



D11.1 – KTH transnational access success story

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ABSTRACT:

This deliverable is about a successful collaboration between Dr. Kęstutis Aidas and Dr. Dovilė Lengvinaitė from the Vilnius University (Lithuania), and prof. Aatto Laaksonen, from the Stockholm University (Sweden), which started through an HPC-Europa3 transnational access visit. This collaboration produced important results concerning intermolecular structure of mixtures composed of imidazolium based ionic liquid and water.

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Materials Science, NMR chemical shifts, room-temperature ionic liquids, quantum mechanics, molecular mechanics, international collaboration, transnational access

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Executive summary

Dr. Kęstutis Aidas and Dovilė Lengvinaitė (PhD student at the time of the first visit) from the Vilnius University, Lithuania, were visiting prof. Aatto Laaksonen, from the Stockholm University, Sweden to work on theoretical modelling of nuclear quadrupolar coupling constants relevant in the field of Nuclear Magnetic Resonance (NMR) relaxation by using molecular dynamics simulations and combined quantum mechanics/molecular mechanics approaches. Very interesting NMR measurements of water mixtures with some imidazolium based Ionic Liquids (IL) have been very recently carried out by the NMR spectroscopy group of Vilnius University, Lithuania. These experimental findings reflected the structural changes of the samples with changing concentration of IL and water. During their visits, Dr. Aidas and his student Lengvinaitė worked on large-scale classical molecular dynamics (MD) simulations of the IL/water systems in order to sample the phase space and record the trajectories. These have been used in the subsequent calculations of NMR shielding constants using linear response quantum mechanics/molecular mechanics approaches. The produced results shed light on the early stages of water pocket formation within the IL and gave valuable theoretical interpretation for the experimental findings. These visits with the help of HPC-Europa3 project have secured a strong collaborative link between the two universities in the field of physics.

In this document, we first give a statistical summary of all KTH visitors and afterwards we detail the success story of the visit of Dr. Kęstutis Aidas and Dovilė Lengvinaitė from the Vilnius University, Lithuania to KTH, Stockholm, Sweden.

1.1 Introduction

1.2 Statistical summary of KTH hosted visitors for the HPC-Europa3 project

KTH Royal Institute of Technology in Stockholm, Sweden, is one of the 9 hosting HPC-Europa3 (HPCE3) partners and it has committed to host 36 visitors during the whole project duration. The role of KTH is to act as a regional access partner with responsibility to accept applicants from Baltic countries along with applications from other countries.

KTH responsibility is also to develop the awareness of HPC usage possibilities in research within these countries. One of the main actions KTH has committed to was to organise an HPC conference in one of the Baltic countries.

Another interesting aspect was the new possibility of HPCE3 project with respect to previous editions to accept visitors from SMEs to universities and vice versa to boost the knowledge transfer between academia and industry. Even in this initiative KTH managed to be active and accepting two visitors to a Swedish SME Airinnova AB (<http://airinnova.se/>).

During the period of May 2017 – April 2021, 50 visits were approved to KTH from 25 countries by overdoing its commitment with about 139%. Out of 50 visitors, 11 (22%) were from the Baltic countries.

Country	Number of visitors	Country	Number of visitors
Latvia	4	Greece	2
Lithuania	6	Turkey	2
Estonia	1	Croatia	2
Poland	2	Slovenia	1
Italy	1	Switzerland	2
China	1	UK	5
Serbia	2	Denmark	1
Belarus	1	Spain	3
Romania	1	Finland	4
Portugal	1	Brazil	2
France	1	India	1
Germany	1	Czech rep	2
US	1		

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KTH also organised the 4th Baltic HPC and cloud conference in Riga, Latvia in collaboration with Riga Technical University (RTU), which was originally planned to take place on 22-23 April 2020. However, due to the COVID-19 pandemic it was postponed to 15-16 of April 2021 (<https://hpc.rtu.lv/4th-baltic-hpc-and-cloud-conference/?lang=en>)



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4TH BALTIC HPC AND CLOUD CONFERENCE



Important: Due to the current situation regarding the COVID-19, the conference has been postponed to April 2021.

Riga Technical University together with the [HPCEuropa3 project](#), University of Tartu, and KTH Royal Institute of Technology cordially invite you to the **4th Baltic HPC and Cloud Computing conference** in Riga on 23-24 April, 2020 (**NB conference has been postponed to April 2021**). This year the conference will feature a lot of new topics – including talks on innovative uses of HPC and Cloud computing and presentations about HPC/Cloud computing services ranging from EuroHPC supercomputers to Machine learning. The conference will be especially relevant for **different research communities that use HPC, including students, HPC experts and companies**.

