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Aggregation-induced emission of non-symmetric C^N*N^C-cyclometallated platinum(II) complexes

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Square-planar platinum(II) complexes are known to be prone to axial π-π and d_{z2}-d_{z2} intermolecular interactions, which lead to the alteration of their photophysical properties, e.g. appearance of aggregation-induced emission (AIE) bands. We report a series of square-planar platinum(II) complexes **Pt1-Pt5** with non-symmetric tetradentate C^N*N^C-cyclometallated ligands (Figure 1A).[1] The complexes exhibit efficient luminescence with a quantum yield of up to 47% and bands' maxima ranging from 560 to 690 nm in degassed solution. Complexes **Pt1**, **Pt2**, and **Pt4** show mechanochromism in the solid state. Upon rapid injection of their THF solution in water, these complexes form nanosized particles with red-shifted AIE, indicating a change in the excited state. TD DFT computational analysis allowed assigning the observed AIE to ^{3}MMLCT excited states of Pt-Pt bonded aggregates of these complexes (Figure 1B). For complex **Pt2**, we stabilized these aggregates inside micellar nanocarrier providing a new approach for near-infrared biosensors (Figure 1C).[2]

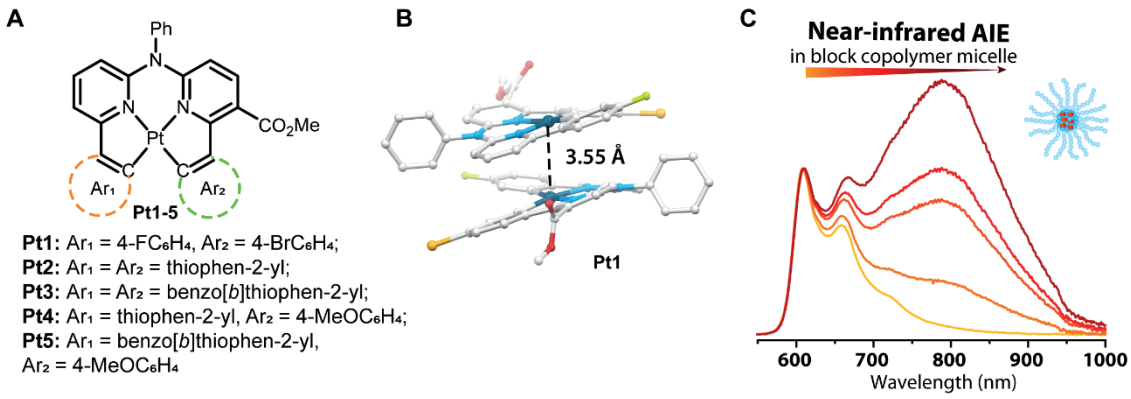

Figure 1. A. Simplified structure of **Pt1**-**Pt5** complexes; B. Optimized geometry of dimer of complex **Pt1** with short Pt-Pt contact; C. NIR-emission of copolymer micelles loaded with different wt. % of complex **Pt2**.

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