VSEPR Theory:

(Valence shell electron pair repulsion theory)

This was proposed by Gillespe & Nyholm

- It mainly deals with repulsions in between $e^{\ominus}_s$ & shapes of molecules.

Postulates:

The electron pairs present in valence shell of central atom will be situated around it so that repulsions are minimum.

- The electron pair shared between two atom is called localised (fixed) electron pair & the bond is called localised electron pair bond.

Order of repulsions in between various Electron pairs:

Lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

- Lone pair is attracted by one nucleus where as bond pair by two nuclei.

  $\therefore$ lone pair occupies more spaces & bond pair less space
- In case of bond pairs, triple bond causes more repulsion than double bond and double bond more than single bond
- The bond pair – bond pair repulsion is influenced by EN of central atom (BP – BP repulsion $\propto$ EN)
- If the central atom contains only bond pairs, the molecule will have regular geometry. If one or more lone pairs are present, it will have irregular geometry

Thus, shape of molecule depends on extent of mutual repulsions between various electron pairs.

Eg : $CH_4 \rightarrow$ 4 bond pairs & no lone pairs.

$\therefore$ Its shape is regular tetrahedral

In ammonia, there are three bond pairs & one lone pair.

$\therefore$ shape is irregular i.e., pyramidal.

In H_2O, these are two bond pairs & two lone pairs

$\therefore$ shape is irregular i.e., angular.

Due to the presence of lone pairs, bond angles are deviated.

VSEPR theory is useful to predict the shapes of molecules, and type of hybridization, based on the no of electron pairs present in valence shell of central atom