Project 6.5. Calculations of the thermodynamic stability and properties at high pressure of fluorides of oxygen and sulphur

Supervisor: dr. hab. Paweł Strąk / dr. hab. Dominik Kurzydłowski

Institute: Institute of High Pressure Physics of the PAS

Unit: Crystallization Laboratory (NL-3)

WWW: https://www.unipress.waw.pl/growth/index.php/theory/general

Background:

Since its birth at the beginning of the 20th century the study of matter at pressures exceeding 1 GPa (= 10 kbar) has developed into a fast growing multidisciplinary field encompassing topics from physics, chemistry, earth sciences, astronomy, and even biology. The often exotic nature of high-pressure transformation has an important impact on our understanding of chemical reactions. Studies of phase transitions and reactivity at large compression are a testing ground for central ideas of chemistry such as atom radii, electronegativity, oxidation state all of which are cornerstones of the so-called “chemical intuition”.

The proposed project aims at exploring a new research avenue within HP sciences, namely the chemistry and physics of fluorine-rich systems at large compression. Fluorine exhibits a unique reactivity at ambient conditions, and the few studies on the high-pressure properties of fluorine containing systems conducted so far strongly indicate that the chemistry of this element becomes even more unique at large compression.

Aim:

The aim of the project is to explore the reactivity of fluorine at pressures exceeding 1 GPa (= 10 kbar). Recent theoretical investigations hinted that the use of this element as a reactant at large compression can enable stabilization of exotic species such as NF_5. We aim to computationally explore the high-pressure affinity of fluorine towards electronegative non-metals: oxygen and sulphur. In particular we plan to study the balance between covalent and ionic bonding in these systems.

Requirements:

- M.Sc. in chemistry, physics, materials sciences or in a closely related field at the time of appointment
- experience in ab initio modelling
- preference will be given to candidates with experience in performing simulations with the use of the Density Functional Theory, especially in the solid state.