Synthesis and study at the micro / nano scale of Poly(Diiododiacetylenes): on the road to carbyne?

<u>Yurii Zubchuk</u>¹, Vincent Malesys², Emmanuel Denys², Severinne Rigolet², Ludovic Josien², Nicolas Blanchard¹, Laurent Simon²

> Université de Haute-Alsace, CNRS, LIMA, UMR 7042¹, Université de Haute-Alsace, CNRS, IS2M, UMR 7361², *3bis rue Alfred Werner 68093 Mulhouse, France* <u>yurii.zubchuk@uha.fr</u>

After the discovery of fullerenes, carbon-nanotubes and graphene, one carbon allotrope described as "illusive"¹ has still not been studied properly: the carbyne.

This allotrope is defined as an infinitely long polyyne molecule $(-[C=C-]n)^2$. It is a major subject of interest with not well known physical properties: Young's modulus, nature of conductivity, charge mobility, possibility of a Seebeck effect etc. Also, its stability remains the major barrier to its large-scale production³, and the definitive evidence of its solid form synthesis has yet to be obtained.

Taking in account that carbyne has been being try to synthesize from other allotrope (CNT or graphene)⁴, by liquid laser ablation (LAL)⁵ and by chemical assembling⁶ we want to propose and develop new alternative method of obtaining carbyne from polydiidodiacetylene or PIDA – a long 1D conjugated polymer, where carbon chain substituted with only single-atom - iodine.

In this work using host-guest topochemical polymerization strategy following N. S. Goroff *et al.*⁷ and L. Luo *et al.*⁸ we developed and optimized the procedure of obtaining Host-PIDA co-crystal in gram-scale. We show using FTIR, Raman spectroscopy, as well as XRD, EDX, and NMR, that it is possible to remove the host molecules and isolate a stable PIDA polymer. We will show our first tentative of producing a PIDA-based Organic Field Effect Transistor (OFET) and first results of electrical measuring.

Next step – transformation of PIDA to carbyne, can be made by de-iodination of the PIDA via several methods: chemically - reaction with bases, physically – thermal, light irradiation or atom by atom using the STM technique.



Figure. Short schema of research project: carbyne synthesis from conjugated polymer

- [1] C. Casari et al., MRS Commun. 2018, 8, 207.
- [2] G. Yang, Mat. Sci. and Eng.: R: Rep., **2022**, 151, 100692.
- [3] R. Baughman, Science, **2006**, *312*, 1009.
- [4] Y. Ando et al., Phys. Rev. Lett., **2003**, *90*, 187401.
- [5] L. Peng et al., Phys. Rev. Lett., 2009, 102, 205501.
- [6] R. Tykwinski, Chem. Rec., **2015**, *15*, 1060.
- [7] N. Goroff et al., Science, **2006**, *312*, 1030.
- [8] L. Luo et al., Patent <u>WO2023097921A1</u>, **2023**.

