FUNCTIONALIZATION OF ZNO NANOWIRES FOR SENSING APPLICATIONS

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There is an increasing demand for portable, reliable and cost effective integrated systems for chemical sensing and biosensing usage. This type of sensor has the potential to provide immediate analysis of blood samples so allowing early detection of diseases. Nanostructures offer novel and unique properties to fabricate such sensors, because the dimension of such structures are similar to those of the target chemical and biological molecules. Biological macromolecules, such as nucleic acids and proteins, are generally charged in aqueous solution and can be selectively detected when sensor molecules are linked to the nanowire surfaces. On the other hand, ZnO is a well known bio-friendly semiconductor with potential applications in electronics and optoelectronics including sensors, field effect transistors, photodetectors and nanolasers. Well-ordered ZnO nanowire arrays with hexagonalcan be grown, making them promising for future multi-functional devices. In this work we employ density functional theory to investigate ZnO nanowires and nanotubes. Bare wires are found to be semiconducting, with band gaps larger than that in bulk ZnO. The band gap decreases as the size of the nanowire increases, revealing strong quantum confinement effects [1,3]. As a first step towards biosensing applications, we have investigated ZnO nanowires functionalized with H and OH groups [5]. We find that the conductivity of these wires can be tuned from semiconductor to metallic, depending on how hydrogen and functional groups adsorb on the nanowire surfaces, thus leading to drastic changes in the ZnO nanowires electrical properties. The size-dependency of atomic relaxations, formation energies, and electronic structures in hexagonal non-passivated ZnO nanotubes was also investigated. The formation energies of thich-walled ZnO hexagonal ZnO nanotubes are mainly dependent on the thickness of the wall and almost independent of tube diameter [2,4]. Thick-walled ZnO nanotubes are energetically more favorable than single-walled ZnO nanotubes. We also show that for ZnO nanotubes confinement strongly affects the shape and energies of the conduction bands, while the valence band maximum seems to be not sensitive to a change of the thickness of the tube.

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