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

Scientific report

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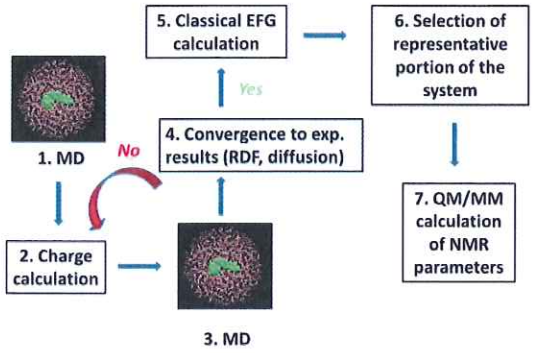

Figure 1. **a)** Molecular electrostatic potential of 1-decyl-3-methylimidazolium chloride (DMimCl) **b)** Proposed scheme for calculation of NMR parameters of ionic liquid

The aim of this project was 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 (IL), and the magnetic relaxation of Cl is highly dependent on the system dynamics.

During my visit to prof. Mocci, we discussed the simulation results obtained on the dynamics of highly charged systems (Figure 1a), and the methods used to analyze it, and to calculate magnetic relaxation parameters.[1] We examined possible strategies to improve the simulation of such systems and the agreement with ^{35}Cl magnetic relaxation data by force field parameterization. I performed preliminary quantum mechanical calculations to improve the charges of DMimCl ionic liquid using Gaussian 09 program, as well as MD simulations using AMBER program to check the influence of assigned charges on the dynamics of system. We made plan for the future work, which is given briefly in Figure 1b. The results of this project might lead to the improved force field parameters for imidazolium-based ionic liquids.

References:

1. Aidas, K.; Agren, H.; Kongsted, J.; Laaksonen, A.; Mocci, F. A Quantum Mechanics/molecular Dynamics Study of Electric Field Gradient Fluctuations in the Liquid Phase. The Case of Na^+ in Aqueous Solution. *Phys. Chem. Chem. Phys.* **2013**, *15* (5), 1621–1631.

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