

Over past two decades lithium ion batteries have become very successful and widespread energy storage devices. Such power sources are vital for sustainable energy development. However, increasing demand, in particular in the view of growing market for electric vehicles, raises concerns about availability of lithium salts, being key ingredient for production of lithium batteries. Resources of lithium are unevenly distributed, with most known commercial resources located in South America, and the prices increased in the first decade of the 21st century. On the other hand, sodium and magnesium are the most abundant elements in the Earth's crust, available everywhere at very low cost. This stimulates increasing interest in sodium or magnesium ion conducting batteries. Non-lithium batteries are seen as one of possible solutions to meet the challenge of increasing demand in a limited-resources world and have potential to become an innovative technology of the future.

Computational modeling methods of theoretical chemistry have been widely used to investigate properties of matter at molecular level and have contributed to success of experimental research through better understanding and interpretation of physical origins of observed phenomena. An ultimate goal of computational modeling is to be able to predict results of experiment.

Development of lithium-based energy storage devices has received continuous support from theory. However, although the experimental research on non-lithium batteries has intensified rapidly, there is only a limited number of computational works focused on this subject. In this project we want to contribute toward development of non-lithium power sources through systematic study of electrolytes used in these devices.

Ion conducting electrolyte is one of key components of an energy storage device and typically consist of a metal salt dissolved in a solvent. In the project we will investigate electrolytes based on sodium, magnesium or zinc salts and organic solvents, ionic liquids and polymers. Quantum-chemical calculations will be used to obtain information on structure and strength of interactions in small ion-solvent aggregates. Simulations of molecular dynamics will yield structures and estimates of the conductivity of bulk electrolytes. We will analyze our results to find correlations between interactions at molecular level and properties of macroscopic system.

Computational methods of chemistry can differ greatly in amount of time required to complete the calculations. Owing to increasing power of computers we will be able to use several advanced techniques. We will compare different methodologies to find those offering best accuracy of results at moderate computational cost.

Outcome of the project will be better understanding of physical processes in electrolytes for non-lithium batteries, relating molecular interactions to observed properties of the electrolyte. This knowledge will be beneficial for enhanced interpretation of experimental results and for rational design of new systems. In this way we will support development of a promising technology for sustainable growth. Achievements of the project in the methodology of calculations will be useful not only in future studies on non-lithium electrolytes but also in modeling of similar condensed matter systems.