The influence of crystallographic defects on the optical properties of MoS2

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Semiconducting transition metal dichalcogenides (TMDC) emerged as promising substitutes for graphene thanks to superior properties and inexpensive production methods. The main advantage comes from quantum confinement effects that enable an indirect-to-direct band-gap transition in single layers that makes TMDC monolayers suitable for nanoelectronic and optoelectronic applications.

The lattice defects in TMDC have been mainly studied from a structural point of view, while their optical properties remain mostly unexplored. Therefore, the analysis of the crystal defects deserves a focused approach to understand how novel optical properties can be engineered by controlling the defect nucleation.

We report on the experimental evidence of near-infrared (NIR) emissions from crystalline defects in MoS_2 multi-layer flakes exfoliated from bulk.

Different kinds of defects have been investigated by Transmission Electron Microscopy (TEM), Electron Energy Loss Spectroscopy (EELS), microRaman spectroscopy, Cathodoluminescence (CL) spectroscopy complemented by *ab-initio* Density Functional Theory (DFT) calculations in order to assess their influence on the optical properties.

In particular, the MoS_2 flake edges present an intense emission peaked at about 0.75 eV due to the high concentration of sulfur vacancies. Moreover, line defects induce a strong red-shift of the indirect band-to-band transition peaked at 1.25 eV.[1]

Lastly, structural and compositional modifications induced by controlled electron beam irradiation experiments have been performed to understand how novel electronic and/or optical properties can be engineered by controlling the nucleation of crystal defects.[2]

References

[1] F. Fabbri *et al. Nature Comm.* **7** 2016 13044
[2] E. Rotunno *et al. 2D Materials* **3** 2016 025024