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Structural and electronic properties of InP nanowires: role of surface dangling bonds on nanowire facets TORU AKIYAMA, KOHJI NAKAMURA, TOMONORI ITO, Department of Physics Engineering, Mie University — InP nanowires are one of intriguing targets in the sources and detectors in fiber optic communications and high-speed electronic applications. In spite of this technological importance, however, understanding of atomic structures and electronic properties of InP nanowires still remain unclear. Here, we present first principles pseudopotential calculations that clarify structural stability and electronic properties of InP nanowires vertically grown on InP(111) substrates. Our calculations with diameter less than 23 Å demonstrate that the nanowires with zinc blende structure are less favorable than those with wurtzite structure, in which the surface dangling bonds on nanowire facets are found to be crucial to determine the stability. An analysis of the nanowire cohesive energy based on the number of the dangling bonds predicts that the nanowires are bistable forming both wurtzite and zinc blende structures at large diameter around 120 Å, which leads to the exhibition of polytypes being consistent with experiments. In addition, the calculated Kohn-Sham energy bands for stable wurtzite nanowires show that the surface dangling bond states determine the band character and the gap energy for the nanowires with diameter less than 9 Å while the gap energy of nanowires with diameter larger than 14 Å is dependent on only the nanowire size.

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