Tight binding parameterization from *ab-initio* calculations and its application

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Motivation for Empirical Tight Binding (ETB)

Shortcomings of ETB

Solutions for ETB’s shortcomings

Summary & Outlook
Motivation for Empirical Tight Binding (ETB)
Shrinking device dimensions call for atomistic level device simulations


Device fabrication

Device design

How to understand device performance?

How to predict device performance?

Device level simulations are needed to understand and predict nanoscale device performance.
Challenges of device level simulations

Strained materials  Low dimensional structures  Interfaces

Complicated systems
- Complicated geometries
- Multiple materials
- Strain, Interfaces, disorders

Challenging simulation domain
- 10000 ~ 10 million atoms (active domain)

Transferable model  Computationally efficient model

What model can we use for device level simulations?
Candidate methods for device simulations

To simulate a real device

**Ab-initio methods**
- First principle
- Use fundamental material information
- A few parameters
- Provide physical insights (E_k, wave functions)

**Empirical methods, e.g. empirical tight binding (ETB)**
- Requires fitting parameters,
- Have been applied to device level simulations

Why are ETB models so efficient?

Accuracy and computational capability are being improved

Software

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**NEMO 5**

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**InGaAs**
ETB is a computationally efficient atomistic model

A few Localized basis functions per atom

- $Y_{lm}(\theta, \varphi)R_{n,l}(r)$
- 10~20 per atom
- No explicitly $R_{n,l}(r)$

Short range Interactions

- Nearest neighbors interactions

Empirical method

- Slater Koster type formula with fitting parameters

Hamiltonian Matrix size:

$N_{\text{atom}} N_{\text{orbitals}}$

Sparse Hamiltonian matrix

Fast Hamiltonian construction

$H_{s,s} = V_{ss\sigma}$

$H_{x,y} = \text{Im}(V_{pp\sigma} - V_{pp\pi})$

How does ETB Hamiltonian look like?
Tight binding model

How do we get the parameters for the ETB model?

- Materials $\rightarrow$ parameters
  - Atoms $\rightarrow$ onsite blocks
  - Bonds $\rightarrow$ interatomic interactions

Sparse Hamiltonian matrix

$N_{\text{atom}}N_{\text{orbitals}}$
Traditional way of parameterizing ETB models has shortcomings.

Unstrained materials
- perfect zincblende structure

Strained materials
- Strained zincblende structure

ETB parameters:
- Fit to theoretical or experimental band structures

ETB models parameterized by traditional fitting have problems!
Shortcomings of ETB
ETB shortcomings

1. Unphysical results in confined structures
2. Ambiguity for heterostructures
### Ideal/Simple systems

<table>
<thead>
<tr>
<th>Unstrained materials</th>
<th>Strained materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>perfect zincblende structure</td>
<td>Strained zincblende structure</td>
</tr>
</tbody>
</table>

### Realistic/Complicated systems

<table>
<thead>
<tr>
<th>Strained nano structures, heterojunctions ...</th>
</tr>
</thead>
</table>

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ETB parameters:
Fit to theoretical and experimental band structures

---

Are ETB models good enough for nanostructures?
- Confined structures (Problem 1)
- Hetero structures (Problem 2)
ETB shortcomings

1. Unphysical results in confined structures
2. Ambiguity for heterostructures
Confined states in H-passivated structures

Confined CB and VB states are expected in H-passivated UTBs

As-H anti-bonding states

As-H bonding states

Quantum well for CB states

Quantum well for VB states

Conduction band (CB) of GaAs

Valence band (VB) of GaAs

Energy

position
Top VB states in a As terminated GaAs UTB

**Ab-initio wave function**

- Confined states
- Explicit passivation

**ETB wave function (existing model/parameters)**

- Un-confined states
- Implicit passivation

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**Problem 2 : unphysical results in confined structures.**

Existing ETB model/parameters

→ unphysical states in some nanostructures
ETB shortcomings

1. Unphysical results in confined structures
2. Ambiguity for heterostructures
ETB shortcomings

1. Unphysical results in confined structures

2. Ambiguity for heterostructures
Problem 2: (example a) Ambiguity for heterostructures

Traditional ETB parameters at interface are not clearly defined → ambiguous results.