Why you should attend?

- A great venue for networking – leading HPC and Cloud Computing community members from Baltic and Nordic countries will be present;
- Unmatched access to the finest HPC minds from Baltic and Nordic countries;
- Latest HPC and Cloud Computing information that you can apply when you return to work;
- Source of inspiration for new ideas and practical uses of HPC and Cloud Computing;
- Practical workshops on HPC and Cloud Computing;
- Meet with leading specialists and solve your HPC or Cloud Computing issues on the spot;

By this, KTH accomplished all its committed goals within the HPC-Europa3 project.

1.3 Summary of the HPC-Europa3 application project of Dr. Kęstutis Aidas and Dovilė Lengvinaitė from the Vilnius University, Lithuania

To model NMR properties of liquid-state molecules, one often relies on the so-called supermolecular approach. This procedure involves geometry optimization of the molecular complex composed of the target molecule and a few important solvent molecules, for example, those which are hydrogen-bonded to the target molecule. The entire molecular complex could also be embedded in some kind of the dielectric continuum which is used to account for bulk solvent effects. The NMR properties are then calculated for this geometry-optimized complex using now standard GIAO technique to remove gauge-origin dependence of the NMR shielding constants. Supermolecular approach is certainly cost-effective, and results of reasonable accuracy are often obtained. However, this scheme suffers from poor description of the long-range electrostatic intermolecular interactions because discrete nature of solvent molecules is neglected by the continuum approaches. Moreover, dynamical and temperature effects are neglected since geometry optimized structure represents just a single point on the multidimensional potential energy surface.

These problems can be very effectively dealt with by using an integrated approach where classical MD simulations are combined with the hybrid quantum mechanics/molecular mechanics, QM/MM, model for the calculation of the NMR properties. MD simulations allow sampling the phase space of the molecular system under proper thermodynamic conditions, whereas QM/MM approaches account for anisotropic distribution of the solvent molecules around the solute in the calculation of the electronic response properties. Moreover, large number of solvent molecules can be easily included in the QM/MM calculation so that the effects of electrostatic interactions are converged. Mutual solute-solvent polarization interactions are accounted for by using explicitly polarizable force fields in the QM/MM calculations. Short-range Pauli repulsion can also be considered by extending the quantum mechanically treated region to include some of the solvent molecules along with the solute. The price to be paid for the increased accuracy of the model is, however, due to the fact that large number of similar QM/MM calculations for molecular snapshots recorded during MD simulation are to be performed, typically on the order of around 100.

The integrated approach has been many times shown to be superior over the supermolecular scheme even for the cases of simple solutes in ordinary isotropic molecular solutions, see for example [1,2]. For IL systems composed entirely of ions, the effect of long-range electrostatic interactions cannot be properly accounted for by just considering a few ion pairs. Moreover, dielectric continuum models will clearly fail to take the heterogeneous nature of the IL into account. Not surprisingly, it was demonstrated that supermolecular approach fails even in the prediction of the ^1H NMR spectrum of imidazolium-based IL [3]. It is the integrated approach which only allows effectively accounting for structural anisotropies and heterogeneities inherent to the IL systems.

Classical molecular dynamics (MD) simulations of RTIL have been attempted soon after the interest in these systems was boosted some 20 years ago. MD simulations of RTIL turned out to be difficult matter due to the ionic nature of these systems [4]. RTIL are typically very viscous substances being by at least an order or two more viscous than liquid water. This implies that the dynamics of the ions is slow. Indeed, very long simulations on the order of tens of nanoseconds are required to reach thermal equilibrium. Even longer simulations are needed if dynamical properties, such as diffusion coefficient, are to be modelled. For example, 20 or 30 ns long mean-square displacement function has to be calculated in order to get converged values of the diffusion coefficient for imidazolium-based IL [5]. Furthermore, due to the long-range nature of electrostatic interactions the simulation

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box has to include at least 400-500 ion pairs to assure size-converged properties of the molecular system.

