

## Electronic properties of P-containing Polycyclic Aromatic Hydrocarbons

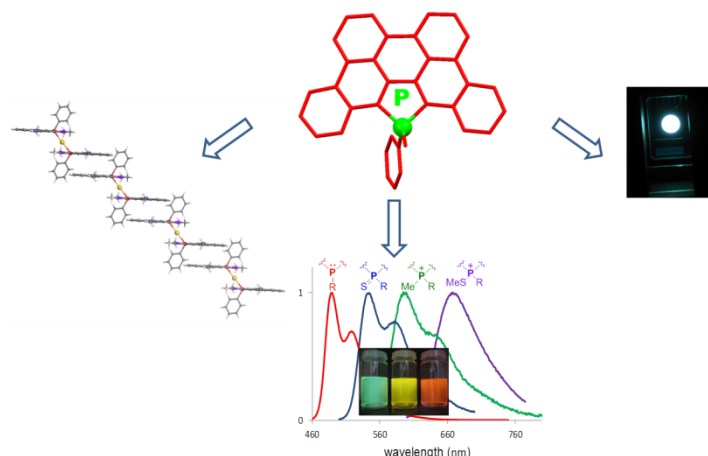
Pierre-Antoine Bouit

*Institut des Sciences chimiques de Rennes, Université de Rennes 1, Campus de Beaulieu,  
35042 Rennes Cedex, France*

*E-mail: pierre-antoine.bouit@univ-rennes1.fr*

Polycyclic aromatic hydrocarbons (PAHs) are of great potential in molecular materials for opto-electronic devices. Their bandgap and supramolecular organization is tunable through modification of the  $\pi$ -system and lateral aliphatic substituents. An alternative original approach uses the versatility of heterochemistry with the successful incorporation of N, O, S or B within the  $\pi$ -conjugated framework of PAHs.[1]

Here, we report that this strategy can be extended to P-modified PAHs.[2] A synthetic route to a family of P-modified PAHs is described. The reactivity of the P-center allows a straightforward HOMO-LUMO gap tuning. The impact of successive addition of fused aromatic rings around the P-ring was also studied. DFT calculations corroborate these studies. Furthermore, the coordination ability of the P-center allows unprecedented coordination-driven assembly of PAHs onto transition metals. The incorporation of these molecules in White emitting OLEDs shows the potential of this new family of compound for opto-electronic applications. [3]



### References:

- [1] M. Stepien *et al.* *Chem. Rev.* **2017**, 10.1021/acs.chemrev.1026b00076.
- [2] P.-A. Bouit, M. Hissler *et al.* *J. Am. Chem. Soc.* **2012**, 134, 6524.
- [3] P.-A. Bouit, M. Hissler *et al.* *Chem. Eur. J.* **2015**, 26, 1351 ; *Chem. Soc. Rev.* **2016**, 45, 5296; *J. Mater. Chem. C.* **2016**, 4, 3686 ; *Dalton Trans.* **2016**, 45, 1896 ; *Organometallics* **2017**, 10.1021/acs.organomet.6b00715.