Optoelectronic and optomechanical properties of atomically thin inorganic nanosheets as revealed by *in situ* TEM

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Free-standing few layered $MoSe_2$ nanosheet stacks' optoelectronic signatures were analyzed by using light compatible *in situ* transmission electron microscopy (TEM) utilizing an optical TEM holder allowing for the simultaneous mechanical deformation, electrical probing and light illumination of a sample [1]. Two types of deformation, namely *(i)* bending of nanosheets perpendicular to their basal atomic planes; and *(ii)* edge deformation parallel to the basal atomic planes, led to two distinctly different optomechanical performances of the nanosheet stacks. The former deformation induced a stable but rather marginal increase in photocurrent, whereas the latter mode was prone to unstable non-systematic photocurrent value changes and a red-shifted photocurrent spectrum. The experimental results were verified by *ab initio* calculations using density functional theory (DFT). The analogous experiments were continued on free-standing few-atomic-layer black phosphorus nanoflakes (Fig. 1) [2]. As compared to other 2-dimensional materials, the band gap of black phosphorus (BP) is related directly to multiple thicknesses and can be tuned by nanoflake thickness and strain. The photocurrent measurements with the TEM showed a stable response to infrared light illumination and change of nanoflakes band gap with deformation while pressing them between two electrodes assembled in the microscope. The photocurrent spectra of an 8-layer and a 6-layer BP nano-flake samples were then comparatively measured. DFT calculations were performed to identify the band structure changes of BP during deformations. The results provide useful pathways for BP smart band gap engineering *via* tuning the number of material atomic layers and programmed deformations to promote efficient optoelectronic applications.

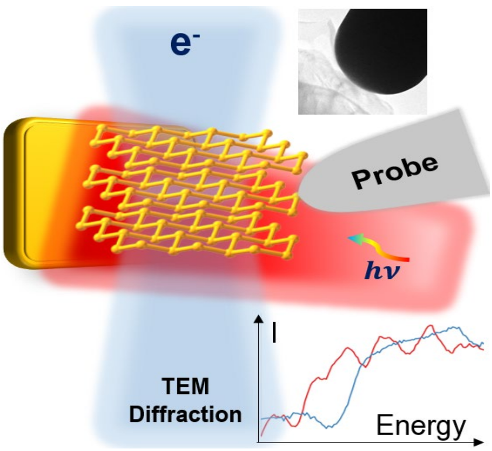

Figure 1. Schematic illustration of the *in situ* optoelectronic TEM setup for black phosphorus nanosheet optoelectronic response measurements. The inset is a low magnification TEM image illustrating the metal probe attached to the nanosheet in the microscope.

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References

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