The accuracy of the QM/MM based calculations of liquid-phase properties depends on several factors. Statistically uncorrelated molecular snapshots have to be considered in the QM/MM calculations to assure that each calculation is statistically relevant. Because of the high viscosity of RTIL, the time-interval between statistically uncorrelated molecular snapshots might be considerably longer than several picoseconds as is the case of ordinary liquids, meaning that longer than usual MD simulations are to be performed. Furthermore, the type and quality of the force field used to represent classical molecules in the QM/MM calculation is of crucial importance. The unique feature of our approach is due to the fact that we can use explicitly polarizable force fields in the QM/MM calculations. Polarizable force fields allow for proper treatment of mutual solute-solvent polarization interactions which are expected to be important for the ionic liquid systems. The size of the quantum mechanically treated region of the total molecular system is yet another important issue to consider. In order to obtain accurate values of NMR shielding constants for molecules in the liquid phases, both solute and some nearest solvent molecules, especially those forming hydrogen bonds with the solute, have to be considered quantum mechanically [6]. This issue is expected to be even more important for IL-water systems and has to be carefully examined.

Very interesting NMR measurements of water mixtures with some imidazolium based IL have been very recently carried out by the NMR spectroscopy group of Vilnius University, Lithuania. Two different RTIL have been considered, 1-butyl-3methyl-imidazolium, C4Mim, and Cl⁻ as well as C4Mim and tetrafluoroborate, BF₄⁻. Interestingly, the H-1 NMR chemical shift of water was found to evolve qualitatively different with the changing concentration of water in the binary solutions of these two IL. When molar fraction of [C4Mim][Cl] is increased, the H-1 NMR chemical shift of water first exhibits an upfield shift with respect to that in liquid water. However, this chemical shift starts to shift downfield starting from certain concentration of the ionic liquid, thus exhibiting a pronounced minimum. On the other hand, the H-1 NMR chemical shift of water was always found to move upfield with the rising concentration of the [C4Mim][BF₄] IL in the binary solution. Similarly, the chemical shift of the H2 proton in the imidazolium ring was found to experience a marked down field shift with increasing concentration of [C4Mim][Cl], but it was seen to be virtually insensitive to the concentration of [C4Mim][BF₄]. Clearly, these experimental findings reflect the structural changes of the samples with changing concentration of IL and water.

The aim of present project is to model the H-1 NMR spectra of [C4Mim][Cl] and [C4Mim][BF₄] RTIL mixtures with water of various concentrations. To this end, we would follow and integrated approach. Large-scale classical molecular dynamics (MD) simulations of the IL/water systems would be carried out in order to sample the phase space and record the trajectories. These would be used in the subsequent calculations of NMR shielding constants using linear response quantum mechanics/molecular mechanics approaches. Our theoretical results are expected to shine light on the early stages of water pocket formation within the IL [7] and give valuable theoretical interpretation for the experimental findings just discussed.

It was clear that in order to achieve these goals, extensive MD simulations on the time scale of nearly 100 ns have to be performed for our IL-water mixtures composed of thousands of ionic pairs and varying number of water molecules. Also, the QM/MM calculations of NMR shielding constants are computationally demanding because the quantum mechanically treated part of the model is expected to include several molecular species simultaneously in order to account for hydrogen bonding interactions properly. These expensive hybrid electronic structure calculations would be needed to perform on hundreds of molecular snapshots recorded during the MD simulations, thus further

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increasing the demand for high-performance computational resources. Computational resources needed to perform MD simulations and QM/MM calculations on this scale were not available at Vilnius University. Furthermore, it was important for Dr. Aidas and his student Ms. Lengvinaitė to establish a viable collaboration with their host Prof. Aatto Laaksonen who is a world-renowned expert in classical MD simulations. Prof. Laaksonen's experience in simulations of RTIL was another strong stimulus for their visits at the PDC center, KTH. Therefore, these visits were the unique chance for this ambitious project to be realized.

1.4 First visit - identification of water binding modes within the ionic liquid with special interest on the formation of aggregates of water known as water pockets.

Dr. Kęstutis Aidas and his PhD student Dovilė Lengvinaitė from the Vilnius University, Lithuania, have applied by sending two HPC-Europa3 (HPCE3) applications simultaneously to the same 3rd HPCE3 call to visit prof. Aatto Laaksonen, from the Stockholm University, Sweden. This 3rd call was open at the end of the 2017 with a closing date 28th of February 2018. Naturally KTH was selected to be the hosting centre. The aim of this first visit was to work on theoretical modelling of the H-1 NMR spectra of [C4Mim][Cl] and [C4Mim][BF₄] RTIL mixtures with water of various concentrations.

