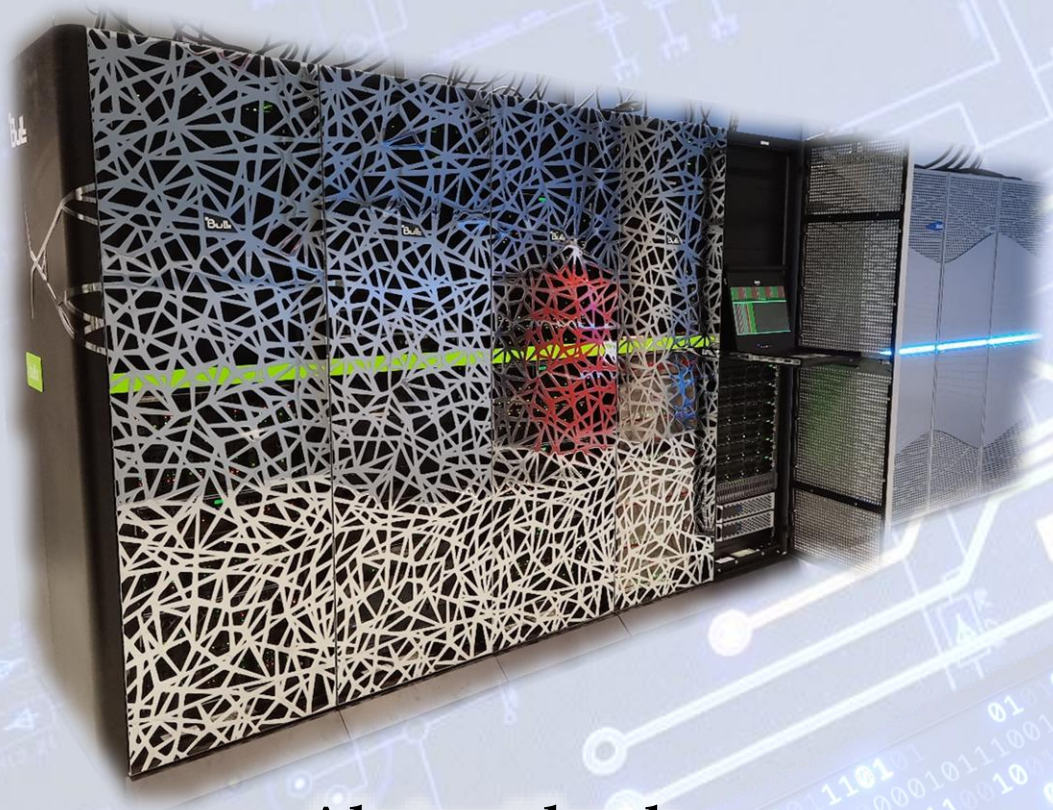
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

https://doi.org/10.5281/zenodo.15754592

https://www.eurocc-lithuania.lt/events_2025-06-27/

June 27, 2025

Vilnius, Lithuania

Hackathon & Workshop organizers

Local organizing committee

Mindaugas Mačernis
Laura Baliulytė

Scientific committee

Mindaugas Mačernis
Laura Baliulytė

Funding

Co-funded by the European Union

EuroHPC Joint Undertaking

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.

Bendrai finansuoja Europos Sąjunga

Projektas bendrai finansuojamas 2021–2027 metų ES fondų investicijų programos (sutartis Nr. 10-051-P-0001).

