CH107 Home Assignment Week-5

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We started this week with our transition from atoms to molecules. We tried to build a model with H_2^+ and then extend the model for other multi-electronic molecules. While writing the Hamiltonian for the H_2^+ and H_2 molecule/ions, we used the Born-Oppenheimer Approximation, which considers that Nuclei are stationary with respect to electronic motion. Hence, the interaction energy term between nuclei ended up having a parametric dependence for different instants. The resultant TISE can be solved under Elliptical Polar Coordinates at one R.

Next, we started chemical bonding with the Valence Bond Theory Model, where we also included ionic contributions in the overall wavefunction. Then, we were introduced to the Molecular Orbital Theory (MOT). A MO is generated by a Linear Combination of Atomic Orbitals and is a Polycentric Wavefunction that spreads throughout the molecule. We then did the Linear Combination of the 1s orbitals of two H atoms to form a bonding and an antibonding MO. Then using the indistinguishability property and the definition of Normalization, we found the Normalization constant for the BMO and ABMO. While doing this, we encounter a new term, which we henceforth labeled as the "OVERLAP INTEGRAL (S)". This integral also makes intuitive sense since it comes out as the product of the two wavefunctions inside the integral, which can be indicative of the common region. Also, this is a function of the parametric constant R_{AB} only which further helps build a picture for the same (Not the same as the common area of overlap!!!)
Further analysis of the overlap integral leads us to realize that S is a qualitative measure of bond strength. We learned to plot the variation curves for S with change in R_{AB}.

An important point to note is that our BMO and ABMO are no longer the Hamiltonian operator's eigenstates (We need to calculate average values!!). Also, to compare if Bond Formation is feasible at all, we looked at the Energy released due to Stabilization, which gave us the Coulomb Integral as well as the Exchange Integral, out of which the latter has no classical analogue. We then were able to calculate energies as a function of internuclear separation, R_{AB}. Then, we concluded that Energy lowering for BMO must be due to the Exchange QM Integral. The contours/surface plots helped us to understand that Electron Density is delocalized over the entire molecule, but the spatial distribution is different for BMO and ABMO.