Surface traps: A key ingredient in the performance of semiconducting piezoelectric materials

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Piezoelectric thin films are widely used in MEMS and NEMS actuators and resonators [1], as well as in mechanical sensors and energy harvesters for IoT applications or wireless sensors networks (WSNs) [2]. Nanotechnology involving piezoelectric thin films and nanocomposites has been identified by the European Community as a key research direction [3], with benefits expected both from nanostructuring and from the replacement of toxic materials, such as the presently widely used PZT (lead zirconate titanate). Vertically-grown piezoelectric nanowires (NWs) of *e.g.* ZnO or GaN, embedded into an insulating matrix, are a typical example of such piezoelectric nanocomposites [4]. They have been employed in proof-of-concept sensors [5] and mechanical energy harvesters [6], featuring unexpectedly high performance, considering that ZnO is normally unintentionally doped during growth and that free carriers should screen the piezo-potential generated under mechanical load.

We will discuss modeling issues, with special focus on the introduction of surface traps and free carriers in the simulation of thin films and nanocomposites of piezoelectric semiconducting materials. Their impact turns out to be crucial [7]. In particular, we compared the piezoelectric response of ZnO NW-based composites to an equivalent ZnO thin film and demonstrated that surface traps explain some puzzling experimental results, such as the exceptionally high piezopotential values that have been measured experimentally in unintentionally doped ZnO NWs, as well as geometrical dependencies like asymmetrical response under bending.

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3. See, for example, *www.nereid-h2020.eu/content/nereid-mid-term-roadmap-download*
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6. Y. Hu *et al.*, *Adv. Mater.* **24**, 110 (2012).
7. R. Tao et *al.*, *Adv. Electronic. Mater*. **4**, 1700299 (2018).