**Assumption 3**

- Interface As atoms → average of GaAs and InAs

\[ E_{\text{As}}(\text{interface}) = \frac{(E_{\text{As}}(\text{GaAs}) + E_{\text{As}}(\text{InAs}))}{2} \]

**E_{\text{As}}(\text{GaAs}) ≠ E_{\text{As}}(\text{InAs})**

Based on assumption without validation
Problem 2: (example b) Ambiguity for heterostructures

Ultra small InAs/GaSb superlattice
- Four different atoms, no common cation/anions
- Or GaAs/InSb superlattice
- Where are interfaces? (Everywhere)

Traditional ETB parameters at interface are not clearly defined → ambiguous results.
Solutions for ETB’s shortcomings
Problems of traditional ETB

1. Unphysical wave functions in UTBs

2. Ambiguities at material interfaces

Can we solve these problems without losing efficiency?
- Keep number of basis functions
- Keep interaction range (1st nearest neighbors)

Solutions and applications

- Parameterization algorithm from \textit{ab-initio} calculations
- Application to unstrained bulk
- Application to ultra thin bodies (UTBs)

- Environment dependent strain model
- Transferability to interface

ETB model: sp3d5s*+SO with 1st nearest neighbor interactions
## Solutions and applications

<table>
<thead>
<tr>
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<th>Description</th>
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<tr>
<td>1</td>
<td>Parameterization algorithm from ab-initio calculations</td>
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<td>4</td>
<td>Environment dependent strain model</td>
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<td>5</td>
<td>Transferability to interface</td>
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Solutions and applications

1. Parameterization algorithm from *ab-initio* calculations
2. Application to unstrained bulk
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4. Environment dependent strain model
5. Transferability to interface
How to improve traditional parameterization?

Ambiguous ETB parameters from traditional parameterization

- Different parameter sets exist
- Fitted to the same targets (band structures)
- Almost Identical band structure ~ Very different parameters

- Degree of freedom exist in pure band structure fitting.
- More fitting targets can be included

Problematic ETB wave functions

Include wave functions into fitting

### Traditional way
- Fitting to experimental band structures.

### This work
- \textit{Ab-initio} calculations + TB parameters construction

#### Problems:
- Ambiguous parameter sets
- Unphysical results in some applications
- Not enough physical insights are considered in fitting

#### Advantages:
- Physical insights from \textit{ab-initio} wave functions
- ETB wave functions match \textit{ab-initio} ones
- Efficiency of the ETB model maintained.

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How to relate ETB wave functions to \textit{ab-initio} ones?
- ETB basis functions
What is missing in the ETB basis function?

Unstrained materials

ETB parameters:
Fit to theoretical or experimental band structures

Basis function: \( Y_{lm}(\theta, \phi)R_{n,l}(r) \)

Radial parts of the basis functions in traditional ETB are missing

Can not get \( R_{n,l}(r) \):
- No fitting parameters for \( R_{n,l}(r) \)
- No targets requires basis functions

Radial parts of the basis functions in traditional ETB are missing
**Process of TB parameterization from *ab-initio* calculations**

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td><em>ab-initio</em> calculations $\rightarrow E(k), \varphi(r), H_{ab-initio}$</td>
</tr>
<tr>
<td>2.</td>
<td>initial TB basis functions $\rightarrow$ radial part $R(r)$ only</td>
</tr>
<tr>
<td></td>
<td>initial TB Hamiltonian $H$</td>
</tr>
<tr>
<td>3.</td>
<td>Represent <em>ab-initio</em> wave functions on ETB basis functions</td>
</tr>
<tr>
<td>4.</td>
<td>Solve TB band structures and wave functions</td>
</tr>
<tr>
<td>5.</td>
<td>Compare the TB band structures and wave functions to <em>ab-initio</em> targets;</td>
</tr>
<tr>
<td>6.</td>
<td>Reconstruct exact TB basis functions.</td>
</tr>
</tbody>
</table>

