Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Stability and structure of free-standing III-V nanorods: An *ab initio* investigation ROMAN LEITSMANN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena — The interest in anisotropic needlelike crystals has been recently stimulated by the potential need as building blocks for nanoscale electronic and photonic devices. Due to their considerable potential for optoelectronics or high-speed electronics nanorods (NRs) consisting of III-V semiconductors are of particular interest. In most cases the growth direction of III-V semiconductor NRs is parallel to the [111] axis of the bulk zinc-blende (zb) structure. However, the crystal structure of the NRs may change noticable, depending on growth conditions and growth method. In particular, changes of the crystal symmetry from the cubic to the hexagonal (wurtzite - w) stacking of the cation-anion bilayers have been observed in many cases. We report ab initio investigations of hexagon-shaped III-V semiconductor NRs with varying crystal structure, varying surface passivation, and varying diameter [1]. Their stability is dominated by the free surface energies of the corresponding facets. We observe a phase transition between local zb and w geometry of the rods versus the preparation conditions of the surfaces [1] J. Appl. Phys. **102**, 063528 (2007)

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Date submitted: 02 Dec 2007 Electronic form version 1.4