Effect of high donor number solvent and electrode morphology on interfacial processes in Li–air batteries

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The work is focused on identifying the factors responsible for different electrochemical activity of carbon cathodes with different morphology in Li–air batteries. Molecular dynamics simulation was used for the interface structure investigation of the high donor number solvent dimethyl sulfoxide (DMSO) at the surface of carbon nanotube, graphene plane, single- and multi-layer graphene edge. It was determined that the solvent has the layered structure at the graphene plane, sidewall of the nanotube, and single-layer graphene edge. Moreover, the sharpness of the solvent layers decreases with increasing surface curvature. The multilayer graphene edge–solvent interface has qualitatively different chessboard structure. It was shown that an adsorption activation energy of O\textsubscript{2} molecules decreases in the order graphene plane, nanotube, graphene edge. Strong solvation of Li\textsuperscript{+} in DMSO prevents ions adsorption, which is qualitatively different from our previous calculations for acetonitrile [1]. It can be concluded from these results, that nucleation and growth of products in DMSO is shifted from the surface towards the solvent bulk that, in turn, leads to capacity increase of Li–air batteries. This work was supported by grant from the President of the Russian Foundation, grant No. MK-7873.2016.3.