Nishant Jindal

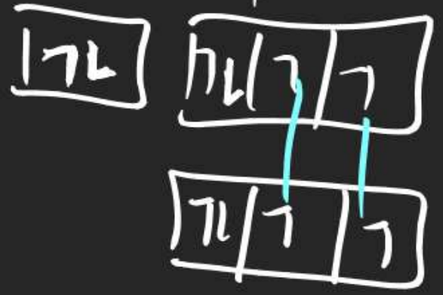
CHEMICAL BONDING

MOT [Molecular orbital theory]

Drawback

acc. to V.B.T O_2 is Diamag. but actually it is Paramag

$O = 1s^2\ 2s^2\ 2p^4$



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(2) V.B.T Can't explain formation odd e^- molecule

(3) V.B.T Can't explain fractional Bond order in diatomic molecule but in polyatomic molecule it is explained by Resonance.

NO

B.O = 2.5

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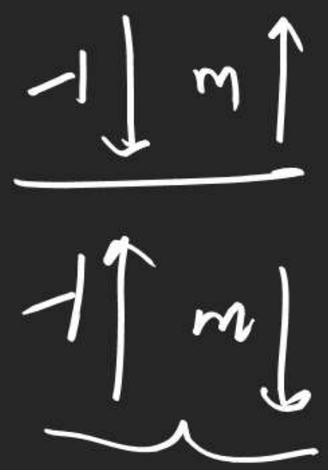
Hund's and mulliken

$$\lambda = \frac{h}{mv}$$



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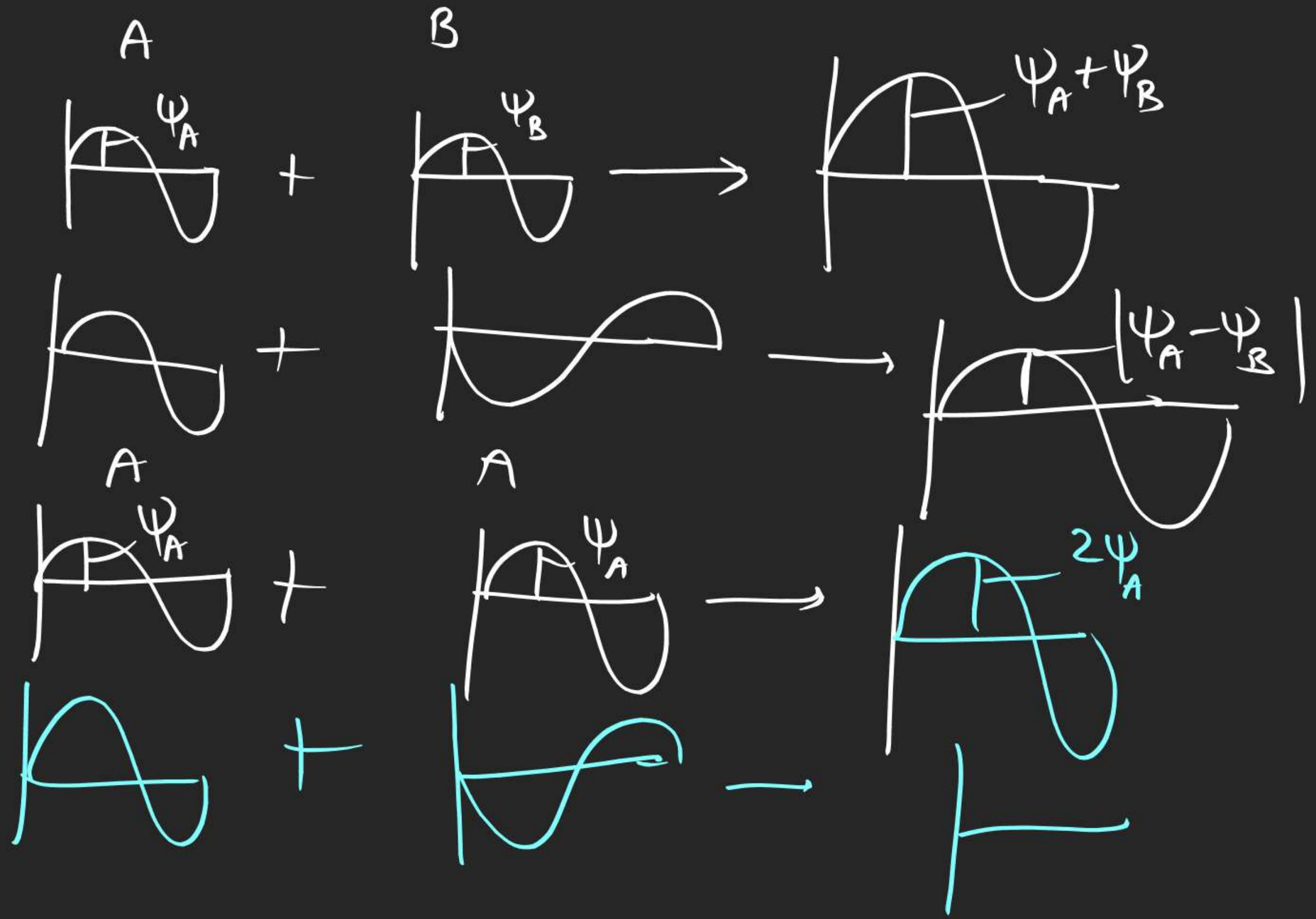

