Remote modification of bidentate phosphane ligands controlling the photonic properties in their complexes: enhanced performance of [Cu(RN-xantphos)(N^N)][PF6] complexes in light-emitting electrochemical cells

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A series of copper(I) complexes of the type [Cu(HN-xantphos)(N^N)][PF6] and [Cu(BnN-xantphos)(N^N)][PF6], in which N^N = bpy, Mebpy and Me2bpy, HN-xantphos = 4,6-bis(diphenylphosphanyl)-10H-phenoxazine and BnN-xantphos = 10-benzyl-4,6-bis(diphenylphosphanyl)-10H-phenoxazine is described. The single crystal structures of [Cu(HN-xantphos)(Mebpy)][PF6] and [Cu(BnN-xantphos)(Me2bpy)][PF6] confirm the presence of N^N and P^P chelating ligands with the copper(I) atoms in distorted coordination environments. Solution electrochemical and photophysical properties of the BnN-xantphos-containing compounds (for which the highest-occupied molecular orbital is located on the phenoxazine moiety) are reported. The first oxidation of [Cu(BnN-xantphos)(N^N)][PF6] occurs on the BnN-xantphos ligand. Time-dependent density functional theory (TD-DFT) calculations have been used to analyze the solution absorption spectra of the [Cu(BnN-xantphos)(N^N)][PF6] compounds. In the solid-state, the compounds show photoluminescence in the range 518-555 nm for [Cu(HN-xantphos)(N^N)][PF6] and 520-575 nm for [Cu(BnN-xantphos)(N^N)][PF6] with a blue-shift on going from bpy to Mebpy to Me2bpy. [Cu(BnN-xantphos)(Me2bpy)][PF6] exhibits a solid-state photoluminescence quantum yield of 55% with an excited state lifetime of 17.4 ţs. Bright light-emitting electrochemical cells were obtained using this complex, and we show that the electroluminescence quantum yield can be enhanced by using less conducting hole injection layers

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