

# Tight Binding analysis of Si/GaAs UTBs with subatomic resolution

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Modern semiconductor devices have reached critical device dimensions in the range of several nanometers. These devices often have confined geometries such as Ultra Thin Body(UTB)-FETs, Fin-FETs and nanowires. In those nano-scale confined geometries, quantitative device analysis requires the reliable prediction of the bandgaps, effective masses and carrier distribution. Recent study by R. Hatcher et,al suggested that the surface carrier distribution in confined systems is strongly geometry and material dependent[1]. The Empirical Tight Binding (ETB) methods are appropriate for device modeling, as ETB methods are proved to be numerically efficient for device level simulations[2]. Traditional ways of ETB parametrization[3] do not provide the explicit TB basis functions, which makes it difficult to predict wave function dependent quantities with high precision. In this work, transferable ETB parameters with explicit basis functions of Si and GaAs are generated by DFT Mapping method[4] which relies on DFT results. The application of the ETB parameters and basis functions to Si and GaAs shows good agreement with DFT E-k diagram and wave functions.

The process of DFT mapping method[4] is shown in Figure. 1. The DFT mapping method make use of the DFT results such as band diagram and eigen functions rather than experimental data. During the Mapping process, TB parameters and TB basis functions are both adjusted to match the corresponding DFT results. The DFT mapping method is applied to bulk/UTB Si and GaAs and sp<sup>3</sup>d<sup>5</sup>s\* ETB model is parameterized. DFT calculations of Si and GaAs systems were performed by VASP package. Hybrid functional HSE06 is used to model the e-e interactions to produce reasonable band gaps. A cutoff energies of 350eV is used for all DFT calcu-

lations. The calculations for bulk and UTB systems are performed on  $6 \times 6 \times 6$  and  $6 \times 6 \times 1$   $\Gamma$  centered Monkhorst Pack k space grid respectively. The band structures of bulk Si and GaAs are shown in Figure. 2 a) and b) respectively. It can be seen that the TB band structures match the corresponding DFT results well. Figure. 3. shows contour of selected localized TB basis functions on x-y plane. The TB basis functions are invariant under crystal symmetry operations. Bulk TB parameters and basis functions is applied to Hydrogen-passivated [100] Si/GaAs UTBs. DFT Mapping method is used to determine the parameters of passivation. E-k diagram and wave functions of 100 Si UTB and GaAs UTB are shown in Figure.4 and 4. respectively. The s orbitals of Hydrogen atoms are included in the TB Hamiltonian. The TB E-k diagrams of UTBs show good agreement with DFT results, suggesting good transferability of the TB parameters. Fig. 6 shows the band gaps of the Si and GaAs UTBs as a function of UTB width. The TB band gaps match the HSE06 band gaps well even for UTBs as thin as 1 to 2 nm. The matching of TB wave functions with DFT ones suggests the TB model with basis function have capability of predicting wave function dependent properties in high precision.

nanoHUB.org computational resources operated by the Network for Computational Nanotechnology funded by NSF are utilized in this work.

## REFERENCES

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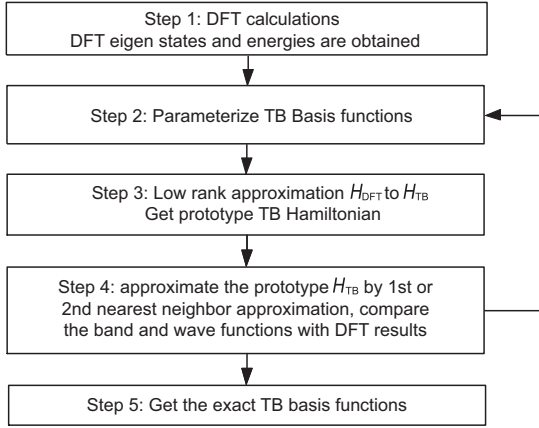


Fig. 1. The process of DFT mapping. ETB parameters and basis functions are extracted iteratively from DFT results.