**Inputs:** *ab-initio* band structures and wave functions  
**Outputs:** TB parameters, TB basis functions

In the fitting process,  
- match TB band structure and **wave functions** with *ab-initio* results.
Solutions and applications

1. Parameterization algorithm from ab-initio calculations
2. Application to unstrained bulk
3. Application to ultra thin bodies (UTBs)
4. Environment dependent strain model
5. Transferability to interface
## Solutions and applications

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</table>
Band structure of bulk GaAs: good agreement between ETB and *ab-initio*

**Bulk GaAs**

ETB band agree with HSE06 calculations in bulk case

HSE06 is a kind of hybrid functional used in *ab-initio* calculations.

sp3d5s* ETB model + nearest neighbor interactions.

ETB Basis functions for GaAs

<table>
<thead>
<tr>
<th></th>
<th>Ga</th>
<th>As</th>
</tr>
</thead>
<tbody>
<tr>
<td>s orbitals</td>
<td><img src="image" alt="Ga-s" /></td>
<td><img src="image" alt="As-s" /></td>
</tr>
<tr>
<td>p orbitals</td>
<td><img src="image" alt="Ga-py" /></td>
<td><img src="image" alt="As-py" /></td>
</tr>
</tbody>
</table>

ETB basis functions:
- Have the feature of sp(d) orbitals
- Highly localized (within 0.4\(a_0\))

Highly localized ETB basis functions are obtained
### Solutions and applications

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ETB models for passivated UTBs

Implicit passivation model

Explicit passivation model

Previous work: implicit passivation model
This work: explicit passivation model
As terminated GaAs UTB: Band structures

- sp3d5s* ETB model + nearest neighbor interactions.
- Bulk GaAs parameters presented are used.
- Use explicit passivation model.

ETB band agree with HSE06 calculations in UTB case.
As terminated GaAs UTB: confined wave functions (top VB states)

- Without basis functions:
  - Discrete
  - Cations and anions form different envelope

- With basis functions:
  - Continuous
  - Subatomic resolution can be achieved

Realspace ETB wave function match HSE06 wave functions well.
What’s the problem of previous results?

<table>
<thead>
<tr>
<th>Previous parameters</th>
<th>Implicit passivation</th>
<th>Explicit passivation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(a)</td>
<td>(b)</td>
</tr>
<tr>
<td>ETB ref + implicit passivation</td>
<td>[Graph]</td>
<td>[Graph]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>parameters by this work</th>
<th>(c)</th>
<th>(d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETB this work + implicit passivation</td>
<td>[Graph]</td>
<td>[Graph]</td>
</tr>
</tbody>
</table>

**ETB ref**: T. Boykin et al. PRB 66, 125207 (2002).

Explicit passivation model and better ETB parameters $\rightarrow$ more physical VB states
**Problem of the previous parameters:**

- **d-orbitals contribute too much**

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<th>UTB wave functions</th>
<th>Bulk wave functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETB $</td>
<td>\psi</td>
<td>^2$</td>
</tr>
<tr>
<td>Previous parameters</td>
<td><img src="image1" alt="Graph showing comparison between Ga and As envelopes" /></td>
<td><img src="image2" alt="Bar graph showing p(As), d(As), p(Ga), d(Ga) contributions" /></td>
</tr>
<tr>
<td>Parameters</td>
<td><strong>New parameters have better quality</strong></td>
<td><strong>Wave function is properly controlled</strong></td>
</tr>
</tbody>
</table>

**In this work**

- **Fitting of ETB wave functions constraint the d contribution**

- **New parameters**

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*Purdue University*
Ø Tight binding parameter obtained from *ab-initio* calculations has better transferability;

Ø TB model with nearest neighbor interactions can work for unstrained bulk and UTBs.

