

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Effective multiband Hamiltonian for InAs in wurtzite phase<sup>1</sup>**

PAULO E. FARIA JUNIOR, TIAGO CAMPOS, CARLOS M. O. BASTOS, GUILHERME M. SIPAHI, University of Sao Paulo, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — Recent advances in nanostructure growth techniques allowed the synthesis of new III-V compounds with wurtzite crystal structure[1]. Although ab initio band structures for these new wurtzite materials can be found in the literature[2], we still lack multiband models and parameter sets that can be simply used to investigate, for instance, quantum confinement effects. In this study, we calculated the ab initio band structure of bulk InAs wurtzite and developed a multiband k.p Hamiltonian to describe the energy bands around the energy gap. In order to correctly describe the spin splitting effects we included the k-dependent spin-orbit term, often neglected in literature. We showed that our model is very robust to describe the important features of the band structure and also the spin splittings with great agreement to the ab initio values. [1] P. Caroff et al., Nat. Nanotechnol. 4, 50 (2009). [2] A. De and C. E. Pryor, PRB 81, 155210 (2010).

<sup>1</sup>CNPq (149904/2013-4 and 88887.110814/2015-00), CAPES PVE (88881.068174/2014-01), DFG SFB 689 and FAPESP (2012/05618-0)

Paulo E. Faria Junior  
University of Sao Paulo

Date submitted: 01 Dec 2015

Electronic form version 1.4