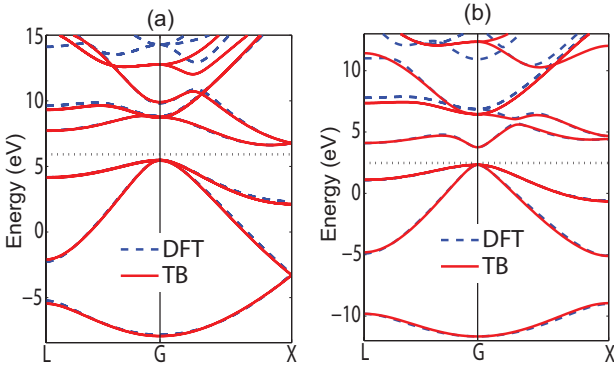


Fig. 2. Band structure of bulk Si(a) and bulk GaAs(b). DFT band structures are based on HSE06 Hybrid functional approach.

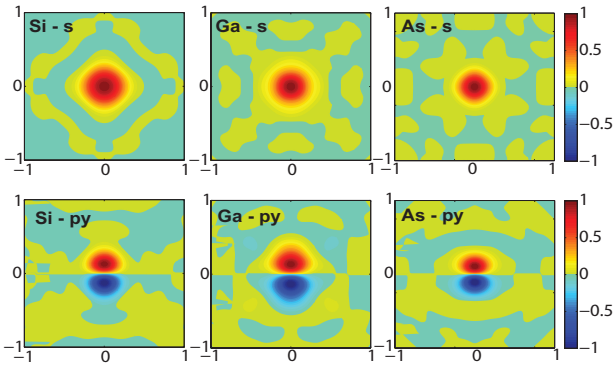


Fig. 3. Tight Binding basis functions of Si, Ga and As atoms. The Orthogonal TB basis functions satisfy crystal symmetries, but has multiple angular parts in each orbital.

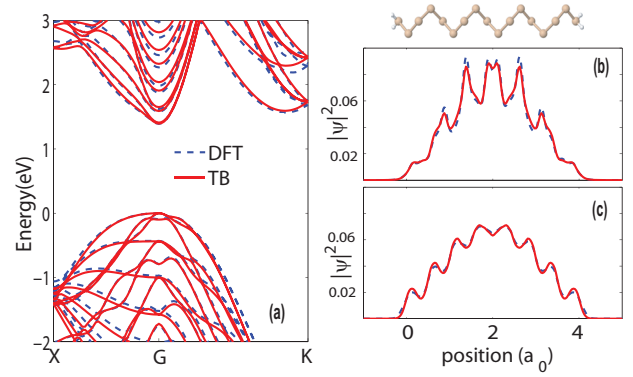


Fig. 4. Si 100 UTB band structure(a) and planar averaged wave functions of lowest conduction bands(b) and topmost valence bands(c). The Si UTB has 17 Si atomic layers, with a thickness of  $4 a_0$ .

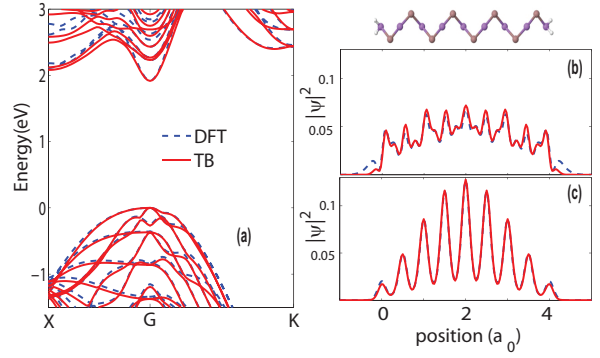


Fig. 5. GaAs 100 UTB band structure(a) and planar averaged wave functions of lowest conduction bands(b) and topmost valence bands(c). The GaAs UTB has 17 atomic layers, and is terminated by As atoms, with a thickness of  $4 a_0$ .

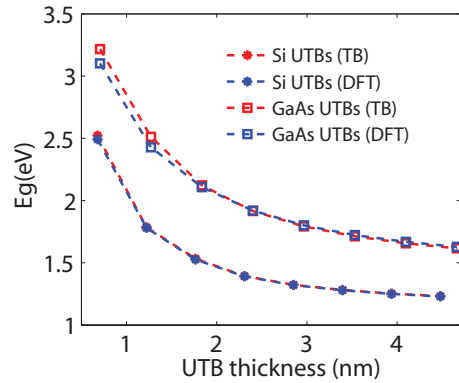


Fig. 6. Band gaps of Si and GaAs UTBs by Hybrid functional and Tight Binding method. The TB bandgap agree well with the Hybrid functional gap for UTBs as thin as 1 to 2nm.