When e^- wave meet in same phase then there would be constructive interferance and e^- probability ↑ between nucleus of both bonded atom due to att; formed molecular orbital named as 'Bonding molecular orbital (B.M.O) which has lower energy than the atomic orbital.

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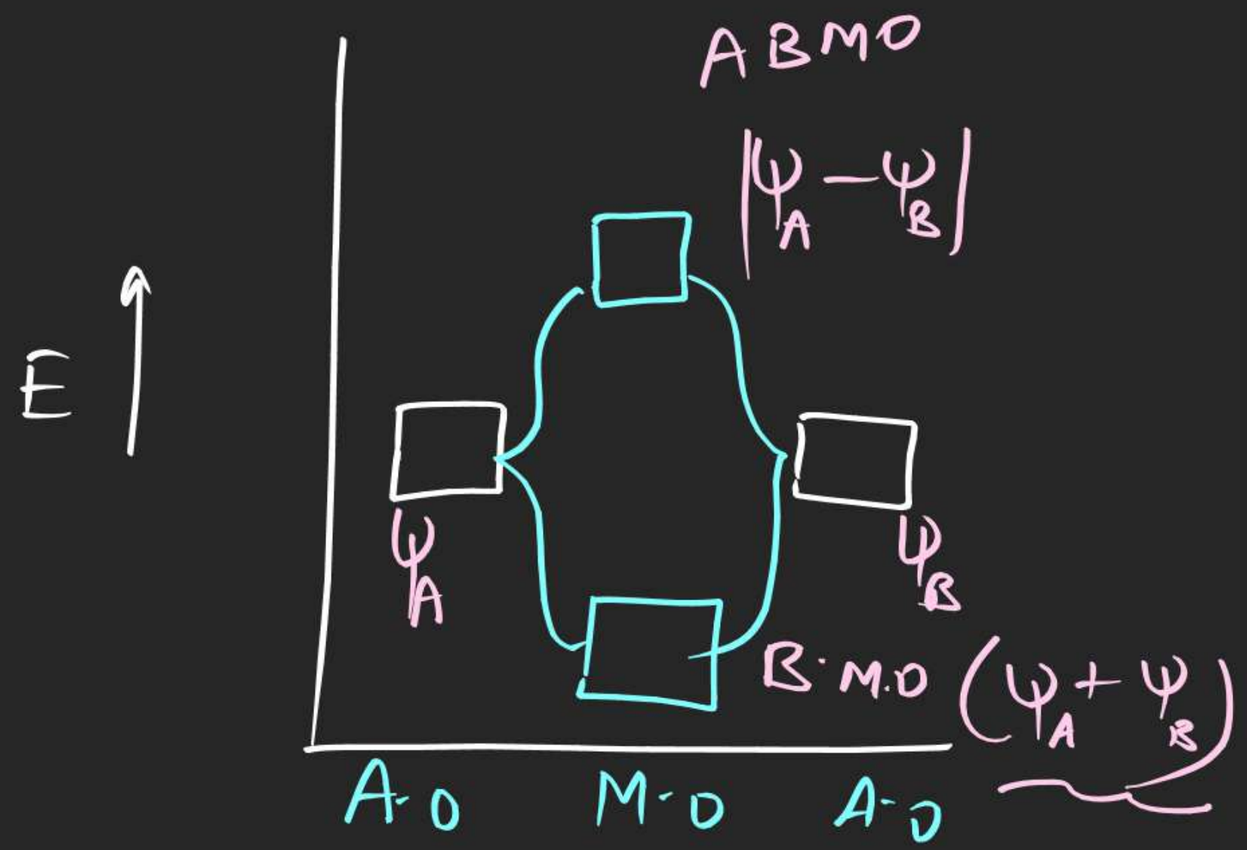

