

Modulation of charge carriers in TMDs using covalent chemistry

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2D materials belong to a class of nanomaterials characterized by extreme thinness down to the nanometer regime and thus often do not have a bulk phase. Apart from this peculiar physical nature, these materials also display a wide variety of interesting electronic and optical properties that are sought in various nanoelectronic applications. One of the representative examples of 2D materials is the subclass of layered materials known as transition metal dichalcogenides (TMD) like molybdenum disulfide (MoS_2). Single layer (sl) MoS_2 in its 1H phase is semiconducting and fluorescent. It also may exist in a metastable metallic phase termed 1T- MoS_2 . Due to its ultrathin nature, the properties of sl- MoS_2 are influenced by various external and internal factors.^[1] Chemical functionalization can be a promising means for controlled modulation of properties in these materials.^[2] A large number of molecular functionalization approaches have focused on the more reactive, metallic 1T-phase to modulate its sensing and catalytic properties.^[2,3] The functionalization on 1H- MoS_2 is less explored, but given its distinctive optoelectronic properties, will also be equally important going forward.

In this contribution, I will present results on the covalent functionalization of CVD grown sl- MoS_2 and using diazonium chemistry. Attachment of aryl groups carrying different functional groups with varying electronic nature ranging from strongly electron donating to strongly electron withdrawing was studied using Raman and photoluminescence spectroscopies. We observe that the changes in the property correlate well with the electronic nature of the functionalization layer.

References

- [1] Schmidt, Henrik, Francesco Giustiniano, and Goki Eda, *Chem. Soc. Rev.*, 44 (2015) 7715-7736
- [2] Stergiou, Anastasios, and Nikos Tagmatarchis, *Chem. Eur. J.*, 24 (2018) 18246-18257
- [3] Simone Bertolazzi, Marco Gobbi, Yuda Zhao, Claudia Backes and Paolo Samori, *Chem. Soc. Rev.*, 47 (2018) 6845-6888

Figures

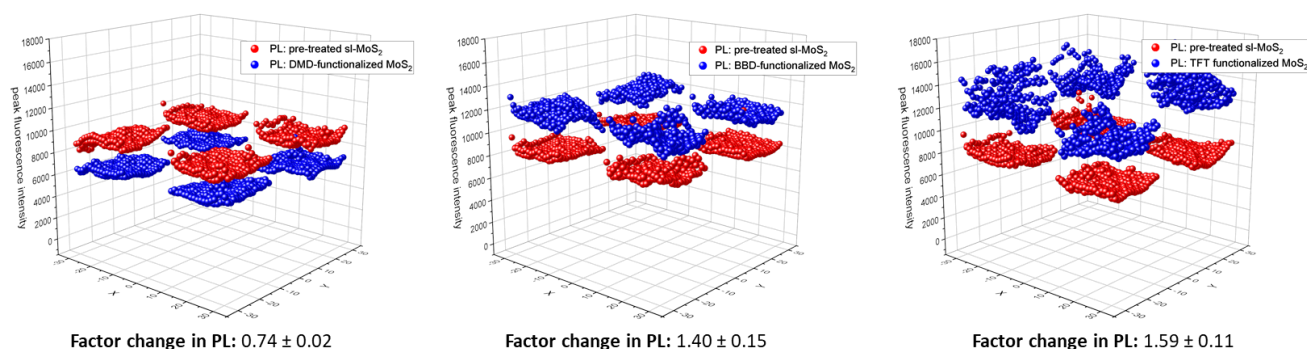


Figure 1: Spatial maps of photoluminescence intensity of single layer 1H- MoS_2 before and after covalent attachment of a functionalized aryl group.