Non-covalent interaction of H_2Pc with CVD-grown transition metal dichalcogenides

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Since the first isolation of graphene, atomically thin two-dimensional (2D) materials have attracted growing interest due to their unique electronic and optical properties. Among them, transition metal dichalcogenides (TMDs) stand out for their tunable bandgaps, strong spin-orbit coupling, and potential in next-generation flexible nanoelectronics and nanophotonic devices [1]. The intrinsic surface sensitivity of 2D materials enables strong interactions with external environments and substrates, offering avenues for precise tuning of their properties. Functionalization strategies, that include mechanical modulation, intercalation, and both covalent and non-covalent molecular interactions, have emerged as powerful tools for modifying TMD behavior [2,3]. While intrinsic defects remain one of the major challenges in the field of 2D materials, they also serve as reactive sites for molecular adsorption, enabling new functionalities [4].

Phthalocyanine (Pc) molecules are highly suited for hybridization with 2D materials due to their planar π-conjugated structure, which promotes strong non-covalent interactions with TMD surfaces. Their tunable electronic properties and strong light absorption make them ideal for modulating the optoelectronic behavior of TMDs. The metal-free variant, H_2Pc, is especially interesting due to its symmetric electronic structure and ability to form uniform, ordered van der Waals interfaces without introducing magnetic or catalytic effects from a central metal atom [5,6].

In this seminar, I will present investigation of organic-inorganic heterostructures, consisting of H_2Pc molecules and CVD grown monolayers: molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2). Using atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM), Raman spectroscopy, and temperature-dependent photoluminescence spectroscopy (PL), we explore the interfacial interactions and their impact on the optoelectronic properties of these hybrid systems. Comparative analysis between MoS_2 and WS_2 highlights material-specific differences in molecular coupling and doping effects, driven by their distinct electronic structures. Our findings provide new insights into organic-inorganic hybrid interfaces, showing clear signatures of defect healing, exciton modulation, and interfacial energy transfer with strong potential for future optoelectronic applications.

Key words: 2D materials, TMDs, Organic-inorganic heterostructures, metal-free phthalocyanine, defect healing, energy transfer

References:

1] Patra, C., Mondal, S., Mukherjee, R., & Nandakishora, Y. (2025). Advanced synthesis and unique properties of 2D transition metal dichalcogenides for realizing next-generation applications. *ACS Materials Au*. https://doi.org/10.1021/acsmaterialsau.5c00015

[2] Daukiya, L., Nair, M. N., Cranney, M., Vonau, F., Hajjar-Garreau, S., Aubel, D., & Simon, L. (2019). Functionalization of 2D materials by intercalation. *Progress in Surface Science, 94*(1), 1–20. https://doi.org/10.1016/j.progsurf.2018.07.001

[3] Brill, A. R., Koren, E., & de Ruiter, G. (2021). Molecular functionalization of 2D materials: From atomically planar 2D architectures to off-plane 3D functional materials. *Journal of Materials Chemistry C, 9*, 11569–11587. https://doi.org/10.1039/D1TC01692G

[4] Liang, Q., Zhang, Q., Zhao, X., Liu, M., & Wee, A. T. S. (2021). Defect engineering of two-dimensional transition-metal dichalcogenides: Applications, challenges, and opportunities. *ACS Nano, 15*(2), 2165–2181. https://doi.org/10.1021/acsnano.0c09666

[5] Xu, X., Lou, Z., Cheng, S., Chow, P. C. Y., Koch, N., & Cheng, H.-M. (2021). Van der Waals organic/inorganic heterostructures in the two-dimensional limit. *Chem, 7*(11), 2989–3026. https://doi.org/10.1016/j.chempr.2021.08.013

[6] Drivas, C., Kennou, S., & Kyriakou, G. (2025). Phthalocyanine interfaces with MoS_2(0001): The effect of the metal centre on the charge transfer. *Applied Surface Science, 682*, 161672. https://doi.org/10.1016/j.apsusc.2024.161672