When e^- wave meet in opposite phase then there would be distructive interferance e^- probability ↓ between nucleus of both bonded atom due to repulsion formed molecular orbital named as antibonding molecular orbital (A.B.M.O), which has higher energy than the atomic orbital.

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V.B.T Can't explain paramag nature of O_2 molecule

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CHEMICAL BONDING

Wave function of molecular orbital is explained by L·C·A·O [Linear Combination of atomic orbital] that may be of two type:
- axial
- sideways

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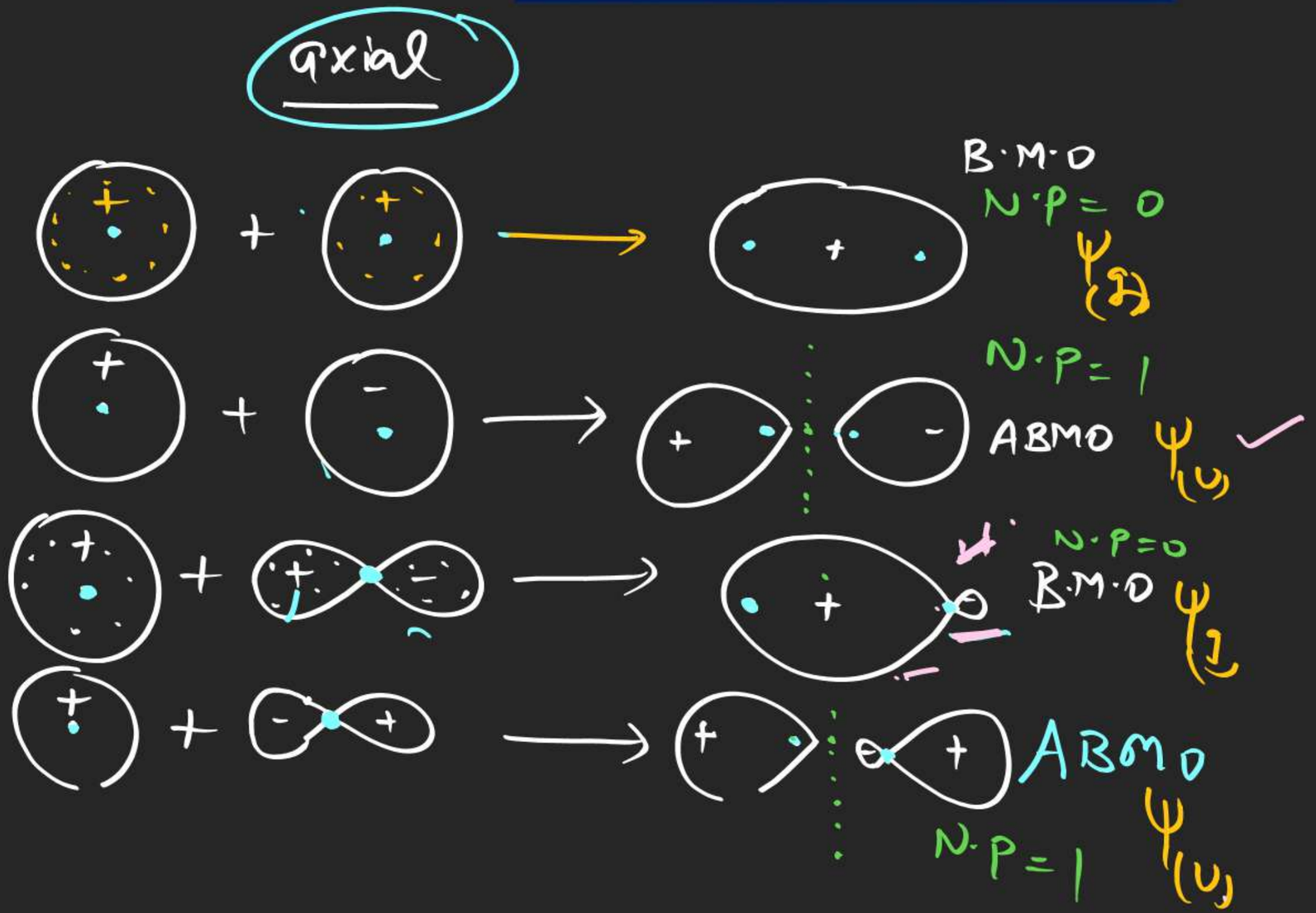
CHEMICAL BONDING



