Mixtures of room temperature ionic liquids with molecular solvents: challenge for the molecular modelling techniques

O.N. Kalugin[a], V.A. Koverga[b,a], B.A. Marekha[b,a] and A. Idrissi[b]

[a] *V.N. Karazin Kharkiv National University, School of Chemistry, Svoboda sq., 4. Kharkiv, Ukraine, E–mail: onkalugin@gmail.com*

[b] *University of Lille, Faculty of Sciences and Technologies, LASIR, Bât. C5, Cité Scientifique, 59655, Villeneuve d'Ascq Cendex, France*

Room temperature ionic liquids (RTILs) have already found an impressive number of applications due to the versatility of their properties which are determined by their composition. In case of electrochemical application of the RTILs the diversity of credible systems can also be expanded by combining RTILs with dipolar aprotic solvents like acetonitrile (ACN), propylene carbonate (PC) and γ-butyrolactone (γ-BL). Many practically important macroscopic properties of these mixtures (such as conductivity, viscosity etc.) are modulated by structure and particle dynamics at microscopic level.

In this contribution we discuss how the results of experimental investigations of the set of imidazolium-based RTILs and their mixture with AN, PC and γ-BL by using conductometry, NMR and Raman spectroscopy and quasi-elastic neutron scattering (QENS) can be explained by utilizing quantum chemical calculations and molecular dynamics simulations [1-11]. Variation in microscopic structure as a function of mixture composition is addressed in terms of competition between inter-ion and ion-molecular interactions as well as the formation of weak H-bonds.

[1] V.V. Chaban *et al. PCCP*, **2011**, 13(17), 7910. [2] V.V. Chaban *et al. J. Phys. Chem. B.*, **2012**, 116, 7719. [3] O.N. Kalugin *et al. Elecrochim. Acta.* **2013**, 105, 188. [4] B.A. Marekha *et al. J. Phys. Chem. B.* **2014**, 118, 5509. [5] B.A. Marekha *et al. J. Raman Spectroscopy*, **2015**, 46(3), 339. [6] B.A. Marekha *et. al. PCCP*, **2015**, 17, 23183. [7] B.A. Marekha *et al. PCCP*, **2015**, 17(26), 16846. [8] B. A. Marekha *et al. J. Phys. Chem. B*, **2016**, 120 (22), 5029. [9] B. A. Marekha *et al. ChemPhysChem*, **2017**, 18, 1. [10] V. Koverga *et al. PCCP*, **2018**, 20, 21890. [11] Kalugin O.N. *et al.* (**2018**) Transport Properties and Ion Aggregation in Mixtures of Room Temperature Ionic Liquids with Aprotic Dipolar Solvents. In: Bulavin L., Chalyi A. (eds) *Modern Problems of Molecular Physics.* Springer Proceedings in Physics, vol. 197. Springer, Cham.