

## **An influence of an effective cation charge on the microscopic structure and solvation dynamics in non-aqueous media**

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Rechargeable batteries based on lithium salts in low molecular weight solvents such as acetonitrile (AN), dimethyl sulfoxide (DMSO),  $\gamma$ -butyrolactone ( $\gamma$ -BL) and propylene carbonate (PC) have become the dominating power source in the market of portable electronics. However, due to the safety problems of such batteries, the rarity and cost of lithium and the increasing energy intensity of the methods for extracting it from the earth's crust, great efforts have been devoted to finding and developing batteries containing other cations as an alternative. One of such non-Lithium candidates is Sodium and Magnesium. Therefore, an investigation of the microstructure and dynamic properties of these cations in non-aqueous solvents remains a relevant task. Molecular dynamics (MD) simulation is an effective tool to achieve this goal, but the problem of ion-molecular polarization especially within the first solvation shell (FSS) of a cation should be considered with a special attention.

With the aim to elucidate this problem, atomistic MD simulations of infinitely dilute solutions of Lithium, Magnesium and Sodium cations with variable charges in AN, DMSO,  $\gamma$ -BL, and PC were carried out by using MDNAES software package. The microstructure of the FSS of the cations was analyzed in terms of radial distribution functions, current coordination numbers and 3D structure of the FSS. Dynamics of cations' solvation was studied in terms of the self-diffusion coefficients and different kind of the time correlation functions. The results indicate the possibility of more accurate reproducing experimental data by variation of the effective cation charges.