S + S ++ , + −

S + P ++ , + −

P + P ++ , + −

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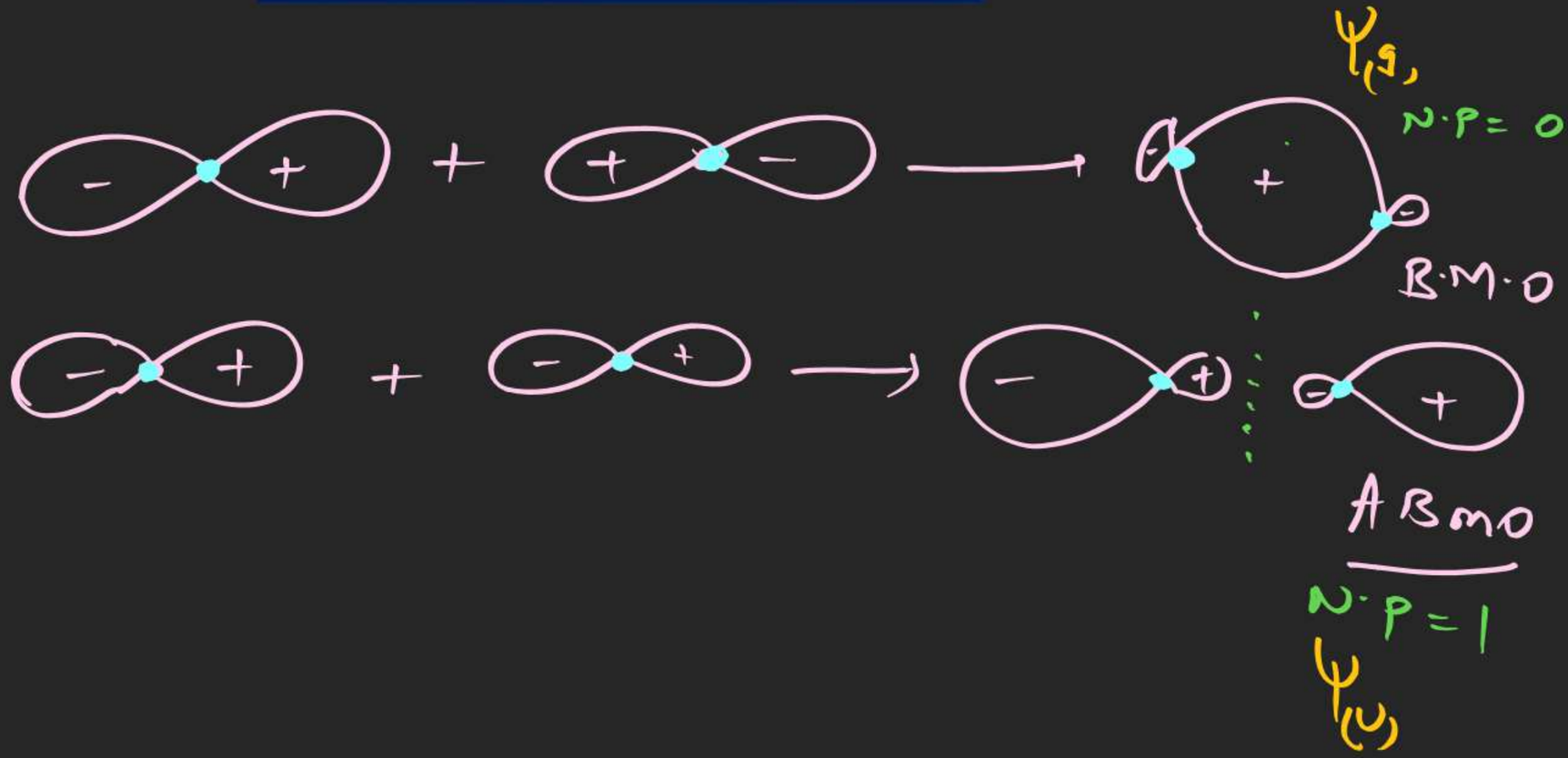
CHEMICAL BONDING