EuroCC2-EuroCC4SEE
Project Organiser

Vilniaus universitetas 1579 Universitas Vilnensis

Project Implementers

Vilniaus universitetas 1579 Universitas Vilnensis — Fizikos fakultetas

Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

ktu kauno technologijos universitetas 1922

VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Structural characterization and accurate ^{1}H NMR spectra modelling of [C_4mim][BF_4] ionic liquid and its aqueous mixtures

Einaras Sipavičius[1], Greta Majauskaitė[1], Dovilė Lengvinaitė[1], Stasė Bielskutė[1,2], Vytautas Klimavičius[1], Francesca Mocci[3], Aatto Laaksonen[4], Kęstutis Aidas[1]

[1]*Faculty of Physics, Vilnius University, 9 Saulėtekio Ave., Vilnius*
[2]*Institute for Research in Biomedicine, The Barcelona Institute of Science And Technology, 10 Baldiri Reixac, Barcelona*
[3]*Department of Chemical and Geological Sciences, University of Cagliari, 09042, Monserrato*
[4]*Department of Materials And Environmental Chemistry, Stockholm University, 10691, Stockholm*

E-mail: einaras.sipavicius@ff.vu.lt

Accurate prediction of spectroscopic features of ionic liquids is challenging because of its nanosegregated intermolecular structure, especially in their mixtures with water. Our previous work [1] showed that NMR calculations of C_4mim$^+$ cation ionic liquids tend to underestimate chemical shift of protons at 2nd position (H2, see Fig. 1 a). We report first accurate prediction of C_4mim$^+$ NMR spectra in [C_4mim][BF_4] ionic liquid (IL) and water mixtures (see Fig. 1 b), including the characterization of intermolecular structure of such systems, especially the local structure around C_4mim$^+$ using radial and angular (Fig. 1 c) distributions. Results were achieved performing molecular dynamics (MD) simulations on four [C_4mim][BF_4]:H_2O mixtures, ranging from 17 % to 100 % IL molar fraction (χ_{IL}), and then extracting 100 configurations from MD trajectories and conducting quantum mechanics / molecular mechanics (QM/MM) calculations for ^{1}H NMR shielding constant evaluation.

We would like to thank to "HPC Sauletekis" for providing us computational resources and Research Council of Lithuania for funding (project no. S-MIP-22-74).

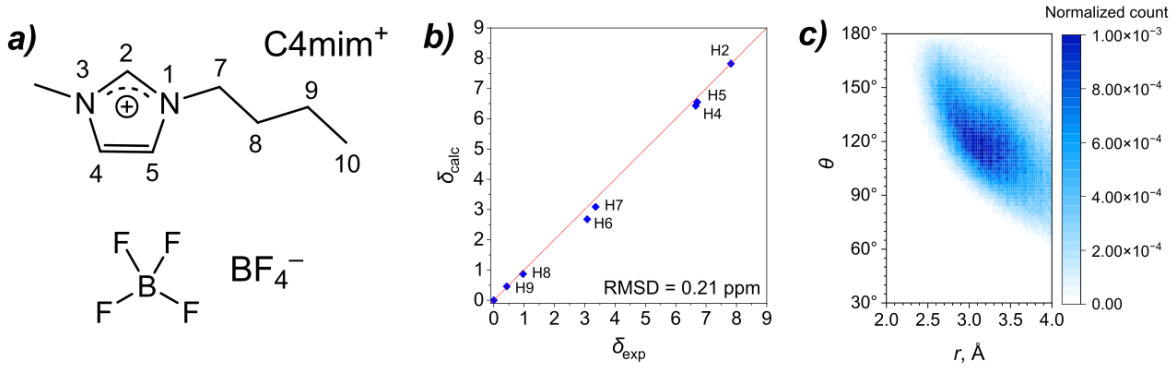


Fig. 1. [C_4mim][BF_4] chemical structure (a), comparison of calculated and experimental ^{1}H NMR chemical shifts of C4mim$^+$ cation relative to H10 protons in the butyl chain in χ_{IL} = 50% system (b), angular distribution of BF_4^- anions around C2–H2 bond of C_4mim$^+$ cation in χ_{IL} = 50% system (c).

REFERENCES

[1] D. Lengvinaitė, S. Kvederaviciute, S. Bielskutė, V. Klimavicius, V. Balevicius, F. Mocci, A. Laaksonen, K. Aidas; *J. Phys. Chem. B* **125** (2021) pp. 13255-13266.