γ-graphyne: A promising electron acceptor for organic photovoltaics

The most significant discovery of recent years is graphene, which consists of a single layer of sp2-hybrid carbon atoms arranged in a two-dimensional (2D) honeycomb lattice nanostructure. Graphynes – a two-dimensional materials similar to graphene, but composed of sp-hybridized carbons periodically integrated into a sp^2-hybridized carbon network. Structure of graphynes were first theoretically proposed in 1987 by Baughman *et al*.[1] More than 20 years later, in 2010, Li et al. developed the first successful methodology for creating **γ-graphdiyne** films.[2] Despite the significant attention from the scientific community, only recently Hu et al. reported the synthesis of **γ-graphyne** with unified long-range crystalline structure.[3]

We demonstrate that **γ-graphyne** is an efficient electron acceptor due to its low LUMO and its ability to delocalize an excess charge.[4,5] Moreover, in contrast to other 2D sheets like graphene its electronic properties are not sensitive to vacancy defects. Investigation of photoinduced electron transfer processes in complexes of **γ-graphyne** with typical electron-accepting and electron-donating partners shows that the lowest excited states with donors are charge separated states formed by the electron transfer from partner to **γ-graphyne**. This electron transfer is thermodynamically favorable and occurs on nano-to-picosecond time scale. In contrast, electron transfer from **γ-graphyne** to strong electron acceptors such as fullerenes or arylenediimides is unlikely.

References:

[1] R.H. Baughman, H. Eckhardt, M. Kertesz, **J. Chem. Phys.** 1987, 87, 6687.

[2] G. Li, Y. Li, H. Liu, Y. Guo, Y. Li, D. Zhu, **Chem. Commun.** 2010, 46, 3256.

[3] Y. Hu, C. Wu, Q. Pan, Y. Jin, R. Lyu, V. Martinez, S. Huang, J. Wu, L.J. Wayment, N.A. Clark, M.B. Raschke, Y. Zhao, W. Zhang, **Nat. Synth.** 2022, 1, 449.

[4] O.A. Stasyuk, A.J. Stasyuk, M. Sola, A.A. Voityuk, **Mater. Des.** 2023, 225, 111526.

[5] O.A. Stasyuk, A.A. Voityuk, M. Sola, A.J. Stasyuk, **Carbon** 2023, 215, 118460.