AB-INITIO CALCULATIONS OF CORE-SHELL CDSE/ZNS NANOWIRES

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We present ab-initio calculations of CdSe nanowires with a surrounding ZnS shell. The influence of a ZnS shell on the structural, electronic and vibrational properties is investigated. The ZnS shell leads to a shortening of the CdSe bond length. The electronic band gap is reduced by the presence of the ZnS shell. In the present study, the CdSe/ZnS multistructure forms a type-II heterojunction, in contrast to plane CdSe/ZnS superlattices forming type-I heterojunctions. The effect of the shell on the Raman-active radial breathing mode (RBM) is analyzed. A comparison with experimental RBM-frequencies will be given.