

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Predicted Band Structures of Wurtzite III-V Semiconductors Based on Empirical Pseudopotentials** AMRIT DE, CRAIG PRYOR, Department of Physics and Astronomy, University of Iowa — The electronic properties of III-V semiconductor nanowhiskers present a problem since the nanowhiskers often crystallize in wurtzite (WZ) form while the corresponding bulk materials are zincblende. Using empirical pseudopotentials, including spin-orbit coupling, we have computed the bulk band structures for non-nitride III-V semiconductors in WZ form, which may be used for electronic structure calculations of nanowhiskers. The calculations make use of transferable model pseudopotentials fit to the zincblende form. We find that due to the stronger breaking of inversion symmetry in the WZ form, there are larger zero field spin splittings than in the corresponding zincblende materials, making WZ nanowhiskers good candidates for novel spin based devices.

Amrit De  
Department of Physics and Astronomy, University of Iowa

Date submitted: 21 Nov 2008

Electronic form version 1.4