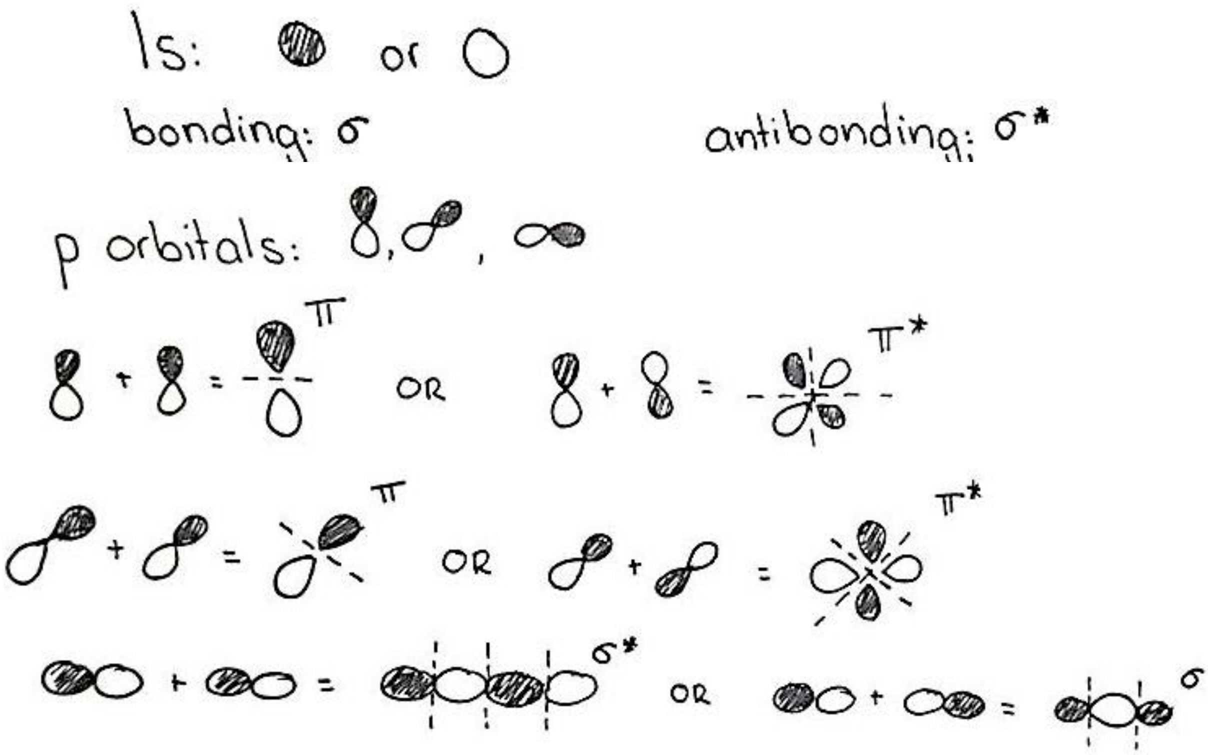
**Bonding – MO Theory ($H_2$):**

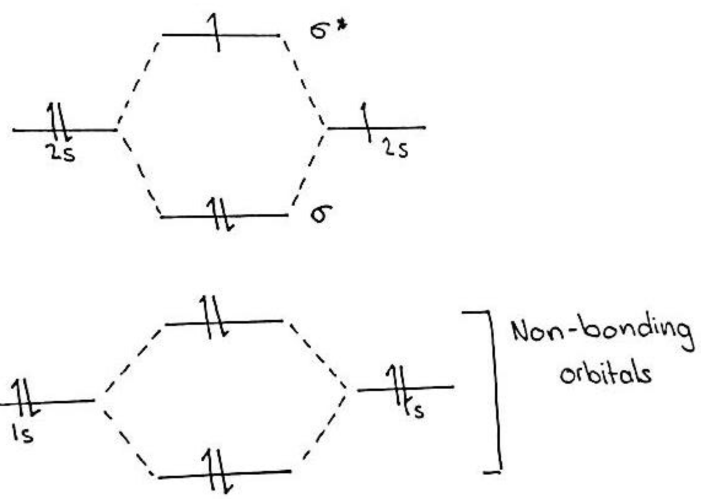
- **Explain how electron sharing leads to lowering of electronic energy in terms of increasing de Broglie wavelength**
  - As atoms come together electrons are shared between the two nuclei, causing wavelength to increase, thus decreasing energy by de Broglie
  - The wavefunctions will add to form a new wavefunction, with one cloud surrounding the two nuclei
  - The lower energy = a more stable situation
- **Recognise a bonding or antibonding orbital from the lobe representation**
  - Orbital created depends on the phases of the joining atomic phases
  - Recall: increasing number of nodes = increasing energy
  - Bonding wants lowest energy possible
  - Antibonding orbitals are created when opposite phases join – they have at least 1 node
- **Recognise a σ orbital and a σ* orbital**
  - Orbitals named looking along bond axis – if they look like s orbitals (i.e. round) then they are sigma bonds
  - * orbital is the antibonding




