

From Frustrated Ligands Towards Thermally Activated Delayed FluorescenceT. von Arx¹, K. Venkatesan^{1,2*}

¹University of Zurich, Department of Chemistry, Winterthurerstrasse 190, CH-8057, Zurich, Switzerland, ²Macquarie University, Department of Chemistry and Biomolecular Sciences, NSW 2109, Australia

Intramolecular frustrated Lewis pairs (FLP) recently gained an intense interest due to their ability to activate small molecules (e.g. CO, NO, SO₂ etc.)^[1]. Especially the reversible activation of H₂ had raised the number of metal-free protocols for catalytic hydrogenations using FLPs^[2]. Since they bear a donor center (Lewis base) and an acceptor center (Lewis acid) which are spatially separated, intramolecular FLPs could be utilized as a suitable ligand-framework for metal centers^[3]. With such a new class of transition-metal complexes we target thermally activated delayed fluorescence (TADF) – as a donor/acceptor interplay in the emitter molecules is known to decrease the T₁ - S₁ energy difference and therefore enhance the reverse intersystem crossing (RISC)^[4].

Hence, our group synthesized and photophysically investigated a series of Au(I) complexes bearing a P/B-FLP and an aryl or an alkyne as ancillary ligand. By altering the donor/acceptor ability of the ancillary ligand we tend to tune the ratio between prompt (prompt fluorescence or phosphorescence) and delayed (TADF) emissions.

[1] D. W. Stephan, G. Erker, *Angewandte Chemie International Edition*, **2010**, 49, 46 – 76.

[2] (a) G. C. Welch, R. R. S. Juan, J. D. Masuda, D. W. Stephan, *Science*, **2006**, 314, 1124 – 1126.

(b) P. A. Chase, G. C. Welch, T. Jurca, D. W. Stephan, *Angewandte Chemie International Edition*,

2007, 46, 8050 – 8053. (c) P. A. Chase, T. Jurca, D. W. Stephan, *Chemical Communications*, **2008**,

1701 – 1703. (d) P. Spies, S. Schwendemann, S. Lange, G. Kehr, R. Fröhlich, G. Erker, *Angewandte Chemie International Edition*, **2008**, 47, 7543 – 7546.

[3] (a) J. Vergnaud, M. Grellier, G. Bouhadir, L. Vendier, S. Sabo-Etienne, D. Bourissou,

Organometallics, **2008**, 27, 1140 – 1146. (b) G. Bouhadir, A. Amgoune, D. Bourissou, *Advances in*

Organometallic Chemistry, **2010**, 58, 1 – 107. (c) A. Amgoune, S. Ladeira, K. Miqueu, D. Bourissou,

Journal of the American Chemical Society, **2012**, 134, 6560 – 6563.

[4] (a) L.-S. Cui, H. Nomura, Y. Geng, J. U. Kim, H. Nakanotani, C. Adachi, *Angewandte Chemie*

International Edition, **2017**, 56, 1571 – 1575. (b) D. Di, A. S. Romanov, L. Yang, J. M. Richter, J. P.

H. Rivett, S. Jones, T. H. Thomas, M. A. Jalebi, R. H. Friend, M. Linnolahti, M. Bochmann, D.

Credgington, *Science*, **2017**, 356, 159 – 163.