Lecture 23

Computational Chemistry

Study Goal of This Lecture

- Molecular orbital theory
- Basis sets
- Density funtional theory

23.1 Preface

The LCAO approach for H_2^+ can be generalized to treat many-electron molecules by using Slater determinant. Silbey's textbook has a nice intro. on this in 11.4&11.5. I understand you are already familiar with this so I will go beyond and introduce some basic terminologies of computational quantum chemistry. Moreover, the valence bond method described in Silbey's textbook 11.6 is also quite useful. But we will basically skip Ch.11.4-11.6. Interested students should read them by themselves, though.

Instead we will briefly discuss the basic of quantum chemistry and how to "calculate" the electronic structures using nowadays computater system.

Solving Schrödinger equation for molecular systems are quite routine jobs nowadays.

Now, we go to slide for more introduing!