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Interfacial Processes at H₂O/III-V Semiconductor Surfaces

Abstract

A photoelectrochemical (PEC) solar cell used for hydrogen production through water splitting offers an efficient approach to the future sustainable supply of energy. However, its performance is directly related to electronic and chemical properties of an electrolyte/photoelectrode interface.

III-V semiconductors exhibit many favorable properties that make them promising candidates for a photoelectrode of a PEC solar cell. Therefore, our recent attention was focused on Ga- and In-based materials for photoelectrodes and their interactions particularly with gas-phase H₂O molecules. We used ambient pressure X-ray photoelectron spectroscopy (AP-XPS) to track the physicochemical processes that occur on the III-V surfaces over wide ranges of pressure and temperature, thus approaching the operational conditions of PEC cells.

We were able to provide a better understanding of III-V surface chemistry at the molecular level and to observe the evolution of surface electrical properties that drive the performances of PEC devices with respect to work function, band bending, surface photovoltage effect, ionization energy, and electron affinity under operando conditions.

In addition, we showed that coupling with first-principles simulations allows one to correlate electronic properties with local interfacial chemistry, and to probe chemical and morphological changes induced by the surface oxidation of III-V photoelectrodes.