Abstract for the general public

Ionic conductors based on cyanido coordination architectures: design and functionalization

Our everyday life strongly depends on electrical energy, which is one of the most important resources in the modern world. The consumption of electricity is growing every year and it is predicted that the global electricity demand will increase by over a half in the upcoming two decades. Increasing the consumption of electricity requires finding new high-performance, low-cost, and ‘green’ solutions for sustainable energy production and storage. Renewable energy sources (wind, hydropower, solar energy) are considered feasible options. However, ensuring constant electricity supply from such intermittent sources requires the construction of grid energy storages based on high-capacity batteries. Another solution for portable and clean energy are fuel cells, which transform chemical energy into electricity. Both of these approaches require the further development of high-performance ion-conducting materials, which will serve as solid-state electrolytes in batteries or robust proton exchange membranes in hydrogen fuel cells. The development of new functional materials for energy technologies constitutes the main research problem we are going to address in this project.

This project aims at the design and synthesis of novel functional ionic conductors based on molecular materials. A great advantage of molecular materials is the fact that their functionalities can be designed on the molecular level through a combination of rationally selected molecular components, which carry the desired properties. Such components react with each other via chemical bonding or supramolecular interactions to form a crystalline material in the self-assembly process. Since ionic conduction is an act of migration of charged species through a medium, it is necessary to design and obtain materials that contain mobile charge carriers and have a structure that provides convenient pathways for their migration. To achieve this goal, we will employ three types of molecular building blocks: anionic cyanido complexes of transition metals, ligand-functionalized transition-metal or lanthanide cations, and charge carriers (i.e. protons or lithium ions). The first two components are meant to form a coordination framework of metal ions connected with a cyanide molecule, which hosts mobile ions ensuring the conducting properties. This ‘scaffolding’ of the cyanido architecture will be designed to enhance the migration of ions to reach highly conductive solids. For a better understanding of the role of molecular interaction in the charge transport in molecular solids, the conductivity of the obtained materials will be analyzed in relation to their structure. Our research will lead to the development of novel materials with a prospective application as solid electrolytes in a new generation of high-performance batteries or fuel cells. Moreover, cynaido-bridged architectures are an outstanding platform for the construction of multifunctional materials, which effectively merge a plethora of functionalities in one compound. Therefore, in this project, we aim at combining ionic conductivity with magnetic properties, luminescence, or non-linear optical effects, as well as making these functionalities responsive to external stimuli (i.e. light, pressure, small molecules). Such multifunctional materials may serve in future molecule-based technologies as molecular switches, sensors, data storages, or information converters. Our project will result in a series of new materials exhibiting the abovementioned features it will significantly contribute to the knowledge of functional molecular materials and ionic conductors.