Molecular dynamics simulation of 1-1'-spirobipyrrolidinium tetrafluoroborate acetonitrile solutions

I. S. Vovchynskyi, Ya. I. Filatov and O. N. Kalugin

V. N. Karazin Kharkiv National University, School of Chemistry, Svobody Sq. 4, 61022 Kharkiv, Ukraine,
E–mail: vovchinsky7898@gmail.com

Electric double-layer capacitors (EDLC) are perspective electrochemical storage of electronic energy due to high power density, short time of charge/discharge and long lifetime. It was established that acetonitrile (AN) solution of 1-1'-spiropyrrolidinium tetrafluoroborate ($SBPBF_4$) is a perspective electrolyte for the EDCLs due to higher conductivity as compared with analogs [1].

Here we present the results of the thorough investigation of microscopic structure of ionic subsystem and transport properties of the highly concentrated solutions of $SBPBF_4$ in AN by using atomistic molecular dynamics simulation (MD) and quantum theory of atoms in molecules (QTAIM) [2]. The cation force field model were generated by ATB [3] builder and then improved to represent conformational diversity. The anions force field model is authors modification of well-known Wu [4] tetrafluoroborate with better reproduction of anions spectral properties. All necessary quantum calculation we carried out on M062X/6-311++G(d,p) level theory. All MD simulations were carried out in NPT ensemble with temperature equal to 298.15 K and 1 atm pressure by using GROMACS package [5].

The results of MD simulation provide a deep insight into the concentration dependence of the transport properties of concentrated solutions of $SBPBF_4$ in AN. Using QTAIM analysis the hydrogen bonds between cations hydrogens and anions fluorines were proclaimed as the main interaction in ionic associates.

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