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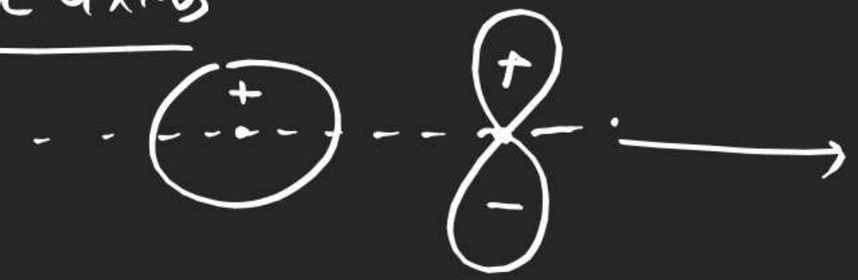
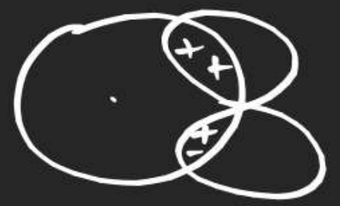
N·B·M·O (non bonding molecular orbital)

if x axias



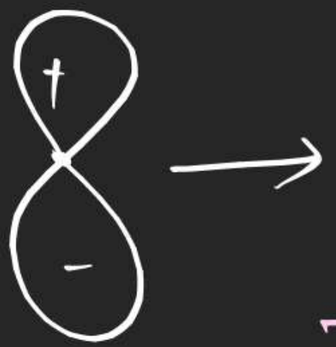
p_y or p_z



N·B·M·O

p_x

+



p_y or p_z

N·B·M·O

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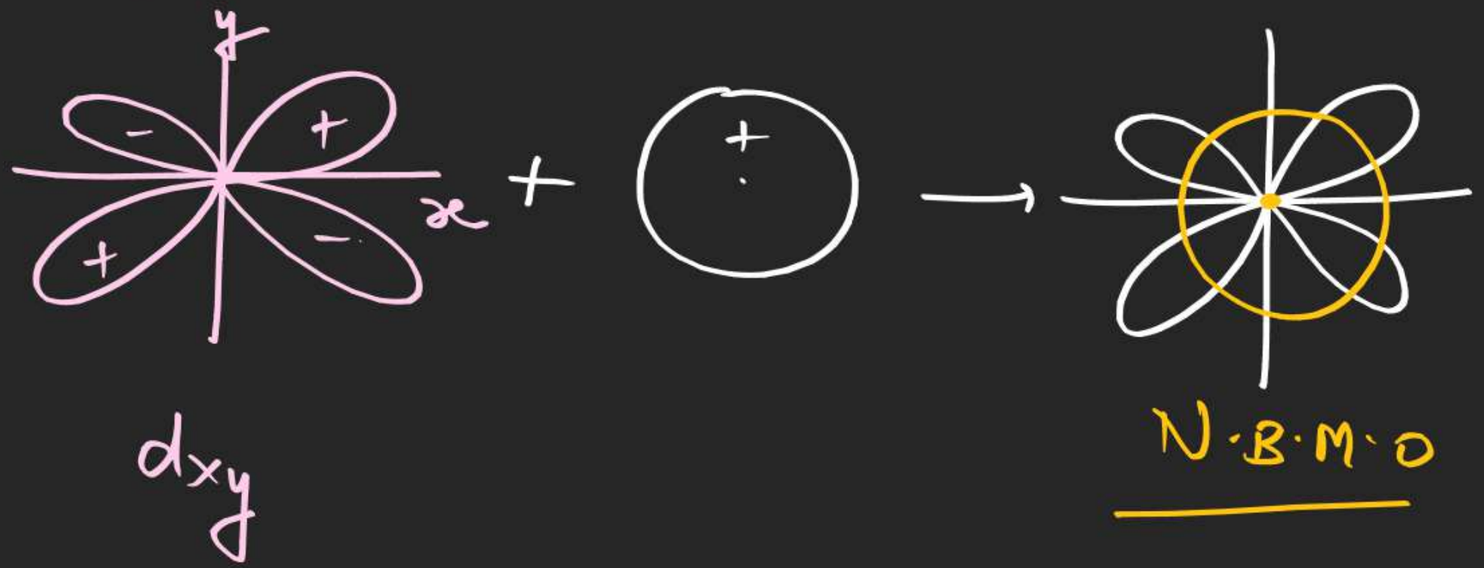
