Understanding photophysical features of (metal-)organic systems via TDDFT studies

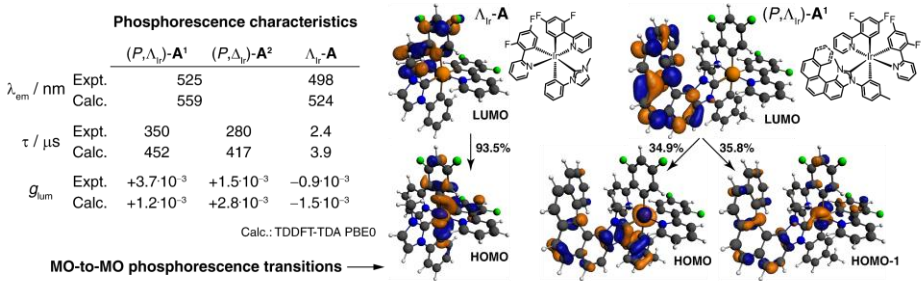
MONIKA SREBRO-HOOPER[1]

[1]*Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland*
monika.srebro@uj.edu.pl

ABSTRACT

Luminescent molecular compounds are continually sought for application in optoelectronic devices including organic light-emitting diodes, in bioimaging and cancer therapy, and as sensors and bioprobes. In the research on such systems the importance of first-principles calculations cannot be understated, since they can provide direct information on the atomic-scale origin of experimentally measured properties. Accordingly, they do not only enable a meaningful interpretation of experimental data, but may also lead to a deeper understanding of the factors responsible for the observed experimental trends. This is the first step in enabling the possibility of designing and proposing new systems with the desired properties.

Recently, a variety of (metal-)organic systems has been successfully studied in our laboratory via extensive combined experimental (in collaboration with Prof. J. Crassous, France; Prof. A. Matwijczuk, Poland) and theoretical research, including, for example, helicene derivatives with a circularly polarized luminescence activity [1] and thiadiazole compounds demonstrating a dual fluorescence emission. Selected results (see, for example, Figure 1) will be presented in this contribution, focusing on our understanding, from time-dependent DFT calculations, of the origin of unique photophysical properties for such systems.



Phosphorescence characteristics

		(P,Λ_{Ir})-$\mathbf{A}^1$	(P,Δ_{Ir})-$\mathbf{A}^2$	Λ_{Ir}-$\mathbf{A}$
λ_{em} / nm	Expt.	525		498
	Calc.	559		524
τ / µs	Expt.	350	280	2.4
	Calc.	452	417	3.9
g_{lum}	Expt.	$+3.7 \cdot 10^{-3}$	$+1.5 \cdot 10^{-3}$	$-0.9 \cdot 10^{-3}$
	Calc.	$+1.2 \cdot 10^{-3}$	$+2.8 \cdot 10^{-3}$	$-1.5 \cdot 10^{-3}$

Calc.: TDDFT-TDA PBE0

MO-to-MO phosphorescence transitions →

Figure 1: Photophysical properties of Ir-based complexes. [1]

References

[1] Ludowieg, H. D.; Srebro-Hooper, M.; Crassous, J.; Autschbach, J. Optical Activity of Spin-Forbidden Electronic Transitions in Metal Complexes from Time-Dependent Density Functional Theory with Spin-Orbit Coupling. *ChemistryOpen* **2022**, *11*, *e202200020*.