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► **To cite this version:**

Muriel Hissler, Pierre-Antoine Bouit, Denis Tondelier, Bernard Geffroy. Organophosphorus emitters for OLEDs. EPJ Web of Conferences, 2022, 266, pp.06006. 10.1051/epjconf/202226606006 . hal-04639775

HAL Id: hal-04639775

<https://hal.science/hal-04639775>

Submitted on 9 Jul 2024

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Organophosphorus emitters for OLEDs

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Abstract. In this paper, we present the development of OLEDs using organophosphorus derivatives as emitters. In this study, we were able to show that the structural variations carried out on phospholes, phosphinines and phosphepines (functionalization of the phosphorus atom, nature of the substituents) make it possible to modulate the emission wavelengths and, thus, the emission colour of the diodes. Using this concept, we were able to develop TADF and chiral organophosphorus emitters and hybrids emitting at different wavelengths which can be used for the development of OLEDs. The diode structures used are simple and provide high external quantum yields.

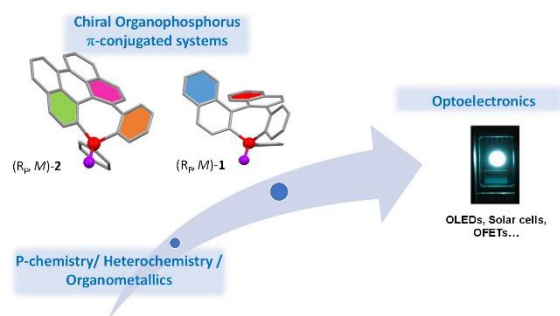
Introduction

The development of technologies based on molecular electronics (field effect transistors (OFETs), light-emitting diodes (OLEDs), solar cells, etc.) has been accompanied by an important development in the synthesis and study of the electronic properties of organic and organometallic compounds with an extended pi-system. [1] Indeed, the development of high-performance "plastic electronic" devices is only possible if the electronic properties and macroscopic organisation of these molecules are controlled. In this perspective, linear oligomers and polymer-conjugates incorporating heteroatoms have received particular attention.[1] Indeed, the introduction of heteroatoms allows the appearance of new geometrical or electronic properties directly related to the nature of the element. The P-rings are used to modify the chemical and physical properties of pi-conjugated systems.[2] The P-rings are also a potential source of chirality that has not been exploited so far in the field of molecular materials. For example, the phosphole has been little studied as a building block for the construction of pi-conjugated systems, although it possesses interesting properties for the construction of pi-conjugated systems[] The phosphole possesses (i) a weak aromatic character which should favour electronic delocalisation in a pi-system, and (ii) a reactive heteroatom which offers the possibility of tuning the energetic position of the HO and BV levels by chemical modifications such as the coordination of the phosphorus atom with a metal. These properties indicate that the phosphole may be a good candidate for the construction of extended pi-conjugated

systems. However, P-heterocycles are not limited to the phosphole family and during the last few years, other pi-systems based on phosphetenes (4-membered unsaturated P-ring),[3] phosphaphenalenenes /phosphinines (6-membered P-ring)[4] or phosphepines (7 membered P-rings)[5] have started to be studied in the context of molecular materials.

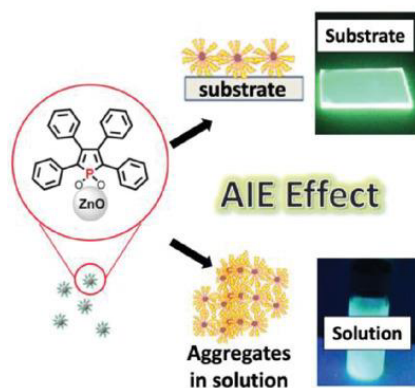
P-rings for optoelectronics

Here, we will report on the stereospecific synthesis of heliceneoid-based phosphepine as well as a chiral P-containing PAH through an axial to central chirality transfer from readily available 2,2'-bis(diphenylphosphino)-1,1'-binaphthalene (BINAP). [6] In these systems, an axial to central chirality transfer takes place from the BINAP moiety to the P-atom. The impact of the molecular design on the structure, the (chir)optical (including circularly polarized luminescence) and redox properties will be presented.



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We will also present the grafting of a hydroxyoxophosphole-based aggregate induced emitter with a POOH function with ZnO or a chiral cinnabar (-HgS) nanoparticle.[7] The restriction of the intramolecular motions of the organic fluorophore, through either aggregates' formation in solution or processing into thin films, forms highly emissive materials due to a strong aggregation induced emission effect. Theoretical calculations and XPS analyses were performed to analyze the interactions between the organic and inorganic counterparts. Furthermore, this combination allowed us to obtain organic-inorganic hybrid nanoparticles capable of emitting circularly polarised light from achiral fluorophores. The impact of the molecular design on the structure, the (chir)optical and redox properties have been investigated using a joint experimental/theoretical approach, highlighting the potential of these chiral derivatives for further applications in optoelectronics. Preliminary results on the use of these nanohybrids as solution-processed emissive layers in organic light emitting diodes (OLEDs) illustrate their potential for lighting applications.



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