

Correlated Structural and Optical Investigation of Excitonic and Vibronic States in Metal-Free Phthalocyanine and Transition Metal Dichalcogenide Heterostructures

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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, H₂Pc, 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 an investigation of organic-inorganic heterostructures, consisting of H₂Pc molecules and different group-6 TMDs. In this research, two approaches for producing samples were used: bottom up (CVD) and top down (gold assisted exfoliation). Using atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM), Raman spectroscopy, temperature-dependent photoluminescence spectroscopy (PL) and modified nanoscale Fourier transform infrared spectroscopy (nano-FTIR) we explore the interfacial interactions and their impact on the optoelectronic properties of these hybrid systems.

Comparative analysis between CVD grown molybdenum disulfide (MoS₂) and tungsten disulfide (WS₂) highlights material-specific differences in molecular coupling and doping effects, driven by their distinct electronic structures [7]. Study of mechanical exfoliated monolayers and bilayers reveal layer dependent behavior. In case of molybdenum diselenide (MoSe₂) we show how molecular emission can be controlled by layer and temperature dependence which is used to control band alignments in HSs. 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

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