Ab initio DFT simulation of the physical properties of InN/GaN multiquantum wells

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Ab initio DFT simulations of InN/GaN multiquantum wells (MQW) were used to obtain electric potential profile in the system that, after appropriate averaging procedure, reveal electric field in the wells and barriers, and also electric potential jumps at the interfaces. The field changes, and the potential jumps were used to obtain the density of the polarization charges and the dipole layer at InN/GaN interfaces, respectively. It was shown that polarization dipoles are confined within one double atomic layer, proving that they have different nature from the dipole layers emerging at the semiconductor surfaces or within p-n junctions.The obtained fields depend on both the well and the barrier thicknesses. DFT data are in good agreement with the continuum polarization analysis results that were obtained accounting the DFT determined potential jumps and using the standard polarization parameters. Built-in electric field causes a spatial separation of carriers, but one of the most important factors, from the point of view of efficiency of the light emission, is the overlap of the hole quantum states at the valence band maximum, and the electron states at the conduction band minimum. The efficiency proportional to the oscillator strength values was obtained from an implementation of the PAW method [1] in an existing plane-wave code supporting non norm-conserving Vanderbilt-type US PP's [2], the Vienna *ab initio* simulation package VASP [3] - [5]. To overcome the Kohn-Sham band gap (BG) underestimation, in comparison to the experimental ones, we have applied an empirical LDA+U correction method [6]. In parallel, a considerable insight was gained in the semiconductor structure properties, including the electronic dispersion relations and the density of states, both total and projected on the atomic layers. Semiconductor bands variation in space projected from partial density of states were inwestigated.

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