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sp3s* and sp3d5s* Tight-Binding Parameter Sets for GaAs, AlAs, InAs, GaSb, AlSb, InSb, GaP, AlP, InP for quantum dot simulations GERHARD KLIMECK, Jet Propulsion Laboratory, Cal. Inst. of Techn., R. C. BOWEN, JPL, T. B. BOYKIN, University of Alabama in Huntsville, Huntsville, AL 35899, T. A. CWIK, JPL — Nano-scaled electronic devices are characterized by material and charge density variations on the length scale of a few atoms. Tight-binding models can resolve spatial material variations on an atomic scale and represent the full crystalline and electronic symmetry of semiconductor materials. While the tight binding approach is systematically appealing, it bears the problem that the orbital interaction energies are related to bandedges and effective masses in a non-trivial manner (15 and 29 "free" parameters). A genetic algorithm approach is used to fit orbital interaction energies of sp3s* and sp3d5s* tight-binding models for the compound liste above. The new parameters are optimized to reproduce the bandstructure relevant to carrier transport in the lowest conduction band and the highest three valence bands. The accuracy of the other bands is sacrificed for the better reproduction of the effective masses in the bands of interest. Relevant band edges are reproduced to within a few meV and the effective masses deviate from the experimental values typically by less than 10%. These new parameters will be useful for nanostructure simulations with tools such as NEMO.

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