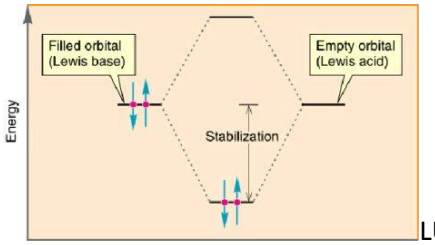
pKa Values

- pKa value < 0 indicates a strong acid
  pKa value > 0 indicates a weak acid
- $HB \rightarrow H^+ + B^-$ (equilibrium)
  $k = [H^+][B^-]/[HB]$
  if k > 1 favoured (more of the top present) and pKa is -ve
  if k < 1 unfavoured (more of bottom present than the top present) and pKa is +ve
- $pKa = -\log_{10}Ka$ therefore pKa = 0 when there is a 50/50 equilibrium
- **Pauling's rules:**
  - In oxy acids of formula $(HO)_xE(O)_y$, pKa = 8 – 5y
    For subsequent deprotonation add 5 to original pKa value
  - E.g. $H_2SO_4 = (HO)_2SO_2$ pKa = 8 – (2x5) = -2
    This is $H_2SO_4 \rightarrow H^+ + HSO_4^-$
  - For $HSO_4^- \rightarrow H^+ + SO_4^{2-}$, pKa = -2 + 5 = +3 (not so easily deprotonated)
  - If there are no hydroxyl groups attached: pKa is 8
    - Such as $Si(OH)_4$, $B(OH)_3$
  - Any variation: could be due to many things
    - Such as H_2CO_3 (carbonic acid): predict +3. Actual pKa is +6.4. Due to equilibrium – lies to the left, on $CO_2 + H_2O$ side – less carbonic acid than expected, so acidity is lower.

Lewis acids and Lewis bases

- Acid – electron pair acceptor (electrophile)
  - H^+ (the Bronsted acid)
  - M^{2+} - gaseous state, bond ligands (such as Co^{2+})
  - Molecules with incomplete octets of electrons: such as BMe_3, $AlCl_3$ (both have 6 electrons)
  - Molecules with complete octets that can rearrange their electrons, such as CO_2 - oxygens withdraw electrons from carbon, leaving the carbon electrophilic (an acidic electron acceptor)
  - Molecules with complete octets that can accept further electron pairs, such as $SiF_4 + 2F^- \rightarrow [SiF_6]^{2-}$ becomes octahedral; uses 3d orbitals to expand from an octet
- Base – electron pair donor (nucleophile)
  - Together they can **form an adduct**: A + B → A-B
    - $BF_3 + NH_3 \rightarrow F_3B\text{-}NH_3$
    - 

    LUMO-HOMO interaction
    - Forms a covalent (dative/coordinate) bond
  - **Displacement reactions** can also occur
    - A stronger Lewis base can displace a weaker Lewis base from its adduct
    - $F_3B\text{-}OEt_2$ + pyridine → $F_3B\text{-py} + Et_2O$