

Theoretical study of fluorine anions solvated in small water clusters

- Determination of the equilibrium geometry: research of different isomers with AMBER program (based on the Molecular Dynamics) and optimization of the geometry with MOLCAS program (based on HF and DFT calculations).
- Calculation of the infrared spectra of each isomers with MOLCAS program.

Contacts: J. Douady – <u>julie.douady@ensicaen.fr</u> – 02 31 45 25 77