CHEM2DMAC

Functionalizing 2D transition metal dichalcogenides with electron-accepting phthalocyanines

Elena A. Mack, Leandro Lourenço, Alejandro Cadranel, Tomas Torres, Dirk M. Guldi Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3A, Erlangen, Germany elena.mack@hotmail.es

Due to the unique properties of 2D transition metal dichalcogenides (TMDs) the preparation of these materials has attracted immense interest, in particular the liquid phase exfoliation and subsequent liquid cascade centrifugation, obtaining size selected TMDs in their semiconducting 2H-phase [1]. This opens up possibilities in tuning the electronic properties though functionalization, particularly pyridyl-zinc phthalocyanines (Pcs) with variable electron accepting strengths [2] awarded positively doped TMD nano-hybrids. We herein report on non-covalent functionalized TMDs with Pcs immobilized onto the basal plane of the exfoliated material [3], which exhibit distinct steady-state absorption and emission spectra. Furthermore, this nano-hybrids present charge transfer character where the electron donor is the 2D-TMD and the acceptor is the Pc which was assessed through steady-state Raman spectroscopy. Furthermore, charge separation was corroborated by femtosecond transient absorption spectroscopy [4] when contrasting to steady-state spectroelectrochemistry.

References

- [1] Synnatschke, K., Cieslik, P. A., Harvey, A., Castellanos-Gomez, A., Tian, T., Shih, C. J., Chernikov, A., Santos, E. J. G., Coleman, J. N., & Backes, C., *Chemistry of Materials*, *31*(24) (2019) 10049–10062
- [2] Wibmer, L., Lourenço, L. M. O., Roth, A., Katsukis, G., Neves, M. G. P. M. S., Cavaleiro, J. A. S., Tomé, J. P. C., Torres, T., & Guldi, D. M., *Nanoscale*, 7(13) (2015) 5674–5682
- [3] Scharl, T., Binder, G., Chen, X., Yokosawa, T., Cadranel, A., Knirsch, K. C., Spiecker, E., Hirsch, A., & Guldi, D. M., Journal of the American Chemical Society, 144(13) (2022) 5834–5840
- [4] Wibmer, L., Lages, S., Unruh, T., & Guldi, D. M., Advanced Materials, 30(12) (2018)



Figures

Figure 1: Excited state dynamics of the Pc-MoS₂ nano-hybrid where distinct spectral features of the radical anion appear around 850nm.