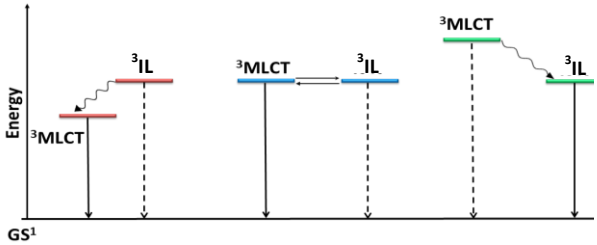
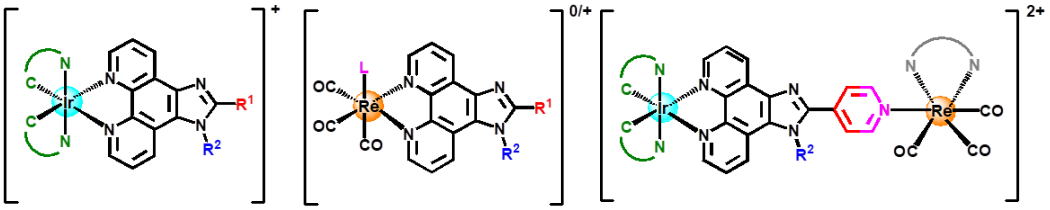
The primary goal of this project is to create new and efficient complexes based on **imidazo[4,5-f][1,10]phenanthroline** (*imphen*) with improved functional characteristics, particularly the intense emission in red wavelengths and extended photoluminescence lifetimes originating from triplet excited states. These attributes will allow to obtain new systems for potential use as photosensitizers. They are strongly desirable for light-emitting materials, sensors, light-harvesting systems, photoredox catalysts, photodynamic therapy, triplet-triplet annihilation for energy up-conversion (TTA UC), and time-resolved bioimaging techniques. Advancements in these technologies require improved triplet emitters with enhanced visible range absorption, improved photostability, solubility, and long excited state lifetimes. Transition metal complexes are particularly attractive for designing photosensitizers, offering tunable absorption and emission optical properties through ligand design and central metal selection. Compared to organic chromophores, coordination compounds offer many more excited states of different electronic nature, such as metal-centered (MC), metal-to-ligand charge transfer (MLCT), ligand-to-ligand-charge-transfer (LLCT), intraligand-centered (IL) and intraligand-charge-transfer (ILCT), or their superposition. Each of these singlet and triplet excited states brings characteristic photophysical properties into the resulting complexes.

Depending on the energies of triplet excited states ^{3}MLCT and ^{3}IL, three scenarios are possible (**Scheme 1**): **(a)** the ^{3}MLCT excited state lies significantly lower in energy than the triplet excited state localized on the organic chromophore (^{3}IL), **(b)** both ^{3}MLCT and ^{3}IL triplet excited states are close in energy, and **(c)** the triplet excited state localized on the organic chromophore lies lower in energy than ^{3}MLCT. In the case of **(b)**, between the ^{3}MLCT and ^{3}IL states sharing similar energy, an excited state equilibrium is established, meaning that the organic chromophore repopulates the luminescent ^{3}MLCT excited state and plays a role of the energy "reservoir".



Scheme 1. Three possible scenarios of ^{3}MLCT and ^{3}IL energy arrangements.

To achieve this scenario, we plan to obtain a series of phosphorescent Re(I), Ir(III), and Ir(III)–Re(I) complexes with *imphen* derivatives (**Scheme 2**). Imidazo[4,5-f][1,10]phenanthroline serves as a planar chelate template, ensuring the formation of thermally and chemically stable transition metal complexes. By adding to the *imphen* ligand various emissive or non-emissive organic chromophores, we aim to create metaloorganic materials with extended phosphorescence lifetimes.



Scheme 2. Proposed Ir(III), Re(I) and Ir(III)–Re(I) *imphen*-based complexes.

Our project employs three strategies for modelling of the ^{3}IL and ^{3}MLCT states:

1. Introduction of **R^2** substituents in 1H-position of the *imphen* ligand. The combination of **steric hindrance** from bulky **R^2** groups with addition of **R^1** substituents will tune the mutual chromophore arrangement, which changes the 3IL energy. An additional advantage of the attachment of **R^2** group is the increase of the solubility and absorption intensity of resulting complexes
2. In Ir(III) compounds, modification of the **C^N cyclometalating ligands** will be used to control ^{3}IL.
3. Last but not least, we plan to examine the electronic and spectroscopic effects exerted by both iridium(III) and rhenium(I) combined into **heterobimetallic Ir(III)-Re(I) compounds**, also examining the impact of **N^N** diimine ligands attached to the {Re(CO)$_3$} core.

Understanding the interplay between ^{3}MLCT and ^{3}IL will enable us to establish reliable structure–property relationship for optimizing the photophysical properties of Ir(III) and Re(I) complexes. The obtained complexes will be investigated using cyclic voltammetry, static and time-resolved spectroscopic methods, and ultrafast transient absorption. Quantum chemical DFT and TD-DFT calculations will complement these methods, providing valuable insights into the behavior and dynamics of photosensitizers at the molecular level. Finally, the stability of the obtained complexes will be tested under physiological conditions, assessing their potential applications in biosciences. This project is of significant importance for developing new functional materials for modern technologies and expanding fundamental knowledge in optimizing the photophysical properties of transition metal complexes, with the expectation of making substantial progress in the rational synthesis of efficient photosensitizers.