***Uncovering the remaining secrets of iridium compounds***

Luminescent iridium compounds play an important role in modern display technology. All of the high-end Smartphones or televisions with displays based on the OLED technology will contain iridium-based compounds in the light-producing layer of the device. Beyond their application in visible OLEDs they play an important role in near infrared illumination, which can be used in night vision technologies, but they are also important in other areas of science: they can be used as photocatalysts – compounds aiding chemical reactions in the presence of light, as well as bioimaging dyes – allowing to take snapshots of living cells and tissues. We have studied luminescent compounds of iridium for many years and scientists believe they have already fully understood them. Or so they thought! It is believed that iridium compounds emit through their longer-lived so-called triplet states, producing phosphorescence. This project aims to study a new luminescent mechanism by which the iridium complexes can emit. The principal investigator (PI) of this project intends to demonstrate not only ways to activate this new mechanism, but also identify iridium compounds in which the scientists have missed it!

The new mechanism is related to the properties of the so-called excited states of molecules – states which occur once the molecule gains energy through absorption of light or electrical excitation. The molecule instead of returning to its initial (ground) state through the lower (and slower!) path *via* phosphorescence from the triplet ($T_1$) state, transitions through an upper, singlet state ($S_1$), returning to the ground state faster, *via* fluorescence. This revolutionary mechanism is named Thermally Activated Delayed Fluorescence (TADF) and is presented in the **Fig. 1**. The energy difference between $S_1$ and $T_1$, $\Delta E_{ST}$, is usually expressed in physical units of energy – electronvolts (eV). Typical values for TADF fluorescent dyes are below 200 millielectronvolts (meV).

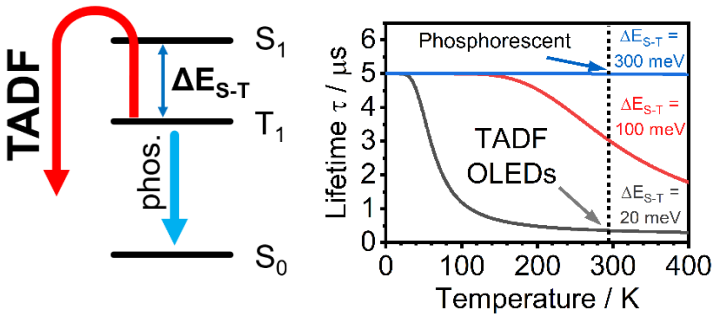


**Figure 1.** (*left*) Schematic representation of TADF mechanism; (*right*) example of how TADF shortens radiative decay lifetime of a metalorganic emitter from its natural phosphorescence rate at 5 microseconds to 500 nanoseconds at RT with $\Delta E_{ST}$ = 20 meV.

One way the scientists measure the rate at which such transitions from excited to ground state occur is through decay lifetime, which is defined in seconds. For example, typical iridium compounds display phosphorescence lifetimes of 1-10 microseconds. The TADF mechanism proposed by the PI allows shortening this lifetime down to 0.1 microsecond.

***But what are the benefits of short luminescent lifetimes?***

Material or OLED stability depends on how long the excited state lives. Many if not most of detrimental processes resulting in emitter degradation occur while the molecule remains in its excited state. Shortening the excited state lifetime by 10-100 fold allows for increased stability of iridium complexes – key aspect for their industrial applications. For example: current OLED technology only uses iridium dyes for red and green pixels, while blue pixels rely on less energy efficient iridium-free dyes. Obtaining stable and blue-emitting iridium dyes would solve critical problems in the OLED industry.

Luminescence quenching in air also relies on the lifetime of the excited state – the shorter the excited state lives the lesser the reduction of light efficiency. This aspect is critical for applications where presence of air cannot be excluded: such as when a luminescent dye is used with tissue or living cells.

In near infrared luminescence dyes are tormented by non-luminescent processes that lead to reduction in light output – one way to sort out the problem is to speed up the rate at which luminescent processes occur, as proposed in this project.

This project not only aims to solve the outstanding problems related to stability and reliability of highly-efficient luminescent dyes, but also broaden the extent of fundamental knowledge about the basic properties of matter. The principal investigator will undertake computational studies to explain the underpinning luminescent mechanisms of iridium compounds in the context of TADF.