

Number of project:

GUKPOST/17/2024

Name of the project:

Triplet Photosensitizers Based on the Coordination Compounds of Rhenium(I) and Iridium(III) with Charge-Transfer in the Deep-Red to Near-Infrared Region

Abstract:

This project is focused on the rational design and synthesis of highly efficient triplet photosensitizers based on bi- and multidentate S,N-heteroaromatic ligands with intramolecular charge-transfer and their complexes with rhenium(I) and iridium(III)-containing blocks, recognized for enhancing singlet-triplet transitions due to spin-orbit coupling (SOC) effect. Target compounds will be selected from a library of proposed structures on the basis of quantum-chemical calculations of absorption spectra, relative energies of singlet and triplet states, SOC matrix elements and intersystem crossing rates, while focusing on photoactivation in the deep-red to near-infrared region. Candidates with the most suitable properties will be synthesized by the applicant in the host institute laboratories, characterized for their singlet-oxygen production and phosphorescence efficiency, and also explored for their potential application in phosphorescent bioimaging and photocatalysis.