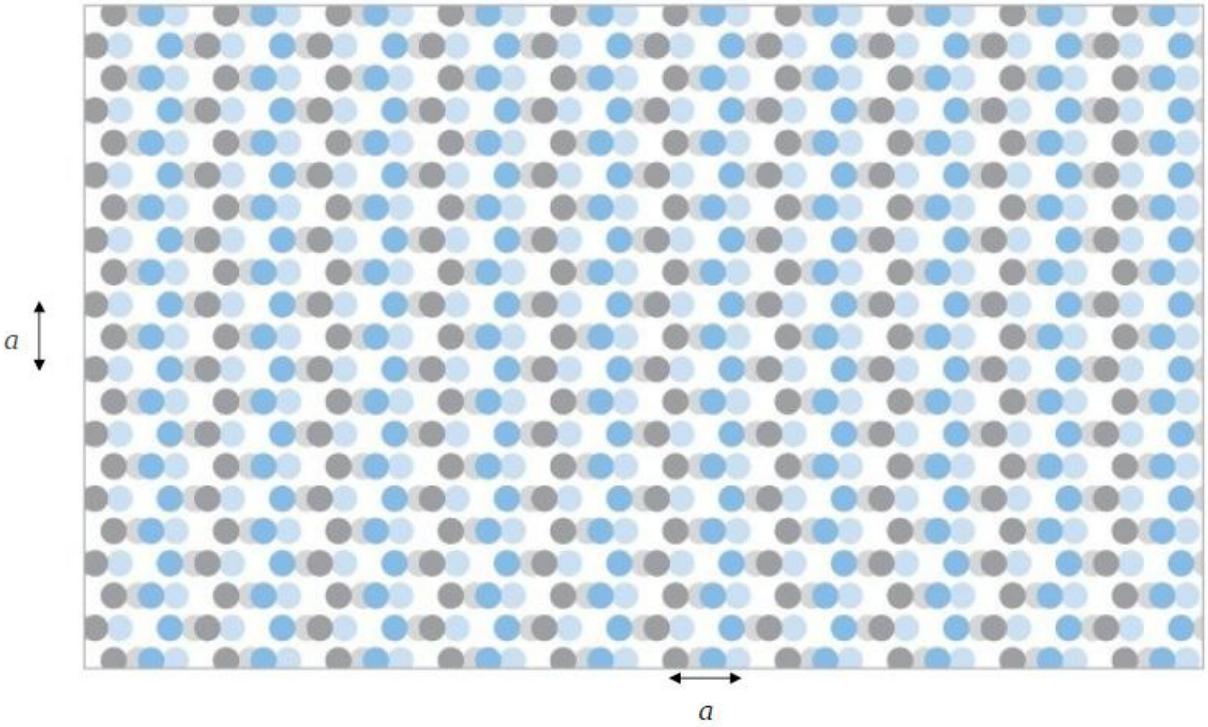
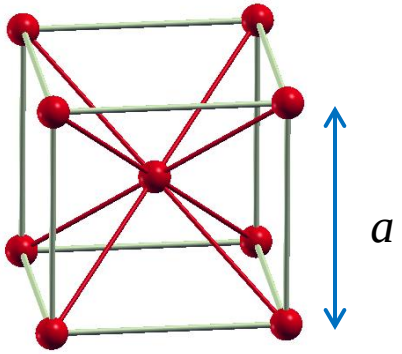
ASESMA 2018
Worksheet 2
Crystal Structures

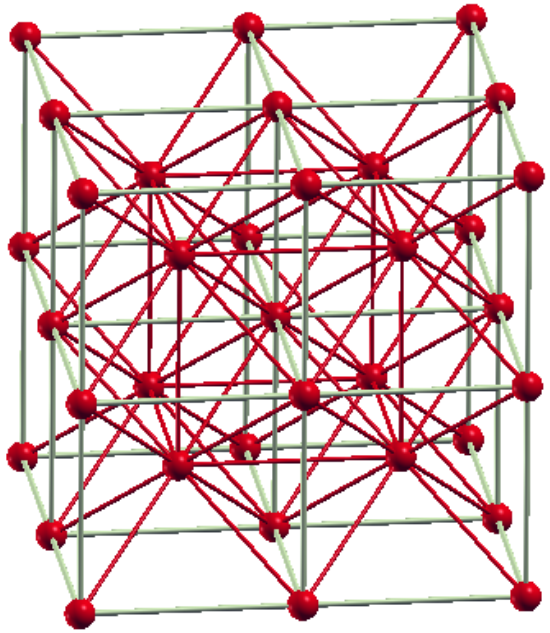
2D Crystals



- Find the 2D Bravais lattice and basis for this (infinite) pattern.
- Draw two (primitive) lattice vectors.
- Find the primitive unit cell. How many atoms (dots) does it contain?

The Body Centered Cubic Structure

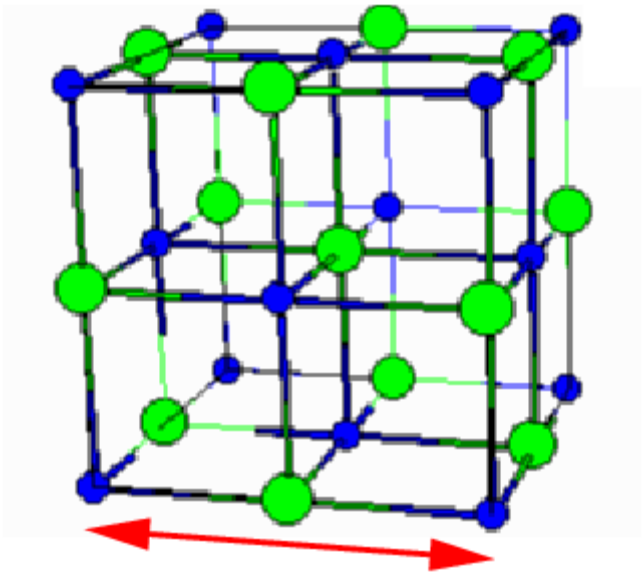




This is a Bravais lattice.
You can do a pwscf calculation with
`ibrav=3`, `nat=1`,`nytp=1`, one atom placed at `0.0 0.0 0.0`

If you instead choose to work with a supercell and `ibrav=3`, give
`nat, ntyp` and `ATOMIC_POSITIONS`

The Rock Salt (NaCl) Structure



- This is obviously not a Bravais lattice! (Why?)
- Find a Bravais lattice and basis.
- Give `nat, ntyp` and `ATOMIC_POSITIONS`