Influence of interparticle correlations on electrophysical properties of solid electrolytes

V. Vikhrenko[a] G. Bokun[a] T. Patsahan[b] D. di Caprio[c] M. Holovko[b]

[a] *Belarusian State Technological University, 13a Sverdlova str., 220006 Minsk, Belarus, E–mail: vvikhre@gmail.com*

[b] *Institute for Condensed Matter Physics, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: tarpa@icmp.lviv.ua*

[c] *Chimie ParisTech, 11 rue Pierre et Marie Curie, 75005 Paris, France, E–mail: dung.di-caprio@chimie-paristech.fr*

Solid electrolytes remain an area of intensive scientific activity due to their great potential in industrial applications like rechargeable batteries, fuel cells, supercapacitors, memory devices, etc. Their models can be considered as mobile charges of one kind in the presence of a compensating background.

A cumulant expansion with respect to renormalized Mayer functions is used for calculating the cell potentials of mean forces and constructing the free energy in the form of a density functional. In the lattice approximation, a system of equations is obtained for calculating the potentials of mean forces. The uncorrelated part of the electric field is accounted for through the Poisson equation. The short-range correlation effects are taken into account through the mean potentials. Correlations between particles are taken into account for the first neighbors only. In the case of sufficiently small electric fields, the distribution of the potential and charge is described by a linear differential equation of the fourth order. Depending on the ratio of the intensities of Coulomb and short-range Van-der-Vaals interactions, its solution shows damped oscillations with varying damping and oscillating constants.

In a more general case, with accounting of the correlations up to third neighbors and without restriction to weak fields numerical solutions for the charge and electric field distributions were obtained. Again, the concentration distribution showed an oscillating behavior. Moreover, the oscillating behavior of the charge distribution was observed without the external electric field at not too small mean charge concentration.

The project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 73427 and the Ministry of Education of Belarus.