New Boron(III) Blue Emitters for All-Solution Processed OLEDs: Molecular Design Assisted by Theoretical Modeling

In one word, how would you describe your research?
Predictive! Modern scientific research, especially synthetic chemistry, tries to reduce experimental procedures needed to obtain the optimized molecular structure for a desired application. Computational predictability is a very useful tool for this purpose.

What is the most significant result of this study?
The perfect synchronism between theoretical modeling and measured experimental properties, which can ultimately lead to material design inspired by calculations.

What was the biggest challenge?
First, optimization of the numerical calculations to compute the molecular structure in order to extract the photophysical properties. Second, optimization of the all-solution processed OLED structures, which were prepared and characterized under ambient conditions.

What was the inspiration for this cover design?
The idea behind the cover picture was the connection of theoretical modeling with molecular design to support synthesis, following specific criteria to achieve the desired molecular properties for application in OLEDs. The experimental electro-luminescence spectrum agrees quite well with that predicted theoretically. The model demonstrates the capability of theoretical methods to predict fluorescence rates and emission colors for these molecular materials, opening new possibilities for realizing novel ideas.

What prompted you to investigate this topic?
The main goal of this work was to obtain an efficient blue-emitting boron complex to be applied in solution processed OLEDs. This was allied to the aim of predicting photophysical properties from theoretical modeling. Also, the lack of easy and accessible computational predictions for real-sized molecules challenged us to investigate whether we could predict an OLED color from scratch by using our newly developed method.

What future opportunities do you see in the light of the results presented in this paper?
Molecular design assisted by theoretical modeling is likely the future of synthetic chemistry. It optimizes time, funds, and natural resources by enabling the ideal molecular structure having the desired properties to be predicted theoretically. We plan to keep improving this approach, to also include more complex systems such as those that present thermally activated delayed fluorescence (TADF) and phosphorescence. It seems that in a near future one would be able to predict not only structure but also photophysical properties to a good precision. This can open many new pathways in chemistry.
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Read more about the story behind the cover in the Cover Profile and about the research itself in the Full Paper by B. de Souza, I. H. Bechtold et al.