The goal of this assignment is to choose a recent paper from the literature and to understand the role of quantum mechanics in the research. This is meant to illustrate the usefulness and importance of quantum mechanics in modern research.

Assignment:

• Pick a full paper (not a communication or letter) published in 2005 - 2007 that includes a quantum mechanical calculation. I suggest looking in JACS, JPCA, or JPCB.

• Your paper may not be longer than 2 typed pages with minimum 1.5 line spacing, 11-pt font, and 1-inch margins. This space restriction includes any figures or additional references. I suggest that you use a spelling checker and possibly a grammar checker.

• The heading of your paper should be the title and authors of the literature paper, with the literature reference (i.e., journal, volume, pages, year). The heading should be centered, and your name should go in the upper right corner.

• The paper should address the following questions:
  1. What are the overall goals of this paper?
  2. What was the quantum mechanical calculation performed?
  3. How did this quantum mechanical calculation help the authors achieve their goals?
  4. What chemical and physical insights were provided by the quantum mechanical calculation?
  5. Provide a personal critique of one or more aspects of the calculation. For example, you could comment on the technical approach (if you are familiar with it), the interpretation, the credibility, the usefulness, or the integration with experiments (if applicable). You could also make suggestions for future calculations.

Your paper should not summarize the entire literature paper, but rather should focus on the quantum mechanical calculation. You do not need to provide any technical details about the calculations. For example, the first paragraph could summarize the overall goals of the paper. The second paragraph could start with a sentence such as: “The authors used the Hartree-Fock method to calculate the wavefunctions and energies of a series of molecules.” Then you could go on to explain how the results of these calculations helped the authors achieve the goals of the paper and provided various types of chemical/physical insight. Due to the space limitations, you should be brief and concise when you address the questions above.