NEMO5

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

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Outline

Motivation for Empirical Tight Binding (ETB)

Shortcomings of ETB

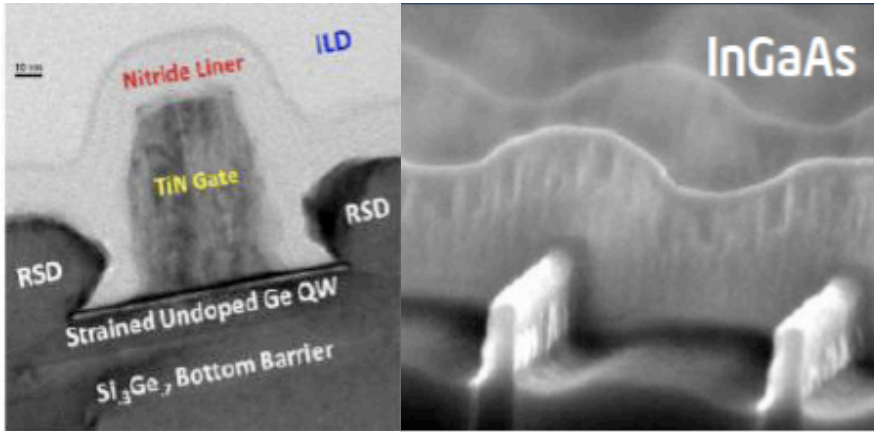
Solutions for ETB's shortcomings

Summary & Outlook

Motivation for Empirical Tight Binding (ETB)

Shrinking device dimensions call for atomistic level device simulations

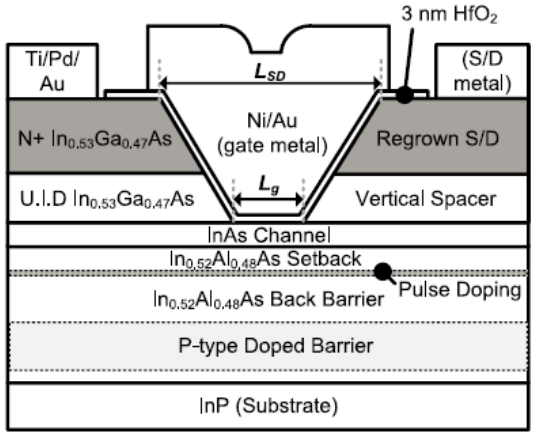
Device fabrication



http://nextbigfuture.com/2011/06/intel-roadmap-from-june-2011-with-7nm.html

How to understand device performance?

Device design

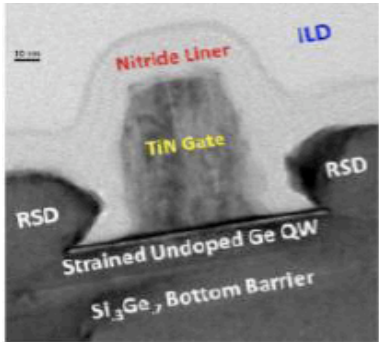


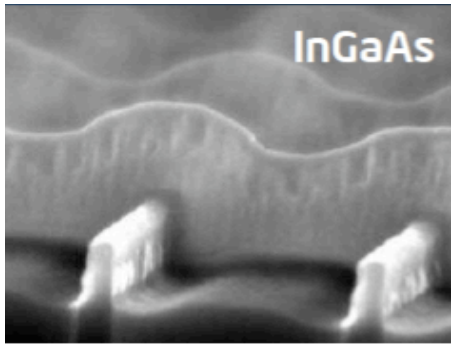
S. Lee, et al. IEEE. Trans. Elect. Dev. Lett, Vol 35, p 621 (2014)

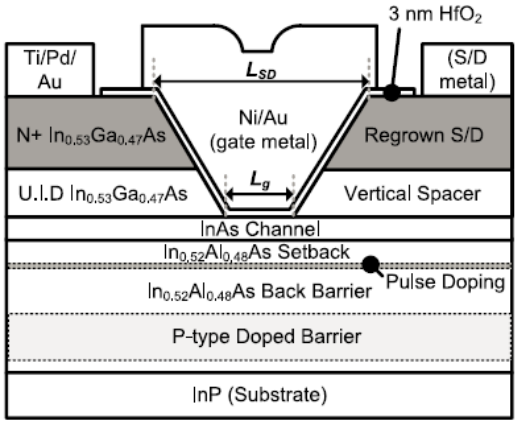
How to predict device performance?

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)

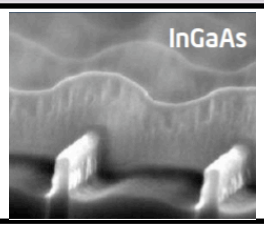
Transferable model

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 (Ek, wave functions)

