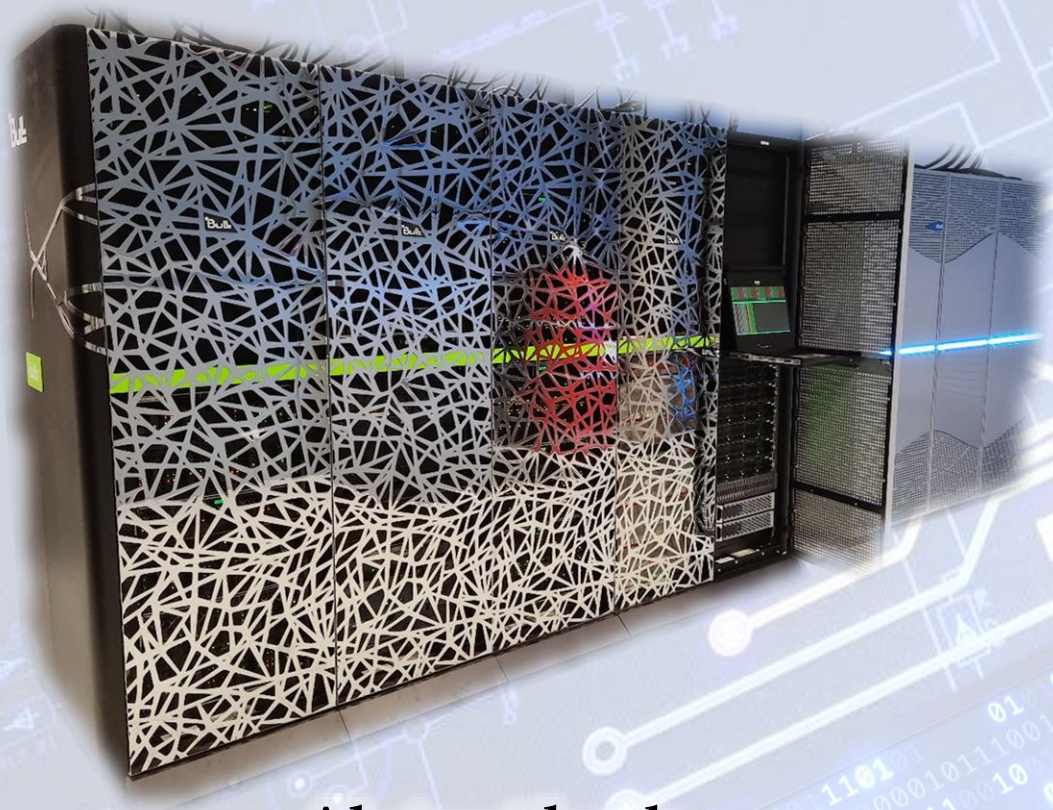
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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ktu kauno technologijos universitetas 1922

VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

QM/MD and NMR study of aqueous mixtures of choline lysinate

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Molecular dynamics (MD) simulations combined with the quantum mechanics/molecular mechanics (QM/MM) models have proven to be a powerful computational technique for accurate predictions of electronic properties of extensive molecular systems. MD simulations are employed to sample the phase space of molecular system of interest under specific thermodynamic conditions, and then QM/MM calculations of electronic properties are performed where the central part of the molecular system is described by an electronic structure method and the rest of the system is modelled by a classical force field.

Aiming to scrutinize intermolecular organization in aqueous mixtures of choline lysinate, [Cho][Lys], ionic liquid (IL), the dependences of the ^{1}H NMR chemical shifts and diffusion coefficients on their composition were measured [1]. To rationalize experimental findings, extensive MD simulations and linear-response QM/MM computations of NMR shielding constants were performed. Analysis of MD trajectories reveals that extent of intermolecular contacts between cations and anions intensifies with the increasing content of the IL in the mixture. Moreover, the tendency of choline cations and the side chains of lysinate anions to self-aggregate was observed as well, leading to the formation of a continuous, highly polar domain composed of choline cations and the carboxylate groups of lysinate anions, as well as a less polar domain formed by the side chains of the anions in IL-rich mixtures. Under these circumstances, isolated water pockets are found to be situated at the interface of the polar and nonpolar ionic domains. The dependences of the measured diffusion coefficients on the composition of the mixture reveals the existence of two dynamical regimes – fast and slow regimes below and above molar fraction of the IL of 11%, respectively. Results of MD simulations suggest that – at this specific molar composition of aqueous [Cho][Lys] mixture – continuous water network ceases giving way to the continuous structure of ionic domains being formed. The QM/MM results for the ^{1}H NMR chemical shifts of aqueous IL mixtures generally agree well with experimental findings and corroborate structural results. The prominent upfield shift of the NMR signal of protons in fast exchange with the rising content of the IL was successfully rationalized [1].

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REFERENCES

[1]E. Sipavičius, L. Mikalauskas, V. Klimavičius, K. Aidas, Intermolecular organization in aqueous mixtures of choline lysinate studied by NMR and molecular dynamics/quantum mechanics, *Phys. Chem. Chem. Phys. (2025)*, https://doi.org/10.1039/D5CP00861A.