Band-offset driven efficiency of the doping of SiGe core-shell nanowires

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One of the main limit of doping of pure silicon and pure germanium nanowires (Si and Ge NWs) is its inefficiency when the diameter is reduced, as a consequence of surface segregation of impurities, strong quantum confinement and dielectric mismatch [1-2]. In the case of doping with boron or phosphorus impurities of Si and Ge NWs the impurity state is deep into the band gap and cannot be electrically activated at typical device temperatures. This phenomenon is responsible of several problems about the real applications of these types of materials for electronic devices.

We present first-principles electronic structure calculations within density-functional theory (DFT) of core-shell silicon-germanium NWs (with diameter of 2.4 nm), showing how this limit can be easily overcome by opportune doping with boron and phosphorus impurities [3]. In these nanostructures, as a matter of fact, the band offset between the two materials causes localization of the valence states on germanium and of conduction states on silicon. As a consequence of this property, with particular doping conditions, a one-dimensional electron (hole) gas at the band edge is created and the carrier density is uniquely controlled by the impurity concentration with no need of thermal activation.

The increased doping efficiency originates from the type II band offset at the Si/Ge interface (Figure 1e, left panel). The position of the impurity state, corresponding to a P at the Ge core, is determined by the wire-confining potential and by the local atomic environment of the Ge-core. In a stand-alone Ge NW as thick as the core, this state would be too deep to be thermally activated. In the core-shell geometry considered, however, the bottom of the conduction band is made up of Si-shell states that stand below any Ge-core state and the impurity state (see Figure 1d). Such an impurity state now does not need be thermally activated and the carriers it provides are available even at low temperature. The impurity state can be tracked back at ~0.34 eV inside the conduction band (see Figure 1b and 1d), while the shell localization of the first four parabolic states at the bottom of the conduction band (see Figure 1c), corroborates the band-offset picture. Similar arguments can be extended to B doping (see Figure 2) and Si core / Ge shell NWs.

SiGe core-shell nanowires provide a system ideally suited for high-mobility heterostructures and in particular for high-efficiency photovoltaic applications, since they fulfil two of their fundamental functions, that is, to separate electron and holes and to render both carriers electrically active.

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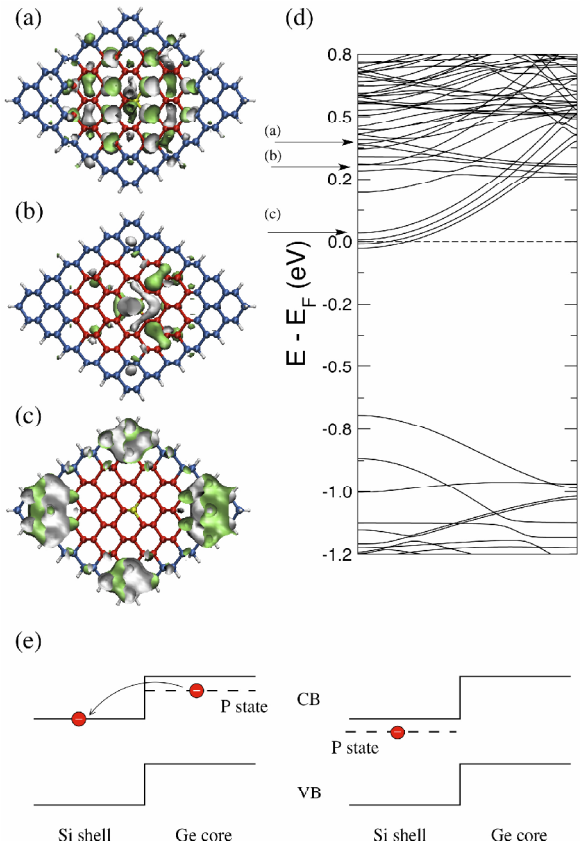

Fig. 1. Band structure of a Ge_{core}/Si_{shell} NW with P doping in the core (d); labeled arrows indicate the states whose real-space distribution is shown in panels (a-c). Lateral panels show the shell character of the bottom of the conduction band (c), the impurity state, 0.34 eV above the band-edge (b), and the lowest energy Ge-core state (a). A qualitative model of the band offset (not in scale) for P-doping of a Ge/Si core-shell NW is shown below (e). Doping of the Ge core yields an electron at the bottom of the conduction band localized in the Si-shell (left-hand side), whereas doping of the Si-shell is similar to the case of an all-Si NW (right-hand side).

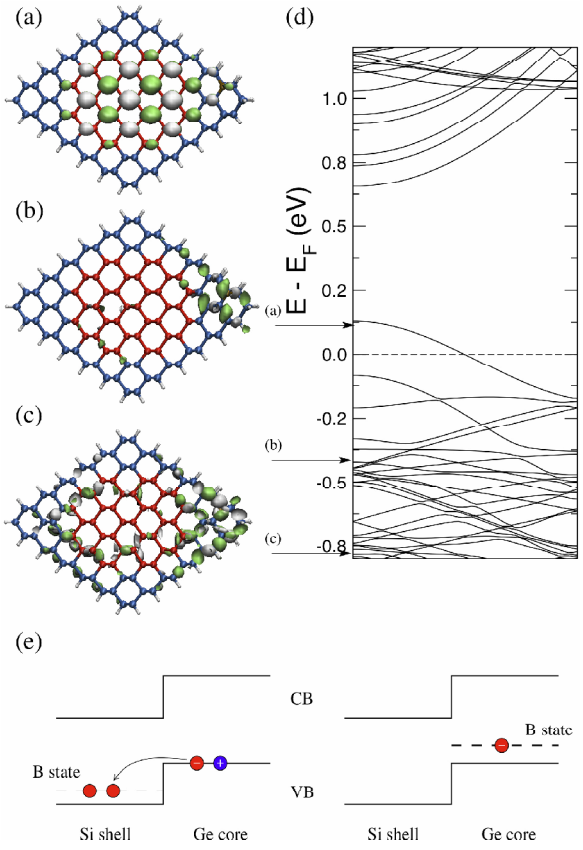

Fig. 2. Band structure of a Ge_{core}/Si_{shell} NWwith B doping in the Si shell (d); labeled arrows indicate the states whose real-space distribution is shown in the side panels (a-c). Lateral panels show the core character of the top of the valence band (a), the impurity state, 0.46 eV below the band-edge (b) and the highest energy Si-shell state (c). A qualitative model of the band offset (not in scale) for B-doping of a Ge/Si core-shellNWis shown below (e). Doping of the Si-shell yields a hole at the top of the valence band localized in the Ge-core (left-hand side), whereas doping of the Ge-core is similar to the case of an all-Ge NW (right-hand side).