Molecular Modeling in Process Engineering

2023/2024

Project 8

Preliminary steps

Download and install the software AIMAII.

The program needs the wfn file from QM calculations (see manual).

Electron Density Analysis

1) Calculate at the B3LYP/6-31G** level the electron density of the following systems: ethane, ethene, ethyne, and benzene (optimize the geometry of the systems)
   By AIMAII search for:
   - Critical Points
   - Molecular graphs
   - BCPs
   - Density at the BCPs
   - Order of the C-C bonds
   - Ellipticity of the bonds

2) Calculate at the B3LYP/6-31G** level the electron density of the systems: water and water dimer (optimize the geometry of the systems)
   By AIMAII search for:
   - Critical Points
   - Molecular graphs
   - BCPs
   - Density at the BCPs

3) Calculate at the B3LYP/6-31G** level the electron density of the systems: H_2, HF and LiF (optimize the geometry of the systems)
   By AIMAII search for:
   - Critical Points
   - Molecular graphs
   - BCPs
   - Density at the BCPs
   - Laplacian of the density at the BCPs
   - Plot the L=-Lpalacian of the density