Generation of Empirical Tight Binding Parameters from ab-initio simulations

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INTRODUCTION

Nanoelectronic semiconductor devices reach critical lengths in the range of 1 to 20nm in two or more dimensions. The active device domain might contain 10,000 to 10 million atoms. Ab-initio methods based on Density Functional Theory(DFT) are usually adopted in the study of nano-materials [1], however, they can only be applied to small systems, thus are not appropriate for device level simulations. However, Empirical Tight-Binding(ETB) can meet the requirements of realistic nano electronic device modeling as demonstrated by the prior modeling results of semiconductor devices [2]. The success of the ETB methods rely on the careful calibration of the ETB parameters [3][4].

The need for ETB parameterizations is growing rapidly as new materials enter device considerations. However, for some exotic materials, no experimental data of the detailed band structure is available. Furthermore the ETB method in general suffers from the lack of an explicit basis representation. Computation of properties such as optical matrix elements and parameters at heterointerfaces require the knowledge of the real space representation of ETB basis functions. This work gives a more fundamental link between ETB and ab-initio methods in order to expand the scope and impact of ETB methods.

METHOD

In this work, a method to extract ETB parameters from ab-initio calculations is developed. The process of the method is shown by flow chart in Fig. 1. The ETB basis functions are defined as

$$\Psi_{n,l,m}(r,\theta,\phi) = R_{n,l}(r)Y_{l,m}(\theta,\phi) \qquad (1)$$

where the radial parts are damped plane wave functions

$$R_{n,l}(r) = \sum_{i=1}^{N}(a_i \sin(\lambda_i r) + b_i \cos(\lambda_i r))r^{n-1}e^{-\alpha_i r} \qquad (2)$$

with parameters $a_i, b_i, \alpha_i, \lambda_i$ to be determined. Once ETB basis functions are known, DFT Hamiltonian is transformed into the ETB basis via low rank approximation [5]. ETB parameters such as onsite energies and two center integrals [6] are obtained from the transformed Hamiltonian. Targets such as band structure, effective mass and wave functions are then evaluated. In order to match ETB targets with the DFT ones, ETB basis functions are adjusted iteratively.

RESULTS AND DISCUSSION

In this work, DFT results are obtained by ABINIT [7]. The method is applied on ETB parameters of bulk Silicon and GaAs. The band structure of Silicon and GaAs by both DFT and ETB are shown in Fig. 2 and Fig. 3. It can be seen that ETB band structures are in good agreement with DFT results. In addition, the parameterization of Equation (2) is chosen such that the eigen functions of the topmost valence bands match with corresponding DFT eigen functions. The radial parts of ETB basis functions of Silicon and GaAs are shown in Fig. 4 and Fig. 5 respectively. The ETB basis functions are localized within the range of lattice constant(5.43Å for Si and 5.65Å for GaAs).

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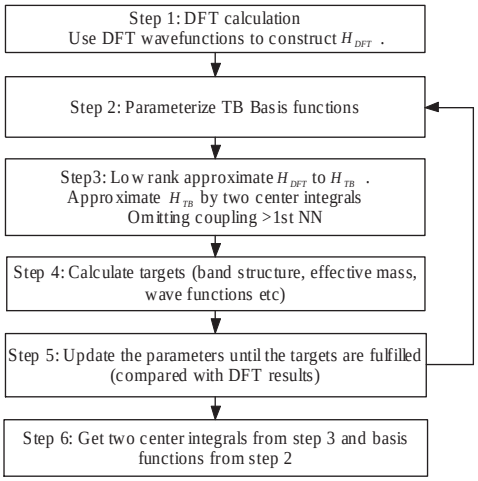

Fig. 1. Process of ab-initio mapping

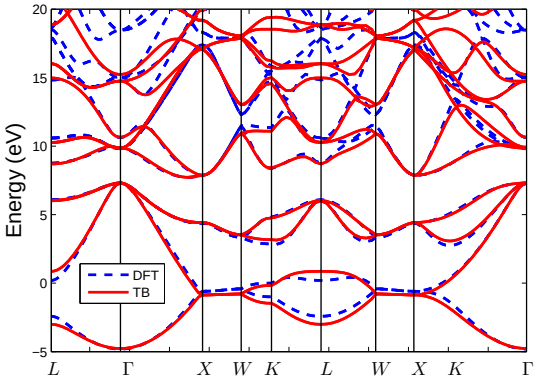

Fig. 2. Band structure of bulk Silicon: Comparison between ab-initio and ETB Band structure

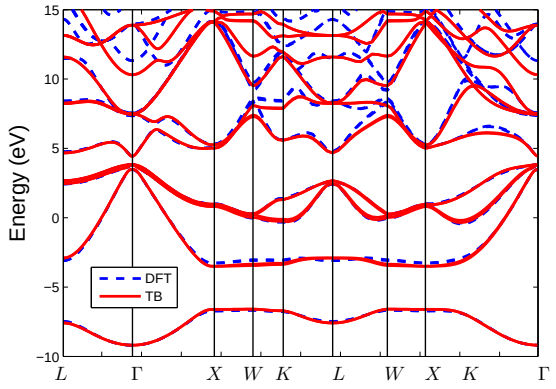

Fig. 3. Band structure of bulk GaAs: Comparison between ab-initio and ETB Band structure

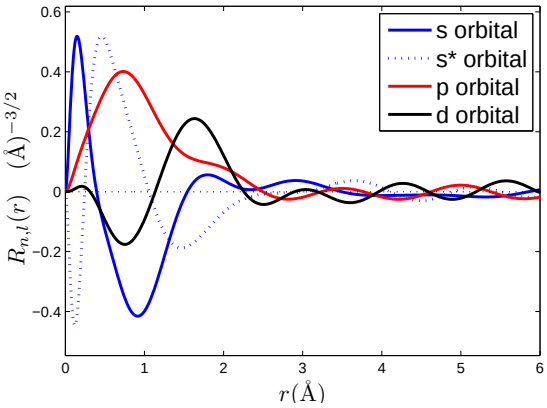

Fig. 4. Radial part of the ETB basis functions of Silicon

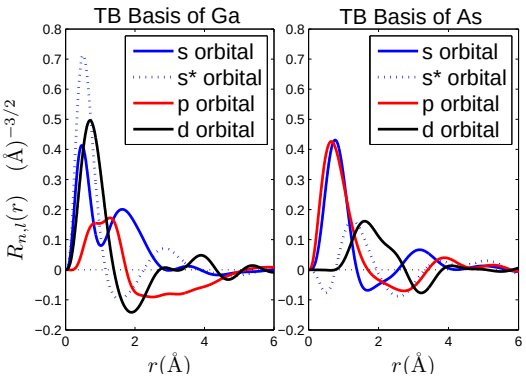

Fig. 5. Radial part of ETB basis functions of GaAs