New Chelating Agents for Selective Extraction of Uranium (URAEXT)

The concentration of uranium in seawater is very low, of the order of 3 μg L^{-1}. However, the total volume of Earth's ocean reserves is roughly 1.4 × 10^9 km^3, which means that seawater contains about 4.5 × 10^9 tons of uranium – a thousand times more than the estimated amount of the metal in terrestrial ores! In other words, Earth's ocean reserves contain a nearly unlimited amount of uranium that is, in principle, available to any country to exploit.

A recent renaissance in the extraction of uranium from seawater has led to a number of novel compounds of which metal-organic frameworks and nanoporous plastic polymers represent some of the latest inventions. However, significant development steps are still required before the extraction technology becomes feasible in practice. Some of the biggest problems to be solved in this area are related to the selectivity of the process as well as the extraction capacity and recyclability of the sorption agent.

Developing highly selective systems for uranium extraction requires insight into the coordination chemistry of the uranyl dication, UO_2^{2+}. The linear shape of UO_2^{2+} differentiates it from other metal cations in aqueous media that have spherical electron densities. Thus, the selectivity of the extraction process can be affected by designing ligands that can bind to the uranyl dication not only through strong metal-ligand bonds but also through interactions between the ligand and the oxo groups of UO_2^{2+}.

The current URAEXT project has at its primary goal a comprehensive computational analysis of metal-ligand bonding in a large number of coordination compounds of the uranyl dication. The aim of the research is to use the acquired knowledge, as well as the data already published, to design tailored ligand systems for uranyl extraction from aqueous media. The use of secondary bonding interactions between the ligands and the oxo groups of UO_2^{2+} to increase the selectivity of the extraction process is a long attempted approach that is yet to be realized.

The second goal of the conducted research is to use computational methodologies to find new materials and compounds that have same functionalities in specified applications as the currently used materials based on critical and/or expensive metals. In this context, the research is being carried out to explore the chemistry of some novel nickel-based coordination complexes that can readily activate small molecules such as NH_3, CO, H_2O and H_2. Such reactions are at the core of a number of basic chemical processes that are used in various fields in the industry.

Researchers working in the project:

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