

# Room temperature phosphorescence in matrix-impurity organic crystals

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## ABSTRACT

In recent years, organic materials exhibiting room temperature phosphorescence (RTP) become a fancy research topic because of their broad range of applications as main components of electronic and optoelectronic devices, among others. Even though RTP in organic materials has been known for over a decade, it was not until 2021 that Chen *et al.* detected that RTP of carbazole was not an intrinsic property of the material but caused by an impurity present in the crystal.[1] In 2021, Ding *et al.* reported the effect on RTP properties of systematically doping an organic crystal with a series of structural isomers.[2] In this work, we present the full characterization of the crystal family in which **1BBI** acts as the matrix while **2BBI**, **4BBI** and **1BPP** are impurities. We use state-of-the-art DFT-based approximations to model the light-triggered processes on embedded monomers and dimers, providing a deep understanding of the RTP mechanism in matrix-impurity systems.

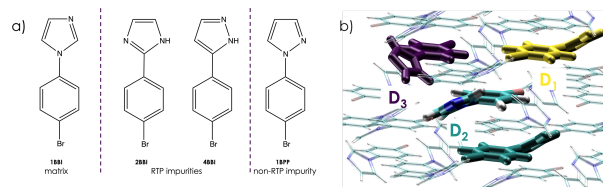


Figure 1: a) Matrix-impurity components b) Embedded dimers.

## References

- [1] Chen, C.; Zhengu, C.; Chong, K.; Bastanov, A.; Yang, Z.; Mao, Z.; Yang, Z.; Bin, L. Carbazole isomers induce ultralong organic phosphorescence *Nature Materials* **2021**, *20*, 175-180.
- [2] Ding, B.; Ma, L.; Huang, Z.; Ma, X.; Tian, -H. Engendering persistent organic room temperature phosphorescence by trace ingredient incorporation. *Science Advances* **2021**, *7*, eabf9668.