- **recognize a π orbital, a π orbital and a non-bonding orbital**
  - Non-bonding orbitals do not take part in the molecular bonding (not valence electrons) – they are orientated in a way that cannot react

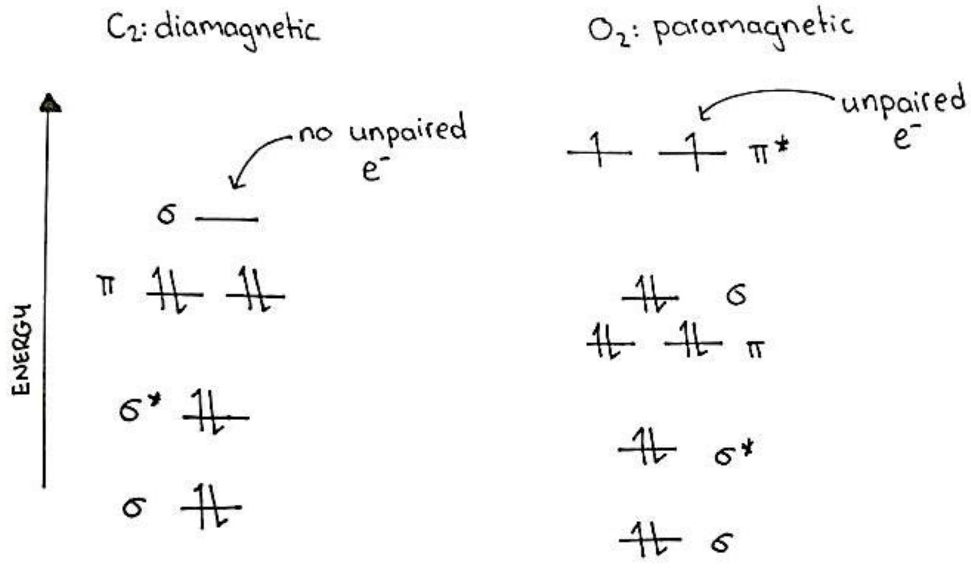
- **Distinguish between polar and apolar bonds in diatomic molecules and relate it to electron attraction of a nucleus (electronegativity)**
    - Asymmetric molecular orbits result in polar (charged) bonds
    - The 1s orbital of two different atoms may have different energy levels due to the distance of the electrons from the nucleus
    - The resulting molecular orbitals are each slightly more like the orbital of closest energy
    - In isoelectronic pairings the more electronegative element will draw electrons slightly more strongly than the other
- **Draw out ground state electronic configurations for molecules and molecular ions given their allowed energy levels**
    - Same rules apply for molecular orbitals as for atomic orbitals
    - Total number of atomic orbitals in component atoms = number of molecular orbitals

$Be_2^+$:




- **Calculate bond order from molecular electronic configurations**
    - $Bond\ Order = \frac{1}{2}(e^-\ in\ bonding\ orbitals - e^-\ in\ antibonding\ orbitals)$
- **Explain the difference between paramagnetism and diamagnetism**
    - Paramagnetism – unpaired electrons cause a net magnetic moment (drawn to magnetic fields)
    - Diamagnetism – no unpaired electrons, weakly repelled by magnetic fields

- **Predict whether a molecule will be diamagnetic or paramagnetic from its orbital energy diagram**
    - Diamagnetic if and only if they are any unpaired electrons




NB: orbitals decreasing energy as $e^-$ are closer to nucleus ∴ more stable.

