Molecular Modeling in Process Engineering

2023/2024

Project 6

1) *Quantum Chemical based Calculation of energies and energy changes: effect of basis set*

The purpose is to compute the impact of basis set on the determination of energies at three different levels of theory.
It is requested to determine the energy change for the reactions:

$H_2 \rightarrow 2H$
$CH_4 \rightarrow CH_3 + H$

At the following levels of theory:

HF, DFT (B3LYP and other functionals of your choice), and MP2.

As basis set you are requested to use at least the Pople and correlation consistent (cc) families of basis sets.
When performing the calculations:
- try to use some of the calculations specifying the basis set in the input.
- perform some calculations using both molpro and gaussian and check if the energies are exactly the same when using same level of theory and same basis set.
- try to impose the symmetry, at least for methane and methyl, when performing the calculations, in order to speed up the calculations. Take note of the symmetry group identified by the code.
- calculate by hand the number of basis and gaussian functions for at least three different basis sets for three different systems.

Remember to include the zero point energy corrections if you want to determine the correct bond energy. The experimental bond energy is 103.2 kcal/mol for H2 and 103.3 for CH4.

2) MEP estimation based on a multireference method

It is required to estimate the MEP for the reaction:

$CH_4 \rightarrow CH_3 + H$

Calculations must be performed with CASPT2 as the level of theory and cc-pVDZ as the basis set.
One active space must be imposed.
Report on excel the energy trend at different C-H distances and compare the values obtained with CASPT2 and those obtained using HF
The use of Molpro as software is recommended. Where in the output file is the information about the basis set used? and the energy of the different types of interaction?