Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

k.p Parameters with Accuracy Control from Preexistent First-Principles Band Structure Calculations[1] GUILHERME SIPAHI, CARLOS M. O. BASTOS, FERNANDO P. SABINO, PAULO E. FARIA JUNIOR, TIAGO DE CAMPOS, JUAREZ L. F. DA SILVA, Universidade de So Paulo — The **k.p** method is a successful approach to obtain band structure, optical and transport properties of semiconductors. It overtakes the *ab initio* methods in confined systems due to its low computational cost since it is a continuum method that does not require all the atoms' orbital information. From an effective one-electron Hamiltonian, the **k.p** matrix representation can be calculated using perturbation theory and the parameters identified by symmetry arguments. The parameters determination, however, needs a complementary approach. In this paper, we developed a general method to extract the **k.p** parameters from preexistent band structures of bulk materials that is not limited by the crystal symmetry or by the model. To demonstrate our approach, we applied it to zinc blende GaAs band structure calculated by hybrid density functional theory within the Heyd-Scuseria-Ernzerhof functional (DFT-HSE), for the usual 8×8 **k.p** Hamiltonian. Our parameters reproduced the DFT-HSE band structure with great accuracy up to 20% of the first Brillouin zone (FBZ). Furthermore, for fitting regions ranging from 7-20% of FBZ, the parameters lie inside the range of values reported by the most reliable studies in the literature.

[1]The authors acknowledge financial support from the Brazilian agencies CNPq (grant #246549/2012-2) and FAPESP (grants #2011/19333-4, #2012/05618-0 and #2013/23393-8).

Guilherme Sipahi
Universidade de So Paulo

Date submitted: 05 Nov 2015 Electronic form version 1.4