

Binary compounds are simple compounds that are composed of only two chemical elements. A discovery of a novel binary compound nowadays represents a considerable challenge and is a scientific achievement akin to the discovery of a novel element a century ago. Moreover, these simple compounds further our understanding of elements and their chemical reactivity. The synthesis and characterization of compounds with elements in unusual oxidation states and novel binary compounds therefore represent a major research challenge in contemporary chemistry. Fluorine is the most electronegative element and the most reactive non-metal, and it is often referred to as the tiger of the periodic table. Fluorine chemistry is usually associated with high oxidation states. As a result low-valent transition-metal fluorides have proven elusive and are hitherto unknown, even though their heavier halogen analogs, typically chlorides, are common and well-characterized substances.

This project aims to explore the high-pressure synthesis and characterization of elusive binary low-valent transition-metal fluorides. The experiments will be performed in diamond anvil cells, which can generate pressures of ten thousand to several hundred thousand atmospheres. Chemistry under these extreme conditions is very interesting and enables the discovery of compounds with unusual compositions and stoichiometries. Experiments in diamond anvil cell will be guided by computational quantum-chemistry modelling, which will also be an invaluable aid in interpretation of the experimental data, and for understanding the chemical bonding in newly discovered compounds and their structural chemistry. A complementary expertise of Polish-Slovenian team will be crucial for tackling this challenging endeavor. The expected results of this project are discoveries of novel compounds, better understanding of binary transition-metal fluorides, and new knowledge about their high-pressure chemistry and structural behavior.