FIG. 3: (Color online) The bare (unscreened) and screened pyro- and piezoelectric potentials along the axis of the nanowire ($t_{\mathrm{QD}} = 4$ nm, $t_{\mathrm{inf}} = t_{\mathrm{sup}} = 8$ nm). The position of the AlN barriers is outlined in gray, and the top surface is at $z = 0$.

$z = 0$ and the position of the AlN barriers is outlined in gray.

The band discontinuities at the GaN/AlN interfaces are clearly visible. The heterostructure undergoes a strong vertical electric field, which is almost homogeneous in the AlN barriers and in the GaN QD. The latter is empty of carriers (electrons and holes). The chemical potential is however pinned at the valence band edge at the top surface of the nanowire, and crosses the conduction band at the interface with the GaN pillar. Electrons therefore accumulate in the GaN pillar, while holes accumulate in the upper AlN barrier.

This redistribution of charges follows from the pyro- and piezoelectric polarizations. Leaving aside piezoelectricity for the moment, the spontaneous polarization in GaN is $P_z = -0.034$ C/m^2, while the spontaneous polarization in AlN is $P_z = -0.090$ C/m^2. This polarization is equivalent to a distribution of charges $\sigma = -0.090$ C/m^2 at the top surface, and $\sigma = \pm(0.090 - 0.034) = \pm 0.056$ C/m^2 at each GaN/AlN interface. Such a charge distribution, if unscreened, would create huge vertical electric fields and potentials of the order of 10 to 20 V in the nanowire (see Fig. 3).

The pyro- and piezoelectric field however bends the conduction and valence bands and tends to draw positive charges at the top of the nanowire, which screen the polarization.

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