Microscopic environment of the D205 dye in $BmimBF_4$ in ground and excited states

D. Stepaniuk[a,b] ,V. Koverga[a,b] , A. Idrissi[b] and O.N. Kalugin[a]

[a] *V.N. Karazin Kharkiv National University, School of Chemistry, Svoboda sq. 4, Kharkiv, Ukraine*

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

The Dye-Sensitized Solar Cell (DSSC) is one of the cheap and easy alternatives for sustainable energy sources. It is based on the applying of room temperature ionic liquid both pure and mixed with molecular solvents as electrolytes and the indoline dyes that serve as antenna to harvest the photons of the incident light. It was shown that the dye D205 (Fig.1) can be used in DSSC caused by high molar light absorption coefficient, electrochemical, photochemical and thermal stability for a long time, ability to absorb photons in all visible range, good solubility in molecular solvents and the presence of anchor -COOH group, binding to substrate.

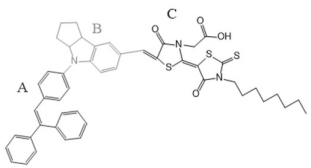

Figure 1: Dye D205: A-donor, B-bridge, C-acceptor

The efficiency of a DSSC depends on the properties of the excited state of the dye used, as well as its ability to electron transfer. All these characteristics are determined primarily by microsolvation of a dye in an electrolyte environment. Here we present the results of the investigation of D205 dye local solvation in ionic liquid $BmimBF_4$. To study the processes occurring at the microscopic level molecular dynamic (MD) simulations were performed by using GROMACS suit. A local solvation of the D205 molecule were analyzed in terms of radial, spatial and combined distribution functions using TRAVIS package. A special attention was paid to a comparison of ground and excited state of D205.