The enterprise of chemistry is about making and characterizing of new chemical compounds. There are 118 chemical elements currently known, but only about 2/3 of them are stable enough to be used for making compounds, which could be used by humans. Chemical compounds consist of different combinations of elements, for example water is composed of hydrogen and oxygen in the ratio of 2 to 1. Fortunately, many elements may adopt several different “oxidation states” that it forms of element differing formally by the number of electrons at a given atomic center. This enables existence of a larger number of combinations of chemical elements – that is, of chemical compounds. For example, one way of changing oxidation state of oxygen in water leads to oxygenated water (so called hydrogen peroxide). With its chemical formula, H_2O_2, different from that of water, H_2O, it also has very different chemical and physical properties.

The oxidation states may be either negative or positive, but for most elements known the oxidation states never surpass the –4 to +4 range, more rarely +5, +6 or +7 and +8. Only one exception is known, that of recently prepared cation of iridium and oxygen, IrO_4^+, where iridium metal adopts the +9 oxidation state (Wang et al., Nature 2014). Some more were speculated by theoreticians. However, there are no systems known to this day, which would be neutral (i.e. carry no total charge) and show the oxidation state beyond +8.

The current project targets theoretical exploration for new chemical species which might contain heavy transition elements of the 6th Period at oxidation states from +9 to +12 or selected lanthanides oxidized up to +5 or +6 state. To enable such high positive oxidation states, the metallic elements have been carefully chosen for this study which would fulfill the preconditions of so called “octet” stability rule – this will increase the chance for success. In isolated molecules, around central ion, with high formal charge it is possible to accommodate only small number of nonmetal atoms, because of small radius of such ion and strong repulsive forces between nonmetal atoms. In spite of limitations in coordination number it is necessary to use the most electronegative ligands with triple-negative charge, i.e. N^{3-}. Moreover, to crown many nonmetals around a metal center (i.e. to increase the oxidation state of a metal) conditions of spatial confinement will be tested, i.e. the regime of very large pressures. At high pressure conditions atoms are pushed towards one another and are forced to make chemical bonds. When this happens to metallic and nometallic elements, new oxidation states of metals may be possible.

The research which we will carry consist of systematic exploration of compounds of iridium, platinum, gold and mercury, and selected lanthanides as they have potential for adopting unprecedented high oxidation states. We will “squeeze” various combinations of these elements with diverse nonmetals using models of the crystal lattice (called unit cells) and applying the state-of-the-art theoretical methods relevant for the calculations for periodic crystals. A broad range of pressures will be tested to explore stability of bulk compounds at high oxidation states. When we find the pressure conditions required to stabilize a compound of interest, we will then perform calculations of selected important properties, which a given compound would have.

By performing this research we hope to respond to the three fundamental questions:

1. Is it possible to increase the oxidation state beyond +8 in neutral compounds?
2. Are pressures required for this small enough that they can be easily accessed in experiments?
3. What key properties would the so-formed compounds have?

We also aim to inspire experimentalists by suggesting a handful of realistic compounds, which could be targeted using high-pressure synthesis in the matrix isolation or pressure regime which are currently available.