr</b>                                  |
| Potassium<br>39.10<br>2-8-8-1                  | Calcium<br>40.08<br>2-8-8-2                                  | Seandium<br>44.96<br>2-8-9-2                      | Titanium<br>47.87<br>2-8-10-2                               | Vanadium<br>50.94<br>2-8-11-2                          | Chromium<br>51.996<br>2-8-13-1                   | Manganese<br>54.94<br>2-8-13-2                               | 55.84<br>2-8-14-2                                     | Cobalt<br>55.93<br>2-8-15-2  | Nickel<br>55.69<br>2-8-16-2                                | Copper<br>63.55<br>2-8-18-1                                   | Zinc<br>63.38<br>2-8-18-2                            | Gallium<br>69.72<br>2-8-18-3   | 72.63<br>2-8-18-4                              | Arsenic<br>74.92<br>2-8-18-5                         | Selenium<br>74.92<br>2-8-18-6                    | 79.90<br>2-8-18-7                                     | 83.80<br>2-8-18-8                                |
| Rb<br>Rubidium<br>85.47                        | Sr<br>Strontium<br>87.62                                     | 39<br>Y<br>Yttrium<br>88.90                       | Zr<br>Zirconium<br>91.22                                    | Nb<br>Niobium<br>92.90                                 | Mo<br>Molybdenum<br>95.95                        | Tc Technetium [98]   | Ruthenium   | Rh<br>Rhodium<br>102.91  | Palladium  | 47<br><b>Ag</b><br>Silver<br>107.87                           | Cd<br>Cadmium  | 49<br>In<br>Indium<br>114.82   | 50<br>Sn<br>Tin<br>118.71                      | Sb<br>Antimony<br>121.76                             | Te<br>Tellurium                                  | 53  | 54<br><b>Xe</b><br>Xenon<br>131.29               |
| 2-8-18-8-1  55  CS Cesium 132.91 2-8-18-18-8-1 | 2-8-18-8-2<br>56<br>Bar<br>Barium<br>137-33<br>2-8-18-18-8-2 | 2-8-18-9-2 57 - 71 Ln Lanthanides                 | 72<br>Hf<br>Hafnium<br>178.49                               | 73 Ta Tantalum 180.95                                  | 2-8-18-13-1  74  W Tungsten 183.84               | 2-8-18-13-2 75 Re Rhenium 186.21                             | 2-8-18-15-1  76  OS  Osmium  190.23                   | 2-8-18-16-1 77 <b>Ir</b> Iridium 192.22                              | 2-8-18-18 78 Pt Platinum 195.08                            | 2-8-18-18-1 80 Au Gold 196-97                                 | 2-8-18-18-2  80  Hg Mercury 200.59 2-8-18-32-18-2    | 2-8-18-18-3  81  Thallium 204.38 2-8-18-32-18-3                        | 2-8-18-18-4  82  Pho Lead 207.2 2-8-18-32-18-4 | 2-8-18-18-5  83  Bi Bismuth 208.98 2-8-18-32-18-5    | 2-8-18-18-6  84  Polonium [209] 2-8-18-32-18-6   | 2-8-18-18-7  85  At Astatine [210] 2-8-18-32-18-7     | 2-8-18-18-8  86  Rn Radon [222] 7 2-8-18-32-18-8 |
| 87<br>Francium<br>[223]<br>2-8-18-32-18-8-1    | 88<br>Radium<br>[226]<br>2-8-18-32-18-8-2                    | 89 - 103<br>Actinides                             | 2-8-18-32-10-2 104 Rf Rutherfordium [267] 2-8-18-32-32-10-2 | 105<br><b>Db</b> Dubnium  [268]                        | 106 Sg Seaborgium [269]                          | Bh Bohrium [270]   | Hassium [277]   | 109<br>Meitnerium<br>[278]<br>2-8-18-32-32-15-2                      | DS Darmstadtium [281]                                      | 2-8-18-32-18-1 111 Rg Roentgeniun [282] 2-8-18-32-32-17-2     | 112<br>Cn<br>Copernicium<br>[285]                    | Nh<br>Nihonium<br>[286]  | 114<br>Flerovium<br>[289]<br>2-8-18-32-32-18-4 | 115<br>MC<br>Moscovium<br>[290]<br>2-8-18-32-32-18-5 | 116<br>LV<br>Livermorium<br>[293]                | 117<br>TS<br>Tennessine<br>[294]<br>2-8-18-32-32-18-7 | 118<br>Og<br>Oganesson<br>[294]                  |
|  |  | 57<br>La<br>Lanthanum<br>138.91<br>2-8-18-18-9-2  | 58<br>Ce<br>Cerium<br>140.12<br>2-8-18-19-9-2               | 59<br>Pr<br>Prascodymium<br>140.91<br>2-8-18-21-8-2    | 60<br>Nd<br>Neodymium<br>144.24<br>2-8-18-22-8-2 | 61<br>Prm<br>Promethium<br>[145]<br><sub>2-8-18-23-8-2</sub> | 62<br>Sm<br>Samarium<br>150.36<br>2-8-18-24-8-2       | 63<br>Bu<br>Europium<br>151.96<br>2-8-18-25-8-2                      | 64<br>Gd<br>Gadolinium<br>157.25<br>2-8-18-25-9-2          | 65<br>Tb<br>Terbium<br>158.93<br>2-8-18-27-8-2                | 66<br>Dy<br>Dysprosium<br>162.50<br>2-8-18-28-8-2    | 67<br>H0<br>Holmium<br>164.93<br>2-8-18-29-8-2                         | 68<br>Err<br>Erbium<br>167.26<br>2-8-18-30-8-2 | 69<br>Tm<br>Thulium<br>168.93<br>2-8-18-31-8-2       | 70<br>Yb<br>Ytterbium<br>173.05<br>2-8-18-32-8-2 | 71<br>Lu<br>Lutetium<br>174.97<br>2-8-18-32-9-2       |  |
|  |  | 89<br>Ac<br>Actinium<br>[227]<br>2-8-18-32-18-9-2 | 90<br>Th<br>Thorium<br>232.04<br>2-8-18-32-18-10-2          | 91<br>Pa<br>Protactinium<br>231.04<br>2-8-18-32-20-9-2 | 92<br>U<br>Uranium<br>238.03<br>2-8-18-32-21-9-2 | 93<br>Np<br>Neptunium<br>[237]<br>2-8-18-32-22-9-2           | 94<br>Pu<br>Plutonium<br>[244]<br>2-8-18-32-24-8-2    | 95<br>Am<br>Americium<br>[243]<br>2-8-18-32-25-8-2<br>Priyamstudyeem | 96<br>Cm<br>Curium<br>[247]<br>2-8-18-32-25-9-2<br>tre.com | 97<br>Bk<br>Berkelium<br>[247]<br><sub>2-8-18-32-27-8-2</sub> | 98<br>Cf<br>Californium<br>[251]<br>2-8-18-32-28-8-2 | 99<br><b>Es</b><br>Einsteinium<br>[252]<br><sup>2-8-18-32-29-8-2</sup> | Fm<br>Fermium<br>[257]<br>2-8-18-32-30-8-2     | Md<br>Mendelevium<br>[258]<br>2-8-18-32-31-8-2       | No<br>Nobelium<br>[259]<br>2-8-18-32-32-8-2      | Lw<br>Lawrencium<br>[266]<br>2-8-18-32-32-8-3         |  |