

CARRIERS SPECTRA OF FUNCTIONALIZED  
SEMICONDUCTING NANOWIRES  
AND CONFORMATIONAL  
TRANSITION IN MOLECULES

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S u m m a r y

The tuning of the spectrum of semiconducting nanowires as a result of the functionalization by a layer of molecules with a conformational transition is investigated. The situation where the electric charge carrier induces the conformational transition with a change of the orientation of the intrinsic electric dipole moments of molecules is expected. The spectrum of a carrier and the parameters of the arising quantum well are determined by the derived self-consistent system of transcendent equations. The system includes the Schrödinger equation for a charge carrier, nonlinear equations for the intrinsic electric-dipole moments, the material equations describing the interaction of an extra carrier in the nanowire and molecular electric dipoles. In a semiconductor nanowire, the hole and electron spectra are symmetric. It is shown that the layer of adsorbed molecules breaks this symmetry when the molecular dipoles create the conditions for a localization of carriers of only one kind, which depends on the charge sign and the orientation of dipoles. The functionalized nanowires can be used as a semiconductor rectifier.