Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-Principle Tight Binding-Like Parametrizations of $\mathbf{GaAs_{1-x}Bi_x}$ and $\mathbf{InAs_{1-x}Bi_x}$ Electronic Structures S.C. BADESCU, Wyle Aerospace/US AFRL, M.E. GRUPEN, US AFRL, J. HADER, J.V. MOLONEY, NLCSTR, US, S.W. KOCH, Marburg Univ., Germany — The anion substitution with Bi atoms in large concentration (1-5%) has been proven to be an effective means for tuning the energy bandgap and the spin-orbit in materials like GaAs and InAs. In order to describe these materials in opto-electronic device simulations it is necessary to use simple and accurate parametrizations of their bandstructures. We describe here tight binding–like parametrizations of first-principle bandstructures to compare the better-know $GaAs_{1-x}Bi_x$ with the newer $InAs_{1-x}Bi_x$. Accurate bandgaps are included via hybrid density functionals, and spin-orbit split-offs of the valence bands as well as the d-orbitals for In are found to be crucial. Essential features such as the strong perturbation of the Luttinger Hamiltonian and the strong anticrossing between valence bands and impurity d-orbitals are captured in a zone-unfolding picture.

S.C. Badescu
Wyle Aerospace/US AFRL

Date submitted: 14 Nov 2014 Electronic form version 1.4