

# Investigation of BN doped PAHs based on a Paracyclophane scaffold

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Boron–nitrogen-doped  $\pi$ -conjugated systems often possess exceptional electronic and optical properties, which qualifies their chiral representatives as promising emitters of circularly polarized light (CPL).<sup>[1]</sup> In previous studies, our group already demonstrated that the attachment of BN doped fluorophores to chiral scaffolds enables synthesis of potent CPL emitters.<sup>[2]</sup>

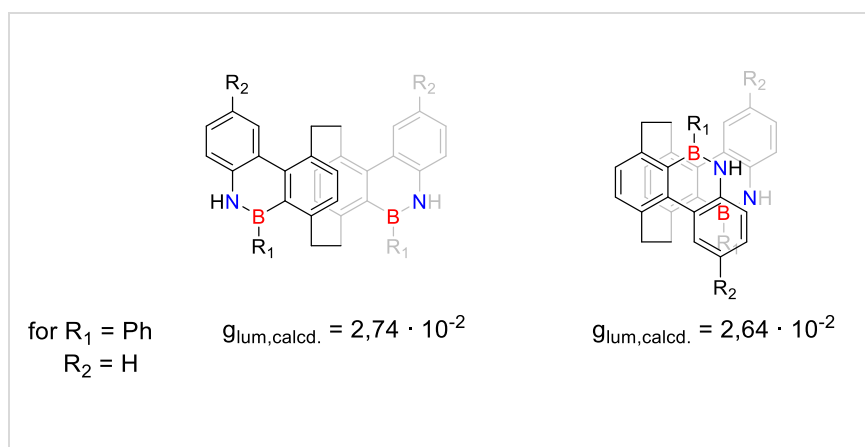


Figure 1: Target Molecules along with the computed dissymmetry factors ( $g_{\text{lum}}$ ) at the TD-M06-2X/def2-TZVP level of theory.

One of our current research projects focuses on the extension and BN-doping of the  $\pi$ - system of [2.2]Paracyclophane. The target molecules (Figure 1) were identified as potent CPL emitters in preliminary computational studies. The synthesis route of these compounds is currently under investigation.

## References:

- [1] X. Chen, D. Tan, D. Yang, *J. Mater. Chem. C*, **2022**, 10, 13499-13532.
- [2] M. Rapp *et al.*, *J. Mater. Chem. C*, **2023**, 11, 15767-15773.