if z is internuclear axis



d_{xy}

N·B·M·O

If

and — if z is internuclear axis
then $d_{x^2-y^2}$ and d_{xy} form N.B.M.O

and — if z is internuclear axis
then $d_{x^2-y^2}$ or d_{xy} form N.B.M.O

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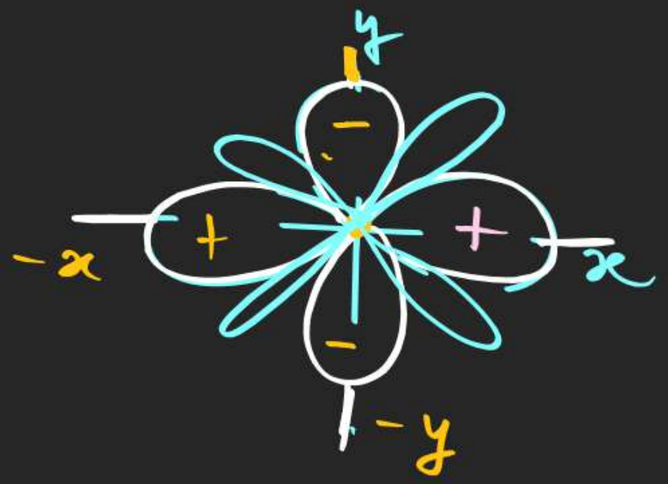
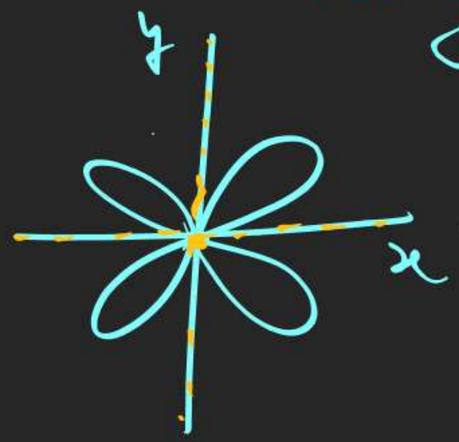


