Artificial Intelligence improved quantum solver of III-V devices

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Downscaling of electronic devices calls for lower bias voltages, which are incompatible with the current CMOS technology because of the limits imposed by the unreducible (thermal) subthreshold swing and not large enough on-currents of CMOS switches. This deficiency can be overcome with tunneling field-effect transistors (TFET). In TFETs, the thermal tail is completely cut off, while the high on-current can be maintained at much lower bias. The tunneling probability of TFET is increased due to the use of III–V compounds which have the band structure properties that make them particularly suited for TFETs. They have a direct bandgap which means that band-to-band tunneling (BTBT) in these semiconductors does not need a phonon assistance. Also, thanks to the electron effective masses smaller than those in Si, the electron wave function deeper penetrates the channel and gives rise to a larger tunneling probability. Additional benefits can be gained in the heterojunction TFET (HTFET), in which lower built-in voltage results in narrower depletion layer and further increased tunneling probability. [1] The issue born by these new concepts is the classification of the charges that enter the Poisson equation which usually is solved consistently with the transport equations. The latter must be derived from quantum methods which catch the physics of the BTBT process. Results of such calculations, made with the nonequilibrium Greens function (NEGF) formalism, are shown in Fig. 1.

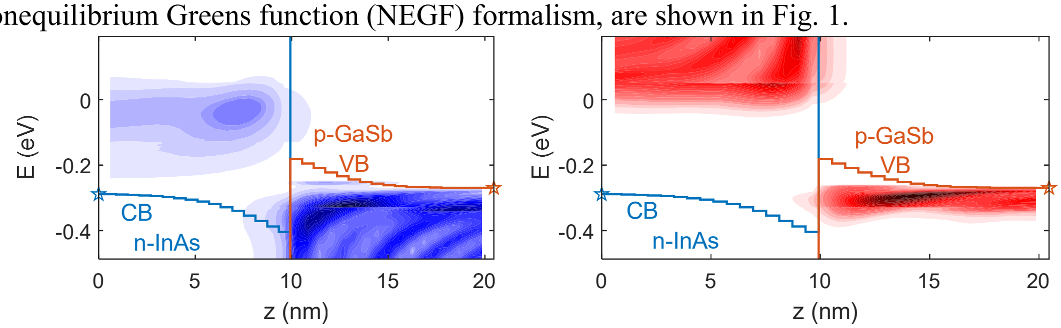

Fig. 1 Density of electrons (left)/holes (right) calculated from lesser/greater Greens functions, for n-InAs/p-GaSb heterojunction.

They refer to a single n-InAs/p-GaSb heterojunction - a part of the flagship HTFETs. As one can see, the electrons and holes penetrate both parts of the junction. When the standard ‘excess charge approach’ of charge counting, i.e., electrons in conduction band (CB) and holes in valence band (VB), is used in the Poisson equation, the parts outside this range are lost. This leads to an incorrect bending of the bands and, in-general, false characteristics. The treatments of this problem include defining some “fuzzy” band delimiters [2] or the full-band, electron-only approaches [3][4]. In this paper, a simple (but yet time-efficient) method of charge classification, which uses artificial intelligence (AI) method – the so-called support vector machine (SVM), is employed to classify charges in the NEGF-Poisson solver of electronic devices. The solver itself uses the 4-band k·p Hamiltonian in the planar orbital basis to estimate the quantity-level characteristic of simulated devices. These results will also be presented. Work is supported by NSC, Poland, Project No. UMO-2020/37/B/ST7/01830

[1] S. Wang, J. Wang, T. Zhi *et al. Physics Reports* **1013**, 1-13 (2023)

[2] M. Luisier and G. Klimeck, *IEEE Electron Device Lett.* **30**, 602 (2009).

[3] T. Andlauer and P. Vogl, *Physical Review B* **80**, 035304 (2009)

[4] Y. Chu, P. Sarangapani, J. Charles *et al. J. Appl. Phys.* **123** 244501 (2018)