Structure-dependent photoelectrochemical properties of transition metal dichalcogenides

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The exfoliation of bulk, layered crystals to single- and few-layered two-dimensional (2D) nanosheets resulted that, the transition metal dichalcogenides (TMDCs) monolayers became one of the first well-studied members of "2D materials family" beyond graphene, because of their high chemical stability and good electrocatalytic properties. [1] The electrochemical properties of 2D nanoflakes −which define the performance of these materials in energy-related applications− depends on their structural properties. For example, the number of layers, the basal/edge planes, and the defect density. [2-3] Therefore, to employ 2D nanosheets for energy conversion and storage we need to understand their fundamental photoelectrochemical (PEC) properties, using a microscopy-based approach with spatial resolution.

In our study, TMDCs samples, $MoSe_2$ and WSe_2, nanosheets were mechanically exfoliated to get bulk, few-layered, and monolayer specimens. The number of layers, and defect density in the separated nanosheets were characterised by Raman spectroscopy and atomic force microscopy. I will show in my presentation our recently developed custom-designed microdroplet cell-based photoelectrochemical approach to identify the structural parts and to measure the PEC activity of the flakes (by 10-50 µm droplets in diameter). PEC measurements, including photovoltammetry (Fig. 1A), photocurrent transient analysis, and quantum efficiency (Fig. 1B) to reveal the role of structural properties on the light harvesting, charge transport, and recombination properties of TMDCs will be presented. We have determined the band diagrams of these materials using bandgap values from PEC studies and work functions achieved from ambient pressure photoemission spectroscopy and surface photovoltage spectroscopy measurements. Finally, I demonstrate the use of model reversible redox species to mimic photoelectrocatalytic processes.

References

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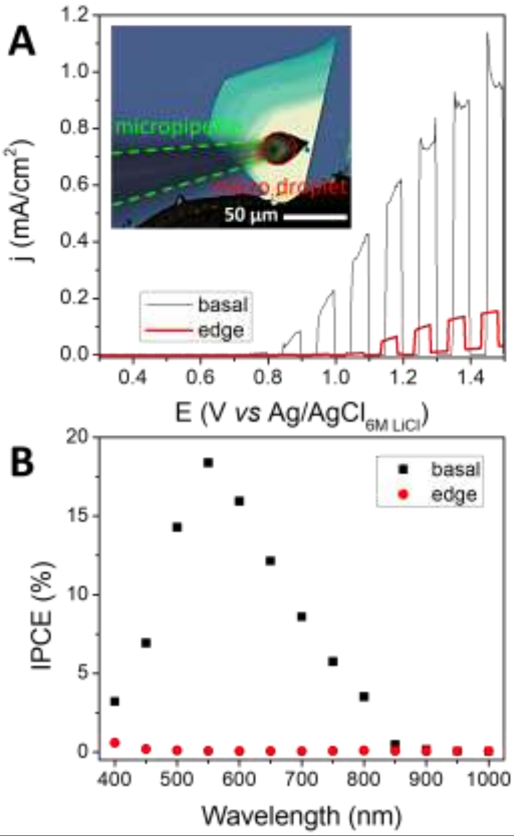

Figure 1: A) Linear sweep photovoltammograms recorded for the illuminated droplets deposited on basal- and edge-planes of bulk $MoSe_2$ flake. Inset depicts an optical micrograph of a droplet deposited on the surface of a bulk $MoSe_2$ flake, the dashed lines indicate the micropipette (green) and microdroplet/flake interface (red). B) Quantum efficiency curves show different behaviours between the PEC activity of basal- and edge-planes of bulk $MoSe_2$ flake.