

# CH 107 Assignment

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## **What I have learnt from this week's lectures:**

This week's content explained the concepts of Valence Bond Theory which I have been studying since 11<sup>th</sup> grade. It was really fun to deeply study the concepts whose results we have been applying blindly till now.

We started off with solving Hamiltonian for  $H_2^+$  and  $H_2$  molecules. We used Born Oppenheimer approximation to eliminate some terms and simplify the expression further. Then we resorted the use of Linear Combination of atomic orbitals of  $H_{atom1}$  and  $H_{atom2}$  to try solving for the Hamiltonian. Later then we came across  $S$  (Overlap Integral), Secular equation,  $J$  (Coulomb Integral) and  $K$  (Exchange Integral) to get the electronic states of  $H_2$ .

From lecture-3 we learn about the hybridisation of orbitals using LCAO starting from  $sp$  hybridisation and ending at  $sp^3$ . We solved for the coefficients of the combining orbitals and proved that even the change of axes will not change the net contribution of  $p$  orbitals or change the hybridisation itself.

## **What I find difficult to grasp in this week's lectures:**

The terms Overlap Integral, Secular Equation, Coulomb integral and exchange integral were a bit hard to grasp at first. Other than those, other topics are clear to me.