Charge Transfer and Hybrid States in Inverted-Gap Core-Shell Nanowires

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Nanowires are rising much interest as a novel nanoelectronic platform for light harvesting, controlled single- or few-photon emitters, and for the realization of topological states e.g. in superconductor proximitized nanostructures. Core-shell nanowires, adding one or more radial layers of a different material to a central nanowire core, expand substantially the possibility to engineer the bandstructure, by tuning the geometric parameters of the sample, its doping profile and the type of band alignment between different materials[1]. In case the radial hetherojunction presents a type-2 inverted-gap alignment[2], electron and hole states coexist at the same energy, and the hybridization of these states takes place. On the one hand, this opens a new rich set of possibilities for quantum technologies, on the other hand, the mesoscopic modeling of such structures is very challenging, as both types of carriers must be taken into account at energies inside the broken gap.

We will present our investigation on the electronic structure of InAs-GaSb core-shell nanowires using a self-consistent, 8-band k.p approach which takes into full account the symmetry and crystallographic directions of the nano-crystal, its realistic hexagonal section and, possibly, external electric fields. Our method, aimed at reproducing the expected charge transfer effects in inverted-gap situations, is based on a real-space finite-element solution. Like the one described in Refs. [3] and [4], we compute the positive and negative charge density contributions separately. It only involves the calculation of a reduced number of the lowest energy eigenstates around the chemical potential, thus resulting in a very efficient approach.

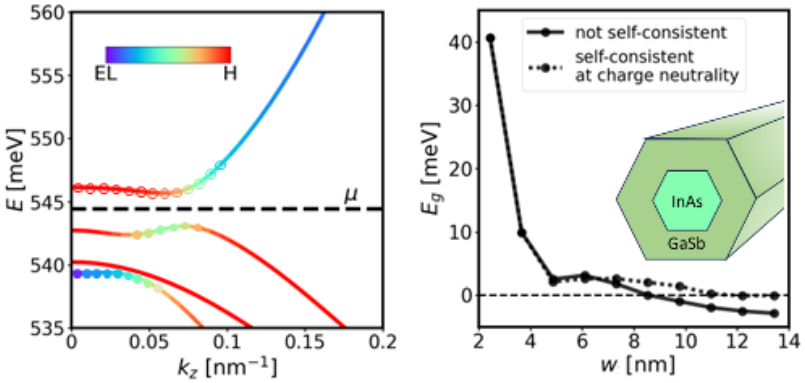

Fig.1. Left: Self-consistent bandstrucutre corresponding to a core radius of 7 nm and shell thickness of 7.3 nm, when the charge-neutrality condition is applied (blue/red color indicate the electron/hole character of the hybridized state). Right: Effective energy gap Eg for different values of the GaSb shell thickness w, with (dashed line) and without (full line) self-consistent effects and sketch of core-shell nanowire simulated.

In particular, we are interested in the fundamental band gap of the system (Fig. 1, left), the hybridization gap which results from anticrossing of the inverted electron and hole subbands. We will illustrate the charge transfer at the interface and how we include such self-consistent effects. Specifically, we extended and implemented approaches previously proposed in the context of InAs-GaSb quantum wells, exposing the substantial effect of the corresponding built-in electric field on the fundamental band gap of the system, which were neglected in previous investigations [5]. We will show how the inclusion of self-consistent electrostatic effects is essential in order to predict the system parameters at which the effective energy gap vanishes.

References

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