Optical bandgap crossing of mono- and bilayer MoS_2 on SiO_2 depending on temperature

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The layered two-dimensional (2D) materials composed of transition metal dichalcogenides (TMDs) such as MX_2 (M = Mo, W, and X = S, Se) have been the centre of attention for applications in next-generation nanoelectronic and opto-electronic devices because of their unusual valley and optical polarization properties. Amongst them, MoS_2 can provide both indirect and direct bandgap transitions depending on the layer thickness [1]. A monolayer (1 L) of MoS_2 is a direct gap semiconductor, whereas bulk MoS_2 is an indirect semiconductor [1]. These findings have boosted the development of 2D materials for high-performance flexible electronic and optoelectronic devices [2]. There has been much interest generated in studying the characteristic optical properties of MoS_2 using photo-luminescence (PL) measurements as well as the valleytronics related to its 2D symmetry [3-5]. However, the electrical and optical properties of the MoS_2 can be greatly affected by its surface and also by the MoS_2/substrate interface. It is therefore important to understand how such interfaces can affect the optical and electronic features of the material. Moreover, the PL intensity depends on the number of layers, indicating that the quantum efficiency can decrease with layer thickness and whether the flake is freestanding or on a substrate [1]. Note that when MoS_2 layers lie on a substrate, each layer undergoes a different strain between the substrate and the MoS_2 layers because the first layer of MoS_2 is in direct contact with the substrate, whilst the other layers interact weakly due to van der Waals bonding between the MoS_2 layers, which can affect the optical transition between the 1L-MoS_2 and the other layers. Here, we present temperature dependent PL behaviour of mechanically-exfoliated 1L- and bilayer (2 L) MoS_2 prepared on a SiO_2 substrate. The PL peak's intensity and energy for the 2L-MoS_2 are stronger and higher than those of the 1L-MoS_2 at low temperatures below 200 K, in contrast to the room temperature measurements, where the opposite occurs as shown in Fig. 1. In order to explain this phenomenon, density functional theory (DFT) calculations are performed taking into account the thermal expansion at the MoS_2/SiO_2 interface.

References

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Figures

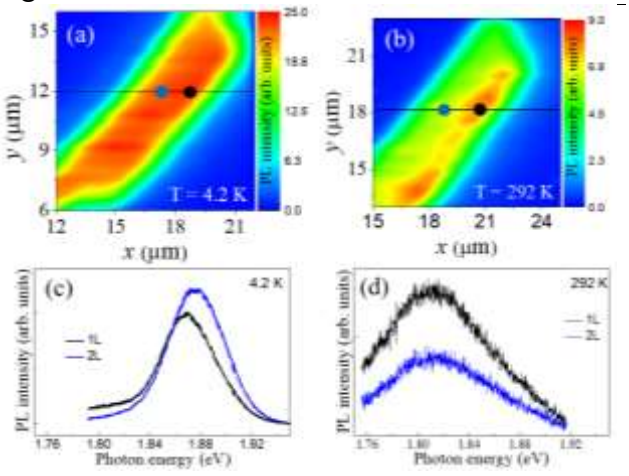

Figure 1: Integrated PL intensity mapping of the 1L- and 2L-MoS_2 flake measured at 4.2 K (a) and 300 K (b). The micro-PL spectra taken from the circle points of the maps at 4.2 K (c) and 292 K (d). The blue and black circles indicate 2L- and 1L-MoS_2.