Molecular dynamics simulation of solvent impact on the association reaction of Li$^+$ and [O$_2$]$^-$ ions

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The impact of solvent on the reaction of Li$^+$ and [O$_2$]$^-$ ions association was studied by molecular dynamics simulation, which is important for the efficiency improvement of Li–air batteries. Three solvents (acetonitrile, 1.2-dimethoxyethane, dimethyl sulfoxide) with various donor numbers (DN = 14, 20 and 30 respectively) are used in the simulation. The potential of mean force for the reaction of ion association in each solvent was calculated. The simulation shows that activation energy of the reaction has the highest value in dimethyl sulfoxide. This fact correlates with the experimental works, which present that the reaction of ion association is better inhibited in high-donor-number solvents than in low-donor-number ones. All computations are carried out using the clusters of JSCC RAS (MVS-100K, MVS-10P). The work was supported by grant from the President of the Russian Federation No. MK-7873.2016.3.