Ø Unphysical TB states in GaAs UTBs are eliminated.
Solutions and applications

1. Parameterization algorithm from *ab-initio* calculations
2. Application to unstrained bulk
3. Application to ultra thin bodies (UTBs)
4. Environment dependent strain model
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<table>
<thead>
<tr>
<th></th>
<th>Traditional ETB model</th>
<th>Environment dependent ETB model (this work)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Onsite blocks</strong></td>
<td>Atom + material</td>
<td>Atom + environment</td>
</tr>
<tr>
<td><strong>Interatomic interaction blocks</strong></td>
<td>Bond + material</td>
<td>Bond + environment</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ga and As atom in GaAs material</th>
<th>Ga-As bond in GaAs material</th>
</tr>
</thead>
</table>

Ga atom and its environment

Ga-As bond and its environment
**Environments:**
*(the status of neighbors)*

<table>
<thead>
<tr>
<th>Atom types of neighbors</th>
<th>Bond lengths</th>
<th>Bond angles</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Atom types diagram" /></td>
<td><img src="image2" alt="Bond lengths diagram" /></td>
<td><img src="image3" alt="Bond angles diagram" /></td>
</tr>
</tbody>
</table>

**ETB model in this work**

- Environment dependent Hamiltonian
- Strains
- Interfaces
The TB model in this work can be applied to hydrostatic strain cases.

With hydrostatic strain:
- Band gaps will change;
- Indirect gap $\rightarrow$ direct gap.
ETB model in this work reproduce the strain valence bands.

Strained effect to conduction bands (X valleys)

ETB model in this work reproduce the strain behavior of CB(X valleys).

ETB model by this work show better result than existing TB model for conduction bands.

Solutions and applications

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Solutions and applications

1. Parameterization algorithm from \textit{ab-initio} calculations
2. Application to unstrained bulk
3. Application to ultra thin bodies (UTBs)
4. Environment dependent strain model
5. Transferability to interface
Existing ETB model shows significant differences in a GaAs/AlAs superlattice.

ETB calculations in this work:
- $sp^{3d5s^*} + SO$
- 1st nearest neighbor interaction
- Negligible built-in potential

ETB in this work can accurately calculate band structure of GaAs/AlAs superlattices
Strained InAs/GaSb superlattices:

Existing ETB model shows significant differences in a InAs/GaSb superlattice.

ETB calculations in this work:
- sp3d5s* +SO
- 1st nearest neighbor interaction
- Negligible built-in potential

ETB in this work can accurately calculate band structure of InAs/GaSb superlattices

Bonds involved:
- In-As, Ga-Sb, In-Sb, Ga-As

BZ

011
010
011
010

G

Energy (eV)

HSE06
ETB
Superlattices with common anions

<table>
<thead>
<tr>
<th>Layers</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>8</td>
<td>12</td>
</tr>
</tbody>
</table>

- 4 layers
- 8 layers
- 12 layers

Band gaps of different superlattices by ETB agree with HSE06 calculations.
Summary & Outlook
Traditional tight binding parameterization has problems;

Tight binding parameterization from *ab-initio* calculations is developed in this work;

ETB parameters with better transferability and explicit ETB basis functions are obtained;

Application to unstrained and strained materials → good agreement with *ab-initio* bands is achieved;

Application to nanostructures (UTBs and superlattice) → good transferability can be achieved with 1st nearest neighbor ETB models.
Motivation:
- *Ab-initio* calculations usually assume zero temperature.
- But device simulations require room temperature tight binding parameters.

Approach:
- Effect of room temperature is approximated by hydrostatic strain.
  \[ E(k, T) \approx E(k, \delta a_0) \]
- Environment dependent strain ETB model
- *Ab-initio* mapping algorithm to extract ETB parameters.

Results:
- *Ab-initio* band structures matching room temperature experimental results are obtained.
- Introduce of strain only change wave function slightly
- ETB parameters for room temperature are obtained.

