Unraveling Secrets of Photoluminescence of Carbon Dots by Computational Chemistry

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Carbon dots (CDs) discovered in 2004 are extensively studied nanomaterials due to their applications in sensing, bioimaging, theranostics and many others. Despite the joint effort of experimental and theoretical approaches a clear link between structure of CDs and their photoluminescent properties has not been established yet. In the talk, I will introduce theoretical tools and models, which provide valuable insights into optical properties of CDs. Particularly, the spotlight will focus on a combination of classical molecular dynamics simulations and theoretical methods for the description of absorption and emission of CDs, mostly time dependent density functional theory providing valuable insights into the nature of the excited states and the source of PL. One of the objectives of this talk is to show that combining the state-of-the art theoretical approaches [1] and modern experimental techniques is very effective strategy in the photoluminescence studies of CDs.

References

[1] Langer M. et al., Appl. Mat. Today, 22 (2021) 100924.