

Title: A quantum mechanics/molecular dynamics study of ^{35}Cl NMR relaxation in the liquid phase

The aim of this STSM is to foster collaboration between the group of Prof. Francesca Mocci (University of Cagliari, Cagliari, Italy) and the group of Dr. Sonja Grubišić (University of Belgrade, Belgrade, Serbia). Within the MOLIM COST action, both mentioned researchers are part of Working Group 1 -Energy-Resolved Methods, being Dr. Sonja Grubišić an MC member and Prof. Francesca Mocci a non-MC member.

During the one week of his visit, the Applicant I. Cvijetić will learn how to compute ^{35}Cl NMR relaxation in the liquid phase, in particular decyl methyl imidazolium, using trajectories generated either using classical mechanics or ab initio method. The integrated computational approach (MD with QM/MM) developed by the group in Cagliari is generally expected to provide reliable estimates of the quadrupolar coupling constants of monoatomic species in condensed phases, by the calculation of the electric field gradients.¹ The quadrupolar coupling stems from the interaction of the nuclear quadrupole moment and the electric field gradient (EFG) due to the surrounding charge distributions. The ^{35}Cl is a spin 3/2 quadrupolar nucleus and is useful probe to study the structure and dynamics of variety ionic and inorganic/organic chlorides. The MD simulations will be carried out using a version of the MDynaMix program, modified by the group in Cagliari to accommodate the calculation of the components of the EFG. The classical MD simulations will be performed using the AMBER program, and quantum chemical calculations on selected portion of the system will be performed using a development version of the Dalton program also in collaboration of Dr Kestutis Aidas of Vilnius University.

The aim of this project is to improve the force field parameters by scaling the charges, which are of importance in the interpretation of the experimental data obtained by ^{35}Cl NMR, since the dynamics of the system seems to be highly affect by the charge adopted for the ionic liquids, and the magnetic relaxation of Cl is highly dependent on the system dynamics. In condensed phases, and especially in aqueous solutions, a detailed description of medium and long-range intermolecular effects, such as electrostatic and van der Waals are required, and ionic liquids have been proved so far to be extremely sensitive to the proper choice and tuning of these parameters. We plan to test the transferability of the developed/improved parameters by performing simulations of the previous investigated systems with pure ionic liquid and its mixtures with water at varying content, and verify the effect on structure, dynamics and therefore magnetic relaxation, of charge scaling.

References

1. K. Aidas, H. Ågren, J. Kongsted, A. Laaksonen and F. Mocci, *Phys. Chem. Chem. Phys.*, 2013, 15, 1621.