Day-31

→ Incorporation reaction :

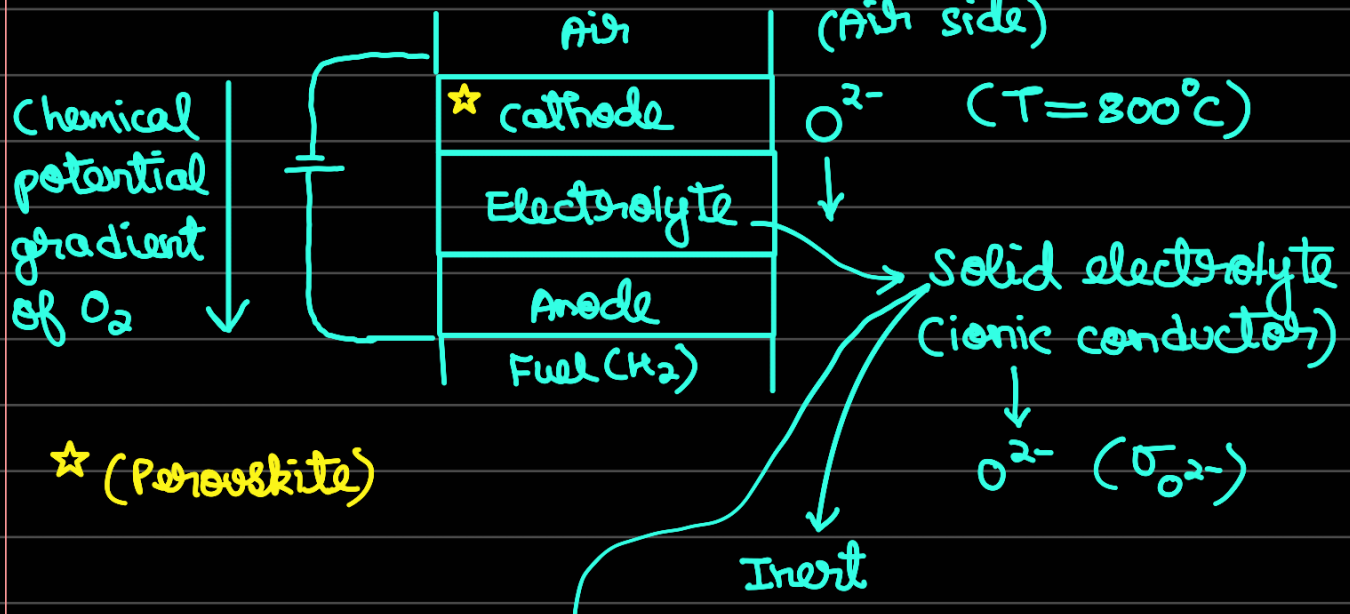
Interaction of the material with an environment (X_2 gas)

Dopant which you introduce introduces a particular → compensating defect → function
→ ionic

Host : Si Dopant : P

$$P \longrightarrow P_{Si}^{\cdot} + e'$$ (n-type)

→ Solid oxide fuel cell (SOFC) :



poor electronic conductor
(Else it will short circuit)

wide band gap material

☆ Create oxygen vacancies (or interstitials) for conducting O^{2-} ions.

Oxygen vacancy $\longrightarrow [V_O^{\cdot\cdot}]$

$\downarrow$

Aliovalent doping

$\sigma_{O^{2-}} = [V_O^{\cdot\cdot}]\, 2|e|\, \mu_{O^{2-}}$

Parent material $\rightarrow ZrO_2$

Schottky: $V_{Zr}^{''''} + 2V_O^{\cdot\cdot}$ (depends on K_s)

N_O' , $Cl_O^{\cdot}$

$$Zr_{Zr}^{x} + 2O_O^{x}\, Cl_2 \xrightarrow{ZrO_2} Zr_{Zr}^{x} + 2Cl_O^{\cdot} + O_2$$

No extra O vacancies here

So N_O' is better choice than $Cl_O^{\cdot}$ (although in practice none used)

3+ , 2+ , 1+

Y_2O_3 CaO Cu_2O

Y_{Zr}' Ca_{Zr}'' Cu_{Zr}'''

$\hookrightarrow$ Size mismatch

go for this (Size near to Zr)

$$Y_2O_3 + 2Zr_{Zr}^{x} + 4O_O^{x} \longrightarrow 2Y_{Zr}' + 3O_O^{x} + 2ZrO_2 + V_O^{\cdot\cdot}$$

8 mol % of Y_2O_3 in ZrO_2

we have $Zr_{1-2x} Y_{2x} O_{2-x}$

→ Anion Vacancies :

cation interstitials → solid state electrolyte for Na-ion Battery

↓

$Na_i^{\cdot}$

$\sigma_{Na} = [Na_i^{\cdot}] |e| \mu_{Na_i^{\cdot}}$

Parent material : $NaZr_2(PO_4)_3$

Aliovalent dopant : $Na_4Zr_2(SiO_4)_3$

$3 Si_P^{'} + 3 Na_i^{\cdot}$

- $LiCoO_2$ → electrode in Li-ion Battery

↓

electronic conductor

Vacancy doping

Li-deficient $LiCoO_2$: $V_{Li}^{'} + h^{\cdot}$

$CoO_2 \xrightarrow{LiCoO_2} 2O_O^{x} + V_{Li}^{'} + Co_{Co}^{\cdot}$ *

(Hopping mechanism of conduction)

* can be written as $h^{\cdot} + Co_{Co}^{x}$ (showing $h^{\cdot}$ is not localised to any site)