CALCULATION OF THE GEOMETRY, DIPOLE MOMENT AND VIBRATIONAL FREQUENCIES OF THE WATER MOLECULE

Use the Gaussian and/or the AMPAC program to determine the optimal geometry (bond lengths and angle), dipole moment, and vibrational frequencies of the water molecule. Comment and compare your results to experimental data.

Project 1: Basis set effects at the HF level : Leo

Perform the calculations at the HF level using various Pople and Dunning basis sets. Analyze the impact of the basis set on the computed properties.

Oral presentation: HF model / Pople and Dunning basis sets / analysis of the results

Project 2: Effects of electron correlation using perturbation theory : Sarah

Perform the calculations at the HF, MP2 and MP4 levels using various Pople basis sets. Analyze the impact of the method and of the basis set on the computed properties.

Oral presentation: HF model / Mollër-Plesset Theory / analysis of the results

Project 3: DFT calculations : Aimery

Perform the calculations at the DFT level using various exchange-correlation functional and Pople basis sets. Analyze the impact of the functional and of the basis set on the computed properties.

Oral presentation: DFT / analysis of the results

Project 4: *Ab initio* and semi-empirical calculations : Benoît

Perform the calculations using various semi-empirical schemes (MNDO, AM1, PM3, PM6), and compare the results to reference HF calculations obtained using various Pople basis sets. Analyze the impact of the semi-empirical parameterization on the computed properties.

Oral presentation: HF / NDDO semi-empirical methods / analysis of the results

Project 5: Semi-empirical Configuration Interaction (CI) calculations : Matthieu

Perform the calculations at the SCF and *full* CI levels using various semi-empirical parameterizations (MNDO, AM1, PM3, PM6). Analyze the impact of the semi-empirical method and parameterization on the computed properties.

Oral presentation: semi-empirical methods / Configuration Interaction / analysis of the results