Structure of aqueous 1,4-dioxane solution via molecular dynamics

Bakulin I K[1,2,@] **and Kondratyuk N D**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] bakulin.ik@phystech.edu

Structure of the aqueous 1.4-dioxane solution is considered using molecular dynamics approach. Dioxane molecules are simulated in a range of force fields: OPLS-AA [1], CHARMM36 [2] and the Smith's model [3]. The structure factor is calculated and the obtained results are compared to the experimental X-ray scattering data [4]. The dioxane cluster analysis is performed. Cluster size, number of molecules comprising a cluster and the life time of a cluster are calculated. All the properties of the solution are considered across the whole range of the dioxane concentrations. Preliminary study of the solution structure presented in [5] show, that at low concentration levels clusters of 2-4 dioxane molecules are predominant in the solution. These findings are in good agreement with the experimental results of Takamuku et al. [4].
The work is funded by the grant 18-19-00734 of the Russian Science Foundation.

[1] Jorgensen W L and Tirado-Rives J 2005 *Proc. Natl. Acad. Sci. U. S. A.* **102** 6665–6670
[2] Klauda J B *et al* 2010 *J. Phys. Chem. B.* **114** 7830–7843
[3] Smith G D, Borodin O and Bedrov D 2002 *J. Comput. Chem.* **23** 1480–1488
[4] Takamuku T *et al* 1999 *J. Mol. Liq.* **83** 163–177
[5] Bakulin I *et al* 2021 *J. Chem. Phys.* **155** 154501