In the era of the rapid development of civilization the energy demand necessary for human life continuously increases. The fossil fuels are becoming more expensive, and, moreover, the climate change risk associated with power generation using fossil fuels is growing. One of the biggest challenges faced by our society is development of new and renewable energy sources. For instance, currently used electric devices consume approximately 19% of the total energy demand. Thus, the scientific and industrial attention is focused on the development of alternative energy sources based on new technologies such as organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs), dye-sensitized solar cells (DSSCs) or organic field-effect transistors (OFETs).
The above-mentioned technologies are the part of intensively developed material science, including also optoelectronics. Optoelectronics deals with the study and the search of novel compounds and their application in electronic devices. The active molecules used in optoelectronic devices can act as absorber or emitter of light due to electron transporting properties. These active materials can be either organic or metalorganic (containing heavy metals) compounds, although the latter are preferred and more often used. The presence of heavy metals in these compounds give rise to increase emission yields. Furthermore, big advantage of using metalorganic compounds in optoelectronic applications is caused by their ease modulation of emitted light via structural modification. In recent years, efficient light emitters based on platinum and iridium have been developed, and there is still rapid progress in the development of novel compounds that may be applied in optoelectronics. In addition, light-emitting platinum and iridium compounds are increasingly being used for bio-imaging. They seem to be more promising than presently applied standard compounds (organic compounds).
Importantly, the analysis in detail the spectral features of chemical compounds based on the results of electronic and vibrational structure calculations may explain the correlation between chemical structure and properties. Enhanced understanding of the theoretical calculations give an opportunity to design the structures of other compounds with modified structure, indicating what kind of changes and in which fragment of the complex molecules should be done.
Thus, the main motivation to undertake the current project is to research more effective and well-designed chromophores based on platinum and iridium compounds. The project is focused on synthesis of iridium and platinum complexes and examination of their physical, optical, and electronic properties. The Iridium and Platinum compounds will contain proper fragments (ligands) allowing to achieve the expected properties, especially luminescent. In addition, the ease modification of chemical structure give the possibility to tune the electronic properties of compounds. The experimental studies will be associated with quantum-chemical calculations using Density Functional Theory.
The absorption and emission spectra, lifetimes, emission quantum yields, oxidation and reduction potentials, and the reversibility of redox processes will be determined and investigated.
The extensive knowledge on the relationship between the structure and properties allows for the rational design and synthesis of new molecules with expected properties which may be promising candidates in optoelectronic and bio-imaging applications.
The project is focused generally on the preparation of novel materials which will be studied as active layers in organic light emitting diodes and agents in bio-imaging. The cooperation with chemists of different specialties, physicists and experts in the material science will allow to test usefulness of the obtained platinum and iridium compounds as photovoltaic cells, organic light-emitting diodes and in bio-imaging technology.