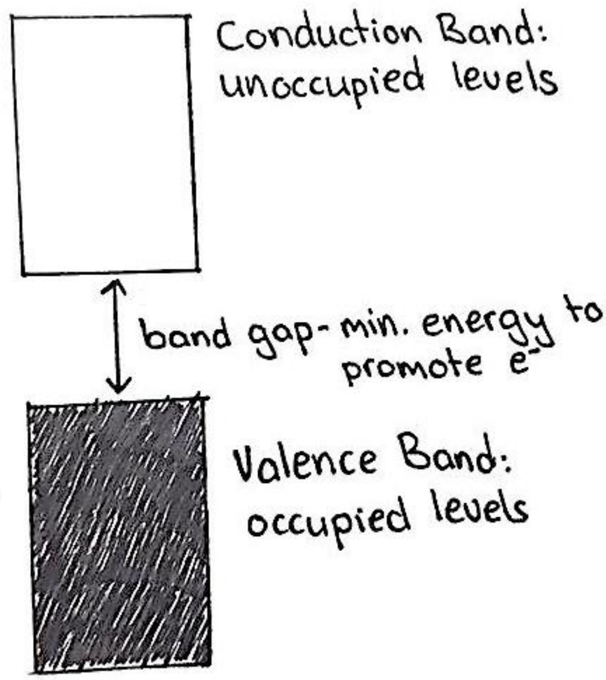
- **Recall the meaning of HOMO and LUMO and determine the lowest energy electronic transition**
    - HOMO: Highest occupied molecular orbital
    - LUMO: lowest unoccupied molecular orbital
    - Lowest electronic transition is the HOMO-LUMO transition i.e. an electron moving from the highest occupied molecular orbital to the lowest unoccupied molecular orbital when provided with energy

<u>**Band Theory: Molecular Orbitals in Solids:**</u>

- **Recall that the number of molecular orbitals increases with the number of atoms in the molecule**
    - Number of molecular orbitals = total number of atomic orbitals
    - Thus, as we increase the number of atoms, the number of molecular orbitals increase
- **Recognise that interactions of σ-orbitals gives rise to a valence band and σ* orbitals give rise to a conduction band in covalent solids**
    - σ-orbitals are filled with electrons, and thus are the outermost or valence band in covalent solids

- σ* orbitals are unoccupied – they form the conduction band of covalent solids that only become occupied if enough energy is provided to overcome the band gap and promote electrons

- **Use, define and explain the concepts of conduction band, valence band, band gap, hole, acceptor level, donor level, n-doping and p-doping**
  - Conduction band: the band of unoccupied orbitals in a molecular solid
  - Valence band: The band of occupied orbitals in molecular solids
  - Band gap: The energy gap between these two bands (i.e. the amount of energy required for an electron to be promoted)




  - Hole: the space in the valence band caused by an absence of an electron – relative positive charge
  - Acceptor level: The level close to the valence band generated in p-type doping, where valence electrons are promoted to
  - Donor level: The level which extra electrons reside in, close to the conduction band, in n-type doping
  - N-doping: doping achieved by substituting with an element with more electrons, thus creating an excess of negative charge carriers
  - P-doping: doping achieved by substituting an element with fewer electrons, thus creating an excess of positive holes

- **Explain the relationship between band gap and electrical and optical properties**
  - Band gap determines colour as it corresponds to the wavelengths of light absorbed by the object
    - Small band gap (e.g. silicon) – absorbs all visible light, thus causing the object to appear black
    - Large band gap (e.g. diamond) – absorbs no visible light, thus appears transparent

- In order to conduct electricity, electrons must have access to the unoccupied energy levels, thus a small band gap is needed so only a small amount of energy is required to promote electrons
  - In metals the valence and conduction bands overlap – this is why they are such good conductors of electricity
- **Explain how n or p doping gives rise to conductivity of electrons and holes**
  - N-type doping is achieved by substituting with an element with more electrons (i.e. to the right on the periodic table), thus creating an excess of electrons (negative charge carriers)
    - These electrons sit in donor levels, just below the conduction band and are easily promoted to the conduction band
  - P-type doping is achieved by substituting with an element that has fewer electrons (i.e. to the left on the periodic table), thus creating an excess of holes (positive charge carriers)
    - Acceptor levels, just above the valence band, are generated and valence electrons are promoted to this level
    - Major conduction due to the holes
- **Explain why the conductivity of semiconductors increases with temperature**
  - Increased temperature provides thermal energy to move electrons into the conduction band, where they are free to move and conduct electricity
- **Recognise a diagram of the band structure of insulators, metals and types of semiconductor**