SterActLEP – structural studies of arsenic and antimony materials containing stereoactive lone electron pairs

ABSTRACT FOR GENERAL PUBLIC

Valence electrons are responsible for the formation of chemical compounds. It is the exchange or sharing of electrons that lead to the formation of various chemical bonds – ionic, metallic and covalent bonds. Sometimes electron pairs do not form chemical bonds but are located in proximity of atoms and influence the spatial arrangement of chemical bonds around them (see Figure 1). We call such electron pairs stereoactive lone electron pairs.

This project entails synthesis and crystallization of chemical compounds build of molecules containing stereoactive lone electron pairs. Inclusion compounds of arsenic(III) oxide and polymorphs of antimony(III) oxide will serve as model compounds. Their synthesis and crystal structure determination at ambient pressure and at high pressure reaching tens of thousands the atmospheric pressure are planned. Subsequently, structural activity of lone electron pairs will be determined quantitatively using bond-valence vector model and the effect of pressure on the structural activity fo the lone pairs will be elucidated. The interactions of lone electron pairs with other molecules, such as hydrogen molecule, present in the inclusion compound and intercalates will be studied. An attempt to understand the interplay between lone electron pairs and intermolecular interactions will be made and the gained knowledge may contribute towards design of better hydrogen-storage materials and to the more effective design of materials with desired thermoelectric, optoelectronic or multiferroic properties.

Accomplishment of the project will deepen our knowledge and understanding of the chemistry of arsenic(II) and antimony(III) oxycompounds and, consequently, contribute to the development of inorganic chemistry. The analysis of lone electron pair stereoactivity in those compounds based on the bond-valence vector model will make it more popular. The proposed project encompasses basic research, but its results will have practical implications for materials design mentioned above.

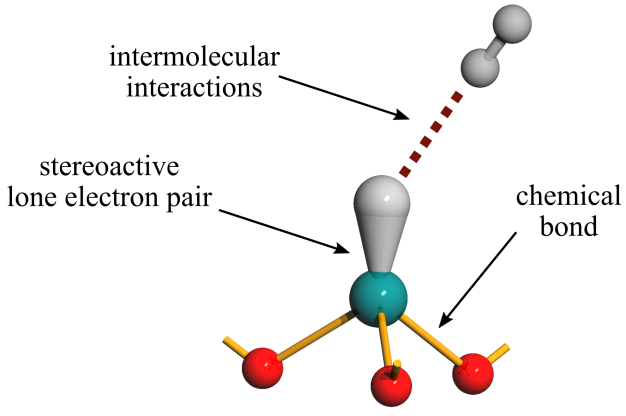

Figure 1. Basic structural unit of arsenic(III) and antimony(III) oxides. Green and red spheres represent arsenic or antimony and oxygen atoms, respectively.