During this first visit, extensive classical molecular dynamics (MD) simulations were performed for [C₄Mim][Cl] and [C₄Mim][BF₄] ionic liquids represented by 1000 ionic pairs with varying concentration of water ($\chi_w=0.05$ and $\chi_w=0.5$, respectively) using OPLS-AA force field for the ionic liquids [8,9]. The standard TIP4Pew potential was utilized for water. All simulations were performed using AMBER program [10]. Extensive equilibration of all molecular systems at the NPT ensemble was performed by heating them gradually to 500 K and then cooling to the desired temperature of 298 K. The final equilibration at ambient conditions of around 16 ns was necessary to get the density converged. We finally switched to NVT ensemble in order to record 10 ns long trajectories for further analysis.

The primary aim of the results of MD simulations was the identification of water binding modes within the ionic liquid with special interest on the formation of aggregates of water known as water pockets. They have initialized their systems by placing a water droplet of appropriate size for a given molar fraction of water within the ionic liquid. At low molar concentration of water, $\chi_w=0.05$, they have observed a rapid disintegration of the water droplet, so that well-separated water molecules are found within the simulation box. In the case of the [C₄Mim][Cl] IL, pronounced hydrogen bonding between water molecules and the chloride anions was observed with the formation of the Cl⁻...HOH...Cl⁻ aggregates. In addition, the formation of the hydrogen bonding between the oxygen atom of water and the acidic C-H bond at the 2nd position of the imidazolium ring was seen for both ILs. This in fact was anticipated due to the analysis of the experimental H-1 NMR spectra of corresponding IL/water mixtures.

At high water concentration, $\chi_w=0.5$, rather different behaviour of water molecules was observed in their mixtures with the [C₄Mim][Cl] and [C₄Mim][BF₄] ionic liquids. In the [C₄Mim][Cl] IL, water molecules were found to persistently form hydrogen bonding with the chloride anions. Interesting chloride sharing water aggregates as shown in Figure 1 were found to be rather ubiquitous. However, no water pocket-like aggregates were seen to be formed in the [C₄Mim][Cl] IL, see Figure 2. On the other hand, small water aggregates as shown in Figure 1 could be identified in the [C₄Mim][BF₄] ionic liquid. This could be expected due to the known hydrophobicity of the BF₄⁻ anions.

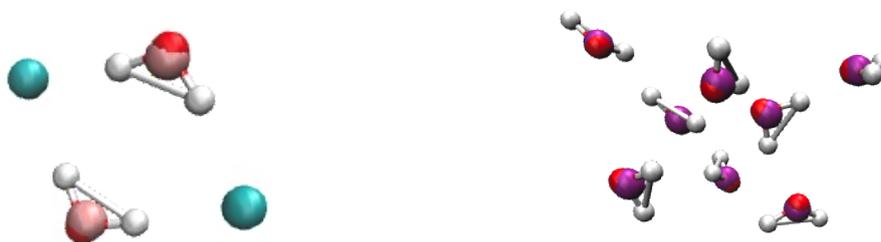


Figure 1: The associates of water molecules in the ionic liquids: $[C_4Mim][Cl]$ (on the left) and $[C_4Mim][BF_4]$ (on the right).

The results proved that the molecular trajectories recorded during present MD simulations should be used in the QM/MM calculations of NMR spectra. The results will hopefully allow for the explanation of non-monotonic behaviour of the NMR chemical shift of water with the changing concentration in the $[C_4Mim][Cl]$ and $[C_4Mim][BF_4]$ ionic liquids.

This first visit was very successful and produced the expected results, however it was obvious that further investigation of the problem was needed, and even more achievements could have been reached in future work. This triggered yet another application for the second visit with the help of HPCE3 calls which otherwise would have been difficult to realise.

