Photophysical and chiroptical properties of rhenium(I) complex bearing pyrazino-phenanthroline helicene ligand

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Organic light-emitting diodes (OLEDs) have gained increasing interest for display and lightening applications. However, the OLED technology still faces some major challenges. Notably, the current portable OLED display devices require the use of anti-glare filters to limit the reflection of external light, which leads to a loss of up to 50% efficiency. In this regard, CP-OLEDs (Circularly Polarized OLEDs) that utilize the circularly polarized luminescence (CPL) emitted by chiral emitters via fluorescence, phosphorescence or thermally activated delayed fluorescence, which could pass the filters with less attenuation [1], offer an attractive alternative.

Metal complexes with helicene ligands such as rhenium(I)-based ones, which have demonstrated a strong chiroptical activity and beneficial CPL characteristics [2], emerge as promising candidates to generate CPL for CP-OLEDS. Recently, a novel Re(I) complex bearing helical π-conjugated pyrazino-phenanthroline ligand has been synthesized (Fig. 1) and its enantiomers have been successfully separated and examined via absorption and emission spectroscopies. To gain comprehensive understanding of experimentally derived photophysical and chiroptical characteristics of both the pristine ligand and the complex, (time-dependent) density functional theory studies have been carried out including simulations of electronic circular dichroism (ECD) spectra and emission features (both non-polarized and CPL) via optimizations of the lowest-energy excited singlet and triplet states and their spin-orbit coupling examinations. The results have been compared with those obtained for the reference non-helicenic systems, highlighting importance of intramolecular charge-transfer states.

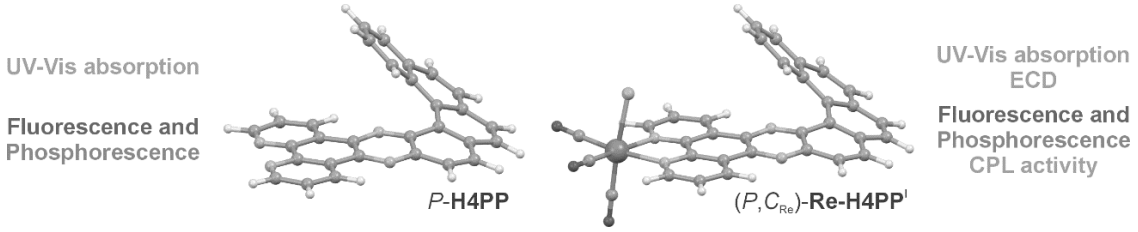

Fig. 1. DFT-optimized structures of the studied ligand and its Re(I) complex.

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[2] Gauthier E. S., Abella L., Hellou N., Darquié B., Caytan E., Roisnel T., Vanthuyne N., Favereau L., Srebro-Hooper M., Williams J. A. G., Autschbach J., Crassous J. (2020) Angew. Chem. Int. Ed. 59, 8394-8400.

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