π-Extension as a Design Strategy in Orthometalated Ligands: From Photophysical Properties to Bio- and Photocatalytic Applications

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Controlling excited-state properties through molecular design is a central challenge in the development of functional organometallic compounds for photoactive applications. In this lecture, I will discuss our recent work on cyclometalated Ir(III) complexes, highlighting ligand π-extension as a versatile design strategy to tune electronic structure, excited-state character and lifetime, aggregation behaviour, and photochemical reactivity. Using half-sandwich and bis-cyclometalated Ir(III) architectures bearing highly π-extended C^N ligands, we have shown that small structural modifications can lead to major changes in photophysical properties and, consequently, in biological and catalytic performance.[1,2]

Ligand π-extension proved particularly effective in transforming half-sandwich Ir(III) complexes into potent photoresponsive systems. The resulting compounds display long-lived excited states and efficient singlet oxygen generation, leading to exceptional photocytotoxicity in both 2D and 3D cancer models, with IC_{50},light values as low as 0.2 nM and phototoxic indices up to 2034. Remarkably, significant activity is retained under red-light irradiation. In contrast, structurally related complexes incorporating the less extended pbpz ligand show reduced photodynamic performance but undergo photoinduced ligand release, pointing to an alternative PACT mechanism that may be particularly relevant under hypoxic conditions. The same ability to generate reactive oxygen species also extends the utility of these complexes beyond biomedicine, enabling their application as multifunctional photocatalysts for aerobic oxidation reactions under mild conditions.[3]

Taken together, these findings identify ligand π-extension as a general design principle for engineering cyclometalated Ir(III) complexes with tailored excited-state properties. This approach provides access to versatile photoactive platforms operating at the crossroads of bioinorganic chemistry, photochemistry, and catalysis.

References

1. J. Med. Chem., 2024, 67, 3, 1783-1811.
2. Inorg. Chem. Front., 2025, 12, 22, 7304-7332.
3. Inorg. Chem. 2026, 65, 15, 8611–8627.

C.V.

Dr Gema Durá is Associate Professor (*Profesora Titular de Universidad*) in the Department of Inorganic, Organic and Biochemistry at the University of Castilla-La Mancha (UCLM), where she co-leads the QuiCAP research group. Her research lies at the interface of inorganic chemistry, materials science, biomaterials, and bioinorganic chemistry, focusing on the design of complexes and multifunctional platforms for biomedical and photoactive applications.

She obtained her European PhD *Cum Laude* from UCLM in 2014, working on coordination polymers and metal–organic frameworks for gas storage and anion exchange under the supervision of Félix Jalón, and subsequently held postdoctoral positions at the University of York and Newcastle University. Her postdoctoral research expanded her expertise from porous and carbonaceous materials to polymer- and protein-based hydrogels, drug delivery systems, rheology, tissue engineering, and 2D/3D cellular models.

Since returning to UCLM in 2020, she has established an independent research line on multifunctional therapeutic platforms, including nanogel-based delivery systems, photoactivatable metallodrugs, advanced photosensitizers, and responsive polymeric nanomaterials for anticancer therapy and photocatalysis. In 2024, she received the **Best Young Researcher Award in Castilla-La Mancha**, granted by **RSEQ-STCLM**.

Beyond her research activity, Gema is strongly committed to science outreach and the promotion of scientific vocations. She has coordinated outreach activities with secondary schools through the Vice-Dean's Office for Students, led the programme **"La Fábrica de Chocolate"**, coordinated the Castilla-La Mancha Science and Technology Olympiad, and participated in numerous public-engagement initiatives, including school talks, hands-on workshops, media interviews, and mentoring activities for young researchers.