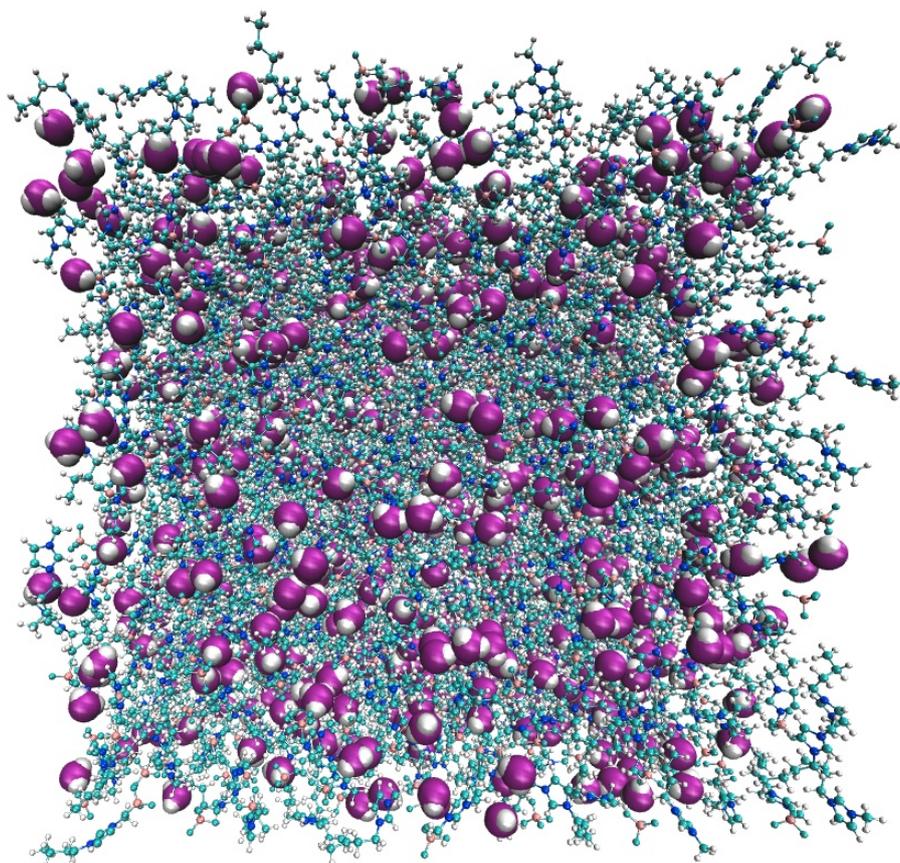


Figure 2: Simulation system of ionic liquid $[C_4Mim][Cl]$ /water mixture at $\chi_w=0.5$ water concentration.

1.5 Second visit – identification of non-monotonically behaviour of the NMR chemical shift of water with its changing concentration in the ILs

The second visit of Ms. Dovilė Lengvinaitė was primarily dedicated for the QM/MM calculations of H-1 NMR isotropic shielding constants for the mixtures of the [C₄Mim][Cl] and [C₄Mim][BF₄] ionic liquids and water. However, very strong hydrogen-bond association of chloride anions with water molecules was found in the [C₄Mim][Cl]/water system even at molar fraction of water equal to 0.5, and thus no pure water cluster were observed which would indicate water pocket formation in this mixture. This called for yet another series of MD simulations for the system of [C₄Mim][Cl]/water where the molar fraction of water is still increased to 0.75. The system was composed of 1000 ionic pairs and 3000 water molecules ($\chi_w=0.75$). The applied force fields and the protocol of simulations were the same as for other systems discussed above.

Based on previous and the new molecular trajectories, we have constructed several sets of molecular configurations to be used in the QM/MM calculations of NMR shielding constants. Each set contains 100 molecular configurations. The QM/MM calculations of the ¹H NMR isotropic shielding constants have been carried out using the QMMM module of the Dalton 2016.1 program [11]. The shielding constants have been computed using the PBE0 exchange–correlation functional along with the def2-TZVP basis set. The point charges representing the ions were the same as in the MD simulations, while for water the point charges from the TIP3P potential were selected.

We have performed QM/MM calculations of the H-1 NMR isotropic shielding constants of liquid water, so that we can reference the isotropic shielding constant of water in its mixtures with the IL with respect to that of the liquid water. Experimentally, the proton NMR signal of water shows an upfield shift with the rising concentration of the [C₄Mim][Cl] IL. Increasing the concentration of this IL still further, the signal changes its direction and shows a marked downfield shift, thus producing a clear minimum of the chemical shift at $\chi_w=0.34$. Our MD simulations show that water molecules form abundant characteristic hydrogen-bonded aggregates with the anions as illustrated in Fig. 1. The QM/MM calculations performed on this specific type of aggregate show that the protons of water molecules are deshielded by around 1.5 ppm as compared to those in pure liquid water. A few small aggregates of water molecules within the [C₄Mim][Cl] IL composed of no more than 3 water molecules were only observed in the simulations where molar fraction of water was equal to 0.75 (see Figure 3 for illustration). We managed to do QM/MM calculations specifically for water molecules in the [C₄Mim][Cl] IL which are hydrogen-bonding to other water molecules but not to the chloride anions. Astonishingly, despite still very ionic nature of the surrounding of these water molecules, the protons were seen to be shielded by around 0.8 ppm more than those of the water molecules in the neat liquid. These computational results suggest that the upfield shift of the H-1 NMR signal of water molecules in the range of small concentration of the IL is due to the water molecules in the second solvation shell of the anions. When the concentration of the IL is increasing still further, the amount of water molecules forming strong hydrogen bonds with chloride anions increases on the relative scale, and less and less water molecules remain without direct hydrogen bonding interaction with chloride anions. Therefore, the NMR signal of water exhibits the downfield shift when molar fraction of IL is over 0.34 and continues to increase. Interestingly, even though our computational results provide solid foundation for the understanding of the above experimental results, the MD simulations we have conducted do not show the formation of the water pockets in the mixtures of [C₄Mim][Cl] and water, as corroborated in Ref. 7.

