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TÉMA

Transport phenomena in nanowires, nanotubes, and other low-dimensional systems

Enrique Montes

Fyzikální ústav AV ČR, v.v.i.

First principles calculations have been implemented to study the ground state and electron transport properties of nanoscale materials and to evaluate its performance in electronic devices (magnetic tunneling junctions, field effect transistors and gas sensors). The ground state properties are studied within density functional theory using the SIESTA code, whereas the transport properties are investigated using the non-equilibrium Green's functions formalism implemented in the SMEAGOL code.

One-dimensional medium-sized nano-structured systems such as nanowires, nanotubes and nanoribbons are believed to be the most important building blocks for the next generation of electronic devices, due to the possibility to control their dimensionality, potentially tunning its physical properties. In particular, Si-based systems are attractive candidates due to their compatibility and ideal interface with the existing Si technology. In order to exploit the high spin coherence of Si a magnetic tunneling junction is built by connecting a <110> Si nanowire to ferromagnetic Fe electrodes. Substantial low bias magnetoresistance of ~200% is observed, which halves for an applied voltage of about 0.35 V and persist up to 1 V. On the other hand, Si nanotube field effect transistors are simulated by making connections to Au electrodes and applying an uniform potential gate. Its performance have demonstrated very high values of transconductance, outperforming the best commercial Si field effect transistors, combined with low values of the subthreshold swing.

As phosphorene (monolayer black P) is the only elemental two-dimensional material besides graphene that can be mechanically exfoliated and have demonstrated to support electronics, P-based systems are a potential platform of study. By specific dislocations of the atoms in the phosphorene lattice it is possible to generate another stable two-dimensional P allotrope with a bucked honeycomb lattice, known as blue P. The structural stability of monolayer zigzag and armchair blue P nanotubes is studied by means of molecular dynamics simulations. These nanotubes are found to be semiconductors with a sensitive indirect band gap that allows flexible tuning. The adsorption of CO, CO2, NH3, NO, and NO2 molecules on their surface demonstrate a high selectivity and sensitivity, surpassing the gas sensing performance of other nanoscale materials and making them superior gas sensors for a wide range of applications.

Field effect transistors with atomic perfect interface, consisting of of black P and blue P nanoribbons are simulated by using armchair nanoribbons as semiconducting channel and zigzag nanoribbons as metallic leads. These devices have been characterized leading to an excellent performance, superior to Si-based devices and commercial Si field effect transistors, with on/off ratio of ~103 , low subthreshold swing of ~60 mV/decade, and high transconductance of ~104 S/m.

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