Excitonic Properties Of Superacid Treated MoS₂ Monolayer

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Optical properties of semiconducting transition metal dichalcogenides (S-TMDs) have been recently intensively studied. This is mainly due to the fact that band gap in these materials changes from indirect to direct when decreasing number of layers. It causes photoluminescence (PL) to be much stronger in monolayer S-TMDs than in bulk crystals. However, even in monolayer MoS₂, the quantum efficiency of PL is very low (below 2 percent), which is associated mainly with vacancies present in the crystal structure of this S-TMD. Recently, it has been shown[1] that by using TFSI (bis(trifluoromethane) sulfonamide) superacid it is possible to increase radiative recombination efficiency even above 90 percent. Moreover, in the low temperature regime, the defect-related PL quenches, leaving excitonic recombination a dominant process[2].

We present the results of PL and reflectance study of superacid treated MoS_2 monolayer. They were obtained by means of a standard exfoliation technique of bulk and then deposited on Si/SiO₂. After initial characterization a certain number of MoS_2 layers were passivated in superacid. The passivation process consisted of several steps, including heating the sample and pouring it in TFSI.

At room temperature no quantum yield enhancement was observed, even though passivation process was performed on several types of samples (for example the natural and synthetic MoS_2 crystals). At low temperature we found that the intensity of defect-related PL is lowered. Most strikingly, contrary to the previous report[2], we observe redshift of the free exciton line.



Figure 1: Low-temperature (T = 5K) PL (left) and reflectance contrast (right) spectra taken from the same flake, before and after each of the passivation processes.

Moreover, two additional features (T_1 and T_2) emerge in the spectra before passivation. We relate them to the intravalley (T_1) and intervalley (T_2) trions with the same charge, but different valley configurations[3]. We discuss a model explaining the observed effects in terms of passivation and homogenization of the monolayer MoS₂.

- [1] Amani et al., *Science* 350, 1065 (2015).
- [2] Cadiz et al., Appl. Phys. Lett. 108, 251106 (2016).
- [3] Plechinger et al., Nat. Commun. 7, 12715 (2016).