Impact:
TB parameters for room temperature materials are available. Devices under room temperature is enabled.
Parameterization of 2D materials

Motivation:
- 2D materials like MoS2 are interested in recent device design, but TB parameters for device level simulation is required.
- Extract TB parameters from DFT results (DFT energy bands & eigenfunctions)

Approach:
- Basis transformation:
  - Plane waves → localized orbitals
- TB model: orthogonal TB model with 1st NN Interactions;
- optimize TB orbitals and parameters to match ab-initio results.
  - targets: ab-initio bands & wave functions.

Results:
- Reasonable parameters and band structure is obtained;

Impact:
TB parameters for TMDs are obtained, device level calculations of TMD transistors are enabled.
Objective:
• Existing four-band tight binding model underestimates band splitting → might affect charge distribution especially if scattering exists.

Method:
• Ten-band ETB model considering 2NN interactions.
• Harrison’s scaling law for bond length dependence of parameters.
• One parameter set for in-plane, one parameter set for inter-layer.
• Optimize parameters by fitting to DFT, for monolayer, bilayer, and bulk.

Results:
• Tight binding parameters for black Phosphorus.
• TB bandstructure well reproduce DFT results.

Impact:
• Atomistic modeling for black Phosphorus transistors are enabled.
Objective:
• Investigate the Si UTB/SiO$_2$ interface and evaluate the normally used hydrogen atom passivation treatment.

Method:
• Passivation for three relevant oxidation configurations are parameterized.
• Parameters are optimized by fitting TB dispersions to DFT-HSE06 calculations.

Impact:
• UTB band structures of TB match well with DFT calculations.
• HGM gives higher DOS compared to hydrogen atom passivation.
• Oxidation configurations involved more oxygen atoms contribute higher DOS.
• DBM and BOM configurations are not well confined, which are suggested to be avoided in experiment.
InAs Parameterization

- Transferable parameters for semiconductors are needed to model disordered systems and interfaces
- Extended Hückel model gives natural treatment of these systems

Parameterization Technique

- InAs fit to $E(k)$ and wavefunction targets from HSE06 calculations
- Work underway to produce bulk parameterizations with more accurate strain behavior than published parameterizations

Extended Hückel Fitting Based on \textit{ab-initio} mapping

Complex semiconductor or-dielectric interface

HfO$_2$, InAs interface. Strain, rearrangement requires high transferability
**Motivation:**
- Extract TB parameters from DFT results (DFT energy bands & eigenfunctions)
- MgO is interested in spintronic devices, but no TB parameters for device level simulation.

**Approach:**
- Low rank approximation: \( H_{DFT} \rightarrow H_{TB} \)
- Constraint:
  - 2\(^{st}\) NNs Interactions,
  - unity overlap matrix;
- Optimize the TB basis functions to get reasonable TB parameters. Targets: HSE06 bands.

**Results:**
- Reasonable parameters and band structure is obtained by mapped TB Hamiltonian;

**Impact:**
TB parameters for complicated material MgO are obtained, device level calculations of MgO based spintronics Transistor are enabled.
Motivation:
- Extract TB parameters from DFT results (DFT energy bands & eigenfunctions)
- Complicated exotic material SmSe is interested in Piezoelectronic Transistor design, but no TB parameters for device level simulation.

Approach:
- Low rank approximation: \( H_{DFT} \rightarrow H_{TB} \)
- constraint:
  - 1st NNs Interactions,
  - unity overlap matrix;
- optimize the TB basis functions to get reasonable TB parameters. 
  targets: LDA+U bands.

Results:
- Reasonable parameters and band structure is obtained by mapped TB Hamiltonian;

Impact:
TB parameters for complicated material SmSe are obtained, device level calculations of SmSe based piezoelectronic Transistor are enabled.
Motivation:
Topological insulators like (CdTe/ HgTe/CdTe QW) are new group of materials. The behavior of topological insulator in device environment is not clear.

Approach:
- 8 band strained k.p model for CdTe and HgTe
- Finite differential method for CdTe/HgTe/CdTe quantum wells.