N·B·M·D

$d_{x^2-y^2}$



Same phase

opposite phase

N·P = 2

B·M·D

A·B·M·D, N·P = 3

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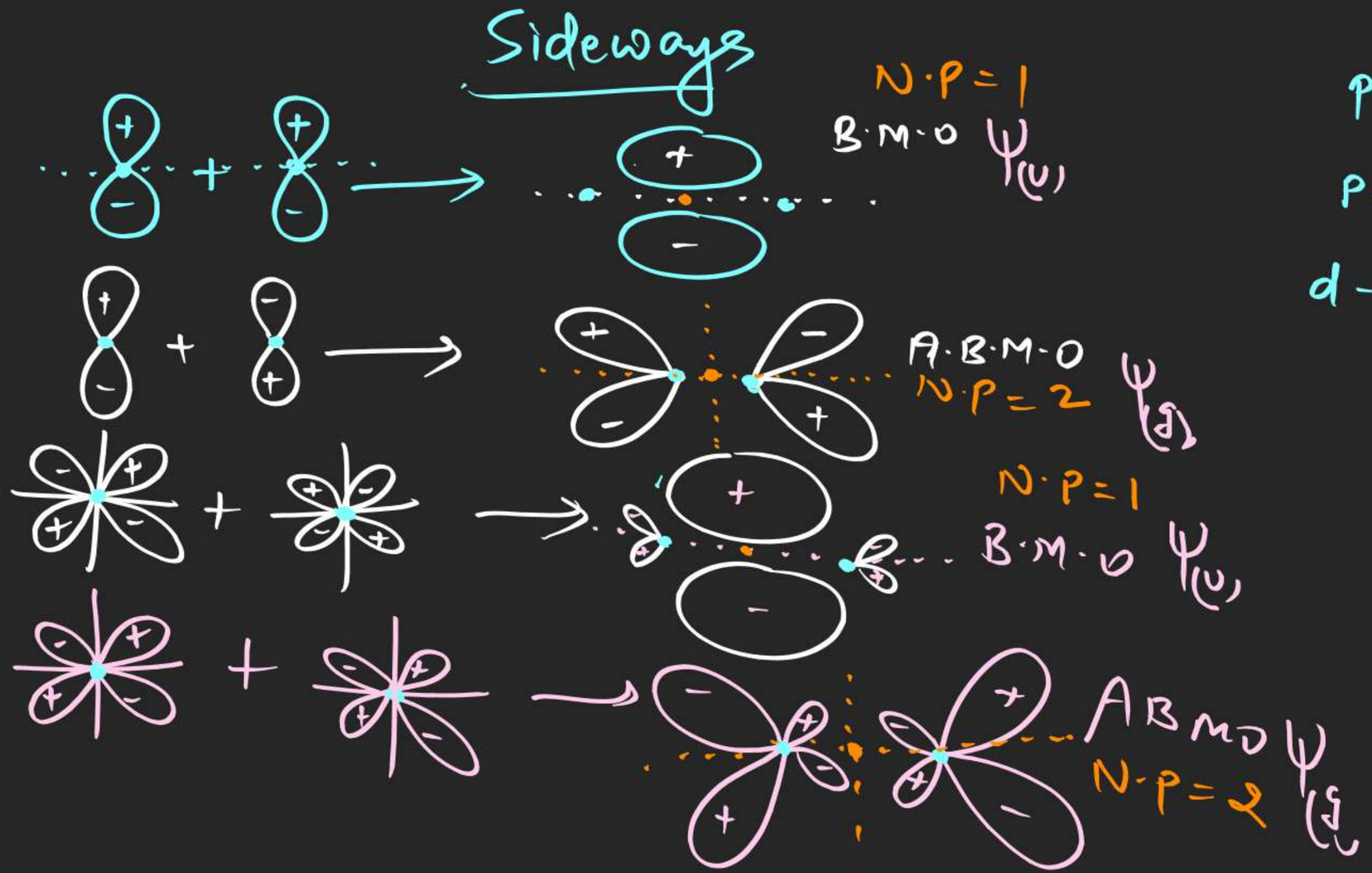
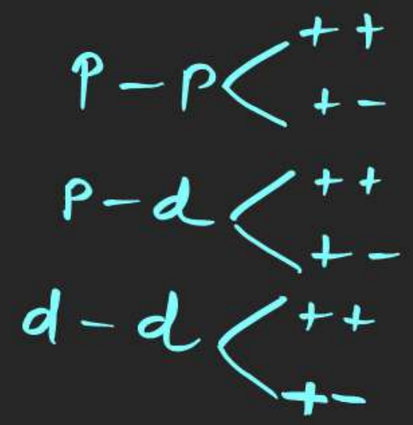
CHEMICAL BONDING





