

Towards quantification of covalent modification on semiconducting MoS₂

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2-dimensional (2D) materials are a recent class of nanomaterials that are characterized by their lack of a bulk state. They are a class of extremely thin nanomaterials that are confined to thicknesses of few atoms in one of the three dimensions. Albeit being a handful in number, this class of materials manage to manifest a wide range of optical and electronic properties among them. These materials have spread their impact to a range of fields from energy and catalysis, nanoelectronics, to drug delivery and biomaterials. One of the most representative examples of such a material is molybdenum disulfide (MoS₂). What makes this material interesting to us is its peculiar phase-dependent optoelectronic properties. MoS₂ has two notable phases: a semiconducting 2H phase, which is fluorescent with a direct bandgap, and a non-fluorescent but metallic 1T/T' phase. There is a growing interest in the research community on modulating and diversifying the properties of such materials. Covalent chemistry offers a solution to this problem as it is a simple and scalable approach for functionalizing these materials and tuning their properties. Different covalent chemical functionalization approaches have been reported on various 2D materials including MoS₂.^[1] But such approaches on MoS₂ have more focused on the 1T phase and defect sites in 2H phase rather than on the 2H basal plane.^[1,2] This can be accounted to the relatively inert nature of the 2H phase towards chemical reactions. Diazonium chemistry tackles these issues with its high reactivity and has recently been proven to be efficient for the covalent modification of 2H-MoS₂ with covalent bond formation between aryl groups and the basal plane of MoS₂.^[3]

We will be discussing the molecular functionalization and modification of semiconducting MoS₂ using diazonium salts towards interfacing these methods to technological applications by controlling and quantifying the modulation in properties. We combine scanning probe microscopy techniques along with Raman spectroscopy and photoluminescence studies to provide a broader understanding of these surface processes and their effect on material properties.

References

- [1] Anastasios Stergiou, Nikos Tagmatarchis, *Chem. Eur. J.*, 24 (2018), 18246-18257
- [2] Simone Bertolazzi *et al.* *Chem. Soc. Rev.*, 47 (2018), 6845-6888
- [3] Lakshya Daukiya *et al.* *Nanoscale*, 13 (2021), 2972-2981