Results:
- Topological states in CdTe/HgTe/CdTe can be modulated by strain/crystal orientation/vertical electric field.
Committee member:
Prof. Klimeck, Prof. Strachan, Prof. Povolotskyi, Prof. Lundstrom, Prof. Boykin (UAH)

Prof. Kubis, Prof. R. Rahman, Dr. J. Huang, Dr. J. Fonseca, Dr. B. Novakovic, Dr. C. Bowen, Dr. P. Sengupta, Dr. M. Salmani, Dr. M. Luisier, Dr. G. Hegde, Dr. S. Park, Dr. L. Zeng, Dr. A. Paul, Dr. S. Lee, Dr. H. Ryu.

Y. Hsueh, Dr. Z. Jiang, Dr. Y. He, J. Geng, K. Miao, P. Long, Y. Wang, D. Mejia, D. Valencia, E. Wilson, M. Tan, F. Chen, H. Ilatikhameneh, K. Wang, Y. Chu, T. Ameen, C. Chen, P. Sarangapani, H. Sahasrabudhe, S. Perez, S. Mukherjee, Dr. X. Wang, Dr. Y. Gao and all other NCN students

NCN Staff members:
V. Johnson, C. Heins, L. Schumacher, A. Byrne, A. Buckles
Thank you!
Related Publication list

### Problem of the previous parameters

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<th>Bulk wave functions</th>
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<tr>
<td><strong>Modified Parameters</strong></td>
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**UTB wave functions**

- Ga envelope
- As envelope

**Bulk wave functions**

- p(As)
- d(As)
- p(Ga)
- d(Ga)

- d-orbital contribute too much.

Smaller d-contribution due to modified parameters

Smaller d-contribution due to modified parameters also eliminate unphysical states
Special distorted systems considered in fitting:
- Four kinds of atom displacements
- Assume no missing nearest neighbor

Hydrostatic strain

Diagonal strains
\[
\begin{bmatrix}
\varepsilon \\
\varepsilon \\
-2\varepsilon
\end{bmatrix}
\]

Two bond lengths change

Off-diagonal strains
\[
\begin{bmatrix}
\varepsilon \\
\varepsilon
\end{bmatrix}
\]
Onsite element:

\[ H^{(0)}_{\alpha_i, \alpha_i} = E_{\alpha_i} + \sum_{j \in \text{NNs}} I_{\alpha_i, j}(d_{ij}) + \sum_{j \in \text{NNs}} O_{i, j}(d_{ij}), \]

Environment dependent terms:
Sum over nearest neighbors
Si under hydrostatic strain

With hydrostatic strain:
- Band gaps will change;
- Gap of X, L and Γ points change at different ratio;
- Transition from indirect gap to direct gap happens;

The TB model in this work can be applied to hydrostatic strain cases
Observation: Ab-initio potential at IIIV interface varies over the range of first nearest neighbor

What is proper interaction radius of TB model?

Is 1\textsuperscript{st} nearest neighbor interaction enough for IIIV hetero structures?

ab-initio local potential of GaAs/InAs superlattice
Superlattice band structure of Xas/YAs

GaAs/AlAs

GaAs/InAs

InAs/AlAs

Energy (eV)

4 layers

8 layers

X G K

X G K

X G K

HSE06

ETB
Folded bands originate from X valleys.

Lowest few conduction bands originate from Γ and X valleys in the fcc BZ.
More superlattices: superlattices with common cations

Superlattices with common **cations**

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Band gaps of different superlattices by TB agree with HSE06 calculations.

- **Band Gap (eV)**
  - **AIAs/AIP**
  - **AIP/AISb**
  - **AIAs/AISb**
  - **GaAs/GaP**
  - **GaP/GaSb**
  - **InAs/InP**
  - **InP/InSb**
  - **InAs/InSb**

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<thead>
<tr>
<th># of layers</th>
<th>HSE06</th>
<th>ETB</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>12</td>
<td>2.5</td>
<td>2.5</td>
</tr>
</tbody>
</table>
Type III superlattice? → confinement opens the band gap