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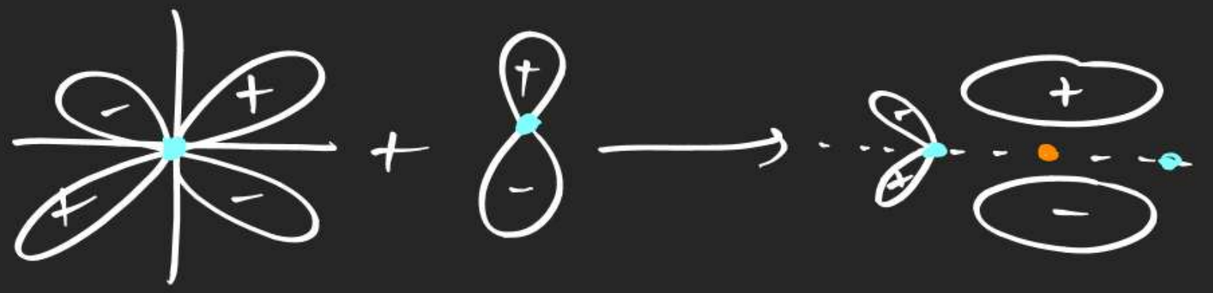
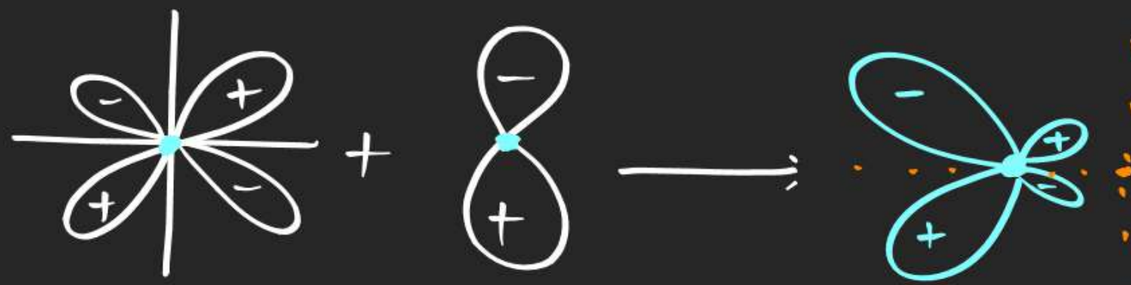
CHEMICAL BONDING



B.M.O

N.P = 1

$\psi_{(u)}$



$\psi_{(g)}$

A.B.M.O

N.P = 2

if N.p is in even number = $\psi_{(g)}$ (geroide)

if N.p is in Odd number = $\psi_{(u)}$ (Ungeroide)

Nodal plane ⇒ Which has zero e^- probability and must be passed through nucleus of atomic orbital

in case of molecular orbital must be passed through mid point of both nucleus.