Conformation Effects and Charge Transfer Excitons in Organic-TMD Heterostructures

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Band alignment in transition metal dichalcogenide (TMD) heterostructures can give rise to a range of newly accessible excitonic states with large binding energies and lifetimes.[1] An alternative route to crystallographic stacking of individual TMD layers is the self-assembly of semiconductor molecules onto a TMD surface. Here the alignment between the band structure of the TMD and organic molecular orbitals can enable spatial separation of charge carriers between the two systems, leading to either free carrier generation or bound excitonic states. We describe the presence of interlayer charge transfer excitons between perylene derivatives (PBI) and bilayer MoS_2, constructed through liquid deposition of the organic molecule.[2] We observe and characterise variations in self-assembly on the MoS_2 surface that give rise to changes in the interfacial charge transfer and the density of interlayer excitons within different regions of the heterostructure. By further investigating the excitation intensity dependence of the intra and interlayer excitons, we find limits to charge transfer rates under poor molecular alignment, which has implications for the application of these materials in optoelectronic devices and sensors.

References

[1] Jiang *et al.*, Light: Science & Applications, 10 (2021) 72.
[2] Bartlam *et al.*, in preparation.

Figures

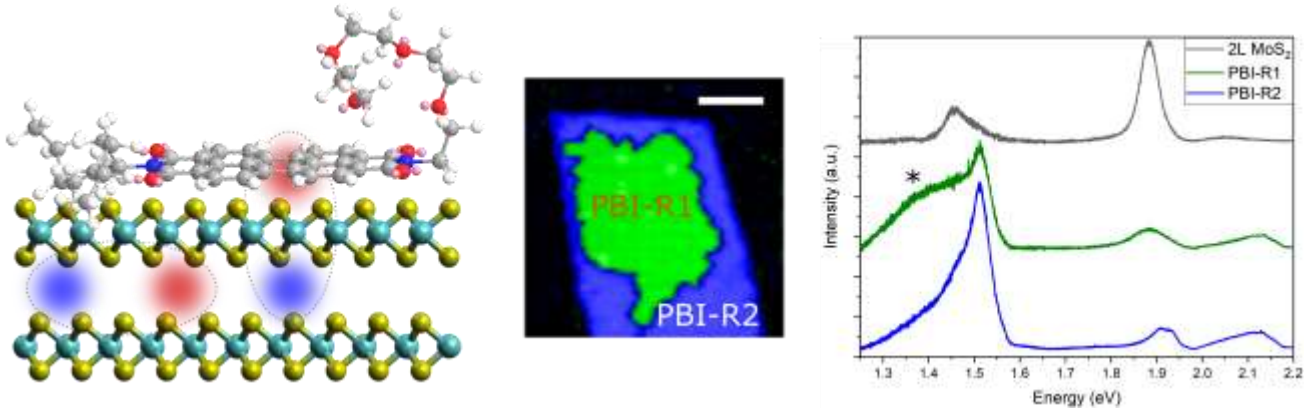

Figure 1: Left – schematic illustrating the presence of both interlayer and intralayer excitons in organic-TMD heterostructures. Centre – Raman map highlighting variations in the crystallographic alignment of the organic PBI molecule on a MoS_2 surface (5 µm scale). Right – Low temperature photoluminescence spectra highlighting the spectral variations between the two regions and an unfunctionalised bilayer (* denotes the energy of the interlayer exciton).