Single nanographenes as quantum emitters

JS Lauret[1]
T. Liu[1], D. Medina-Lopez[2], H. Levy-Falk[1], T. Huynh Thanh[1], S. Osella[3], C. Tonnelé[3], Y. Chassagneux[4], C. Voisin[4], L. Rondin[1], D. Beljonne[3], S. Campidelli[2]

[1]Université Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS, LuMIn, Orsay, France
[2]CMN, Université MONS, Belgium
[3]Université Paris-Saclay, CEA, CNRS, NIMBE,LICSEN, 91191 Gif-sur-Yvette, France
[4]LPENS, PSL, CNRS, Université de Paris,

lauret@ens-paris-saclay.fr

Recent years have shown an increasing number of studies focused on new light emitters for various applications and in particular for quantum technologies. In this context, nanographenes have great assets since bottom-up chemistry allows a total control on the structure, which opens the way to wide customization of their optical, and spin properties [1–3]. The full benefit from these opportunities needs addressing nanographene intrinsic photophysical properties. To do so, single molecule photoluminescence experiment is a powerful tool [4].

Here, we will focus on small nanographenes where electrons a confined in the three dimensions of space, the so-called graphene quantum dots (GQDs). We will show that our degree of control on the structure allows us to address both the influence of the size and of the symmetry of the GQD on its properties: emission wavelength, polarization selection rules, oscillator strength... We will report on experiments performed at the single molecule level and from room to cryogenic temperatures. We will show that the experimental results are well predicted by extensive DFT/TDDFT calculations combined with molecular dynamics simulations. [5-7].

References

[1] M. G. Debije, J. Am. Chem. Soc. 126, 4641 (2004)
[2] X. Yan, X. Cui, and L.-s. Li, J. Am. Chem. Soc. 132, (2010), 5944
[3] A. Konishi *et al*, J. Am. Chem. Soc. 132, (2010), 11021
[4] S. Zhao *et al*, Nature Communications, 9, (2018), 3470
[5] T. Liu *et al*, Nanoscale, 14, (2022) 3826 – 3833
[6] T. Liu *et al*, Journal of Chemical Physics 156, (2022), 104302
[7] D. Medina-Lopez *et al*, under review