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In the mixtures of $[C_4Mim][BF_4]$ and water, the H-1 NMR signal of water molecules shows consistent upfield shift with the rising concentration of the IL component over the entire concentration range. Our MD simulations do show the formation of the complexes between the water molecules and the tetrafluoroborate anions. However, the QM/MM calculations for the H-1 NMR shielding constants of water molecules hydrogen bonded to these anions show that the protons here are shielded by around 1.1 ppm more than in the liquid water. We have observed more abundant aggregates of water molecules in this IL as compared to that based on the chloride anion when the molar fraction of water is equal to 0.5. The QM/MM calculations on the water molecules forming hydrogen bonding to other water molecules but not the anions show that the protons here are shielded by around 0.5 ppm more than in the liquid water. Thus, the increased shielding is observed also for this type of aggregate, but this effect is lesser in magnitude in the $[C_4Mim][BF_4]$ as compared to the $[C_4Mim][Cl]$ IL. The qualitatively different behaviour of water H-1 NMR signal in the mixtures of $[C_4Mim][BF_4]$ and water as compared to those involving $[C_4Mim][Cl]$ IL is thus due to the known weak hydrogen bonding abilities of the tetrafluoroborate anions. As these anions are hydrophobic, the formation of water pockets in the $[C_4Mim][BF_4]$ IL cannot be ruled out, although our simulations of the mixtures of this IL and water at $\chi_w=0.34$ show only minor aggregates of water molecules at best (see Figure 1), and are thus inconclusive.

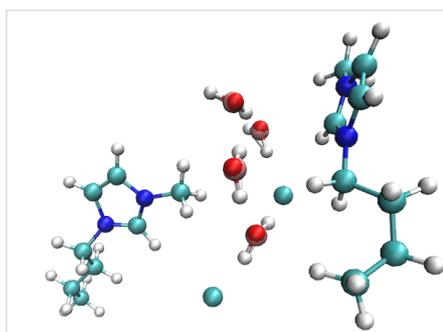


Figure 3: The associates of water-chlorine anion and water-water in the ionic liquid: $[C_4Mim][Cl]$.

1.6 Role of HPC-Europa3

The research interests of Prof. Aatto Laaksonen from the Dept. of Materials and Environmental Chemistry are focused on Sustainable Chemistry. Using advanced theoretical and computational chemistry methods his group has been designing green solvents and a new generation of lubricants based on room temperature ionic liquids. The research visit of Prof. Aidas and Ms Lengvinaite within the HPC-Europa3 programme was therefore most welcome. The group of Aidas is developing and applying the high-end computational tools to study these chemical most complicated liquids with all possible molecular interactions in effect. As the number of possible ionic liquids through different combinations of molecular cations and anions can be order of 10^{18} , *in silico* techniques in designing them for different applications is the only feasible way before starting to synthesize them. In our case, the HPC-Europa program was simply an ideal way to connect high-level research and high-performance computing to produce green chemistry products and application. The highly professional and extremely friendly staff at PDC did provide the perfect circumstances to perform the work.

Dr. Aidas shared that computational resources provided by the PDC at KTH through the HPC-Europa3 programme were instrumental in making these expensive calculations possible. An extended visit at KTH was extremely fruitful also because they had excellent conditions for uninterrupted work and great technical support from PDC. He strongly believes that the obtained computational results lead to important insight concerning the behaviour of water molecules in the highly heterogeneous systems of ionic nature such as the ionic liquids are. The success of this project will facilitate further computational studies of ionic liquid systems.

Ms Lengvinaite reflected “These two visits were very useful to me as a young scientist, PhD student. During this visit, I had the opportunity to work independently, to test different computing capabilities, to meet the challenges. Get acquainted with great scholars and get in touch. These let us to realize this project in much faster way and produce the expected results. The publication is under preparation, to be finished this summer.”

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