Abstract Submitted
for the 4CF11 Meeting of
The American Physical Society

***Ab initio* study of wurtzite InAs and GaAs nanowires** PHIVU NGUYEN, ANDREW COPPLE, XIHONG PENG, Arizona State University — The unique properties of one dimensional semiconductor nanowires have inspired extensive research efforts during the past decade. In particular, group III-V semiconductors are promising building blocks for a wide range of applications such as field-effect transistors, light-emitting diodes, and optical sensors. A clear understanding of the fundamental properties of those materials, especially the electronic properties, and their tunability are critically important toward the applications. In this presentation, we report first principles density-functional theory study on the electronic properties of wurtzite InAs and GaAs nanowires along (0001) direction with the diameter of the wires up to 3 nm. The band gap of the nanowires increases with the reduction of the nanowire diameter, mainly due to quantum confinement effect. In addition, the band gap can be further tuned through uniaxial strain. The effective masses of charge carriers and work function of the nanowires are also reported.

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Date submitted: 15 Sep 2011 Electronic form version 1.4