Day-14

→ materials used in SOFC : → chemical energy (fuels) → electrical energy

Cathode : electronic conductor
Anode : ↗

Electrolyte medium → ionic conductor
↓ solid ↓ oxide

Electrolyte : ZrO_2

Cathode → Perovskite (ABX_3 → a)

CF lattice

n times the stoichiometric unit

→ CF : Zr at (0,0,0)
O at (1/4, 1/4, 1/4), (1/4, 3/4, 1/4)

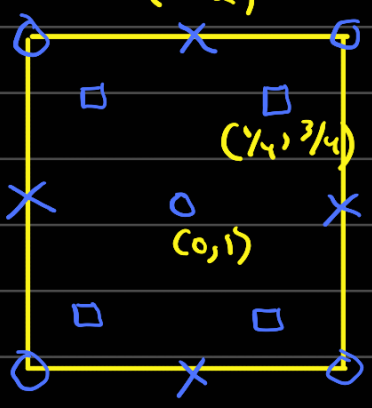
a.) 2D proj. ⊥ to [001]

b.) motif ?

c.) O–Zr–O Bond angle

d.) Distance between nearest neighbour O^{2-} ions and how many for each O^{2-} ?

Ans) a = (1/2)



b.) Zr at $(1/2, 1/2, 0)$, O at $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$ and $(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$

c.) $\vec{p} = (\frac{1}{4}, \frac{-1}{4}, \frac{1}{4})$

$\vec{q} = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

$$\vec{p} \wedge \vec{q} = \cos^{-1} \frac{1 - 1 + 1}{\sqrt{3} \times \sqrt{3}}$$

$$= \cos^{-1} 1/3$$

d.) $d = \frac{5.4}{2} = 2.7 \text{ Å}$

No. of nearest neighbours = 6

→ Perovskite : ABX_3

Eg: $SrTiO_3$ (1 motif / u.c.)

CP → Sr at (0, 0, 0)
O at face-centres
Ti at body-centre

$Sr^{2+} Ti^{4+} 3O^{2-}$

Dipole moment = 0 (μ) → paraelectric

$\frac{\mu}{V}$ → electric polarization
↳ volume

If $\mu \neq 0$, ferroelectric

Distort slightly the c-axis of $SrTiO_3$
↓ ↓
order of pm $\mu \neq 0$, tetragonal.

→ $BaTiO_3$ (distorted perovskite)

If: Ba at (0,0,0)
Ti at (½, ½, 0.482)
O at (½, ½, 0.016), (½, 0, 0.515),
(0, ½, 0.515)

$a = 3.999$ Å, $c = 0.4018$ nm

a) Draw [010] projection of the crystal
b) calculate μ/V.

→ ASSIGNMENT

→ complex motifs: $C_6H_{12}NCl$

→ Alternative ways:

Lattice + motif → crystal structures

metallic structures → crystal structures adopted by metallic elements.

→ Close Packing of hard spheres

↓

Hard sphere model of crystals