Minicolloque n° CPR 24 **X Oral** **☐ Poster**

Robust 2D semimetallic inclusions boost performances of III-V/Si heterostructures for water-splitting

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Hybrid materials taking advantage of the different physical properties of materials have become highly attractive for numerous applications in today's science and technology. For years, Anti-Phase Boundaries (APBs), generated during the non-polar III-V epitaxial growth on the polar Si substrate were considered as detrimental defects [1]. Recent researches gave the hope to develop phase-engineering strategies in III-V/Si samples [2-4]. In addition, the optoelectronic and vibrational properties of stoichiometric APBs were recently clarified [5]. Here, we demonstrate that epitaxial bi-domain III-V/Si are hybrid structures, composed of bulk photo-active semiconductors with 2D topological semi metallic vertical inclusions endowed with ambipolar properties. By combining structural, transport and photoelectrochemical characterizations (e.g. Fig. 1(a)) performed on various III-V/Si samples with first-principle calculations (e.g. Fig. 1(b&c)), it is shown that the bi-domain III-V/Si materials are able within the same layer to absorb light efficiently, separate laterally the photo-generated carriers, transfer them to semimetal singularities, and extract both electrons and holes vertically, leading to efficient carrier collection (Fig. 1(d)). The original topological properties of the 2D semi-metallic inclusions are also discussed. This work opens up new horizons for energy harvesting, photonics, electronics or computing device applications.

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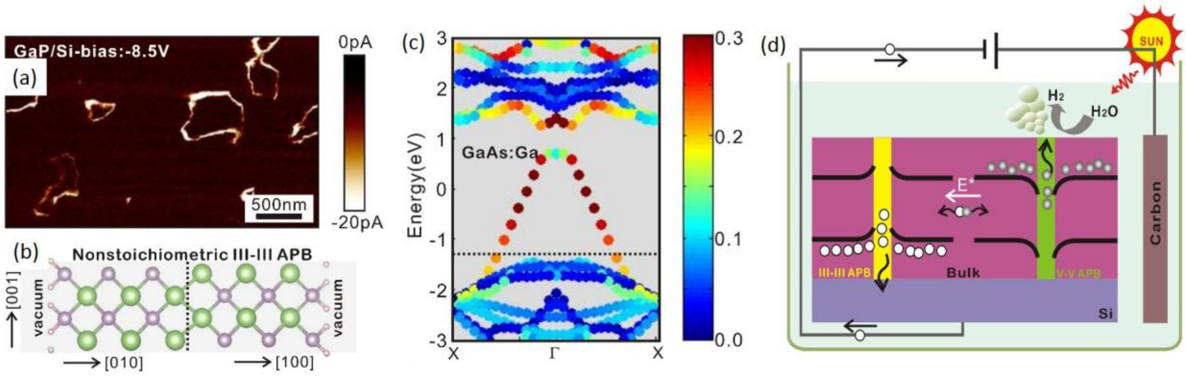

Figure 1 : (a) Conductive-AFM measurements highlighting the conduction by APBs, (b) Atomistic description of a non-stoichiometric APB, used for DFT calculations, (c) the semi-metallic bandstructure observed for an APB in GaAs, (d) Scheme of the carriers photogeneration and extraction in a III-V/Si sample for solar hydrogen production.