Superhalogen anions are chemical compounds with very unique properties, which can be described using simple general formula: MX_{k+1}^- (*M* means central metal atom, *X* is a halogen ligand, while *k* stands for the maximal formal valence of atom *M*). Superhalogen anions are characterized by very high values of vertical electron detachment energy (VDE), which is a factor describing the strength of excess electron binding by chosen molecule. Electron affinity of neutral superhalogens is definitely higher than analogous values obtained for the most electronegative atoms in periodic table – fluorine and chlorine. Hence, superhalogens bind the excess electron very strongly and are able to "withdraw" an electron from almost any molecule located in their surrounding area (even as stable and weakly-reactive compounds as water, benzene and some noble gases, e.g. xenon and krypton). A lot of types of superhalogen anions are known thus far, for example: mononuclear anions (containing one central atom), polynuclear anions (containing two or more central atoms), alternative superhalogen anions (non-metal atom plays the central atom role) and hyperhalogens (other non-modified superhalogens as ligands in superhalogen system). Due to their possible impact on the chemistry of noble gases and other almost non-reactive compounds (e.g. methane), the search for novel superhalogens (characterized by electron affinity values even higher than those of superhalogens described before) is justified.

The goal of this research project is to design and describe novel superhalogen anions (nano-superhalogen anions and metal-mixed superhalogen anions), whose vertical electron detachment energy values could be higher than 13.87 eV (the largest VDE value estimated thus far). Discovery of such strongly bound anions could enable the ionization process of another noble gases (e.g. argon and neon). Due to their unusual shape and size (spatial geometric figures containing empty cavity inside), nano-superhalogen anions could also play the molecular trap role and could be used to transport other molecules inside their cavities.

All research scheduled in this project will be performed using theoretical chemistry methods – computer calculations. Novel superhalogen anions will be constructed by applying adequate graphical computer program and then their geometry will be optimized in order to achieve the global energy minimum (the most stable structure). Analysis of data obtained will allow to describe novel superhalogen anions properties and potential applications reliably. Our theoretical results could also inspire experimental investigations of such molecules in the future.