Work Plan

The main goal of my short-term scientific mission (STSM) will be to work on a reliable computational protocol for obtaining effective electric and optical molecular properties (linear and nonlinear susceptibilities), i.e. the properties modified by the environmental effects. The work will be focused on the assessment of the quality of various implicit and explicit solvent models in the evaluation of electric and optical properties of selected organic molecules in solution. Specifically, we plan to focus on the following issues:

- The use of polarizable force fields in MD simulations of a solvated NLO system

  Since our work uses solvents of different multipolar character it would be interesting to compare the application of polarizable force field (FF) description with non-polarizable FF and QM/MM (DFT-B) approaches.

- Calculations of vibrational contributions to electric properties of *para*-nitroaniline in solution.

  One of the important things we need to take into an account are the vibrational contributions. These are highly important for a molecule of *para*-niroaniline thanks to the non-planar amino group.

- Further practice with the rigorous local field (RLF) explicit solvation model.

  The RLF model has been applied in our previous work, but it is necessary to learn more about its possible developments. Calculations of local fields were also done using local software LORCHI which was written by Dr. Heribert Reis who would be able to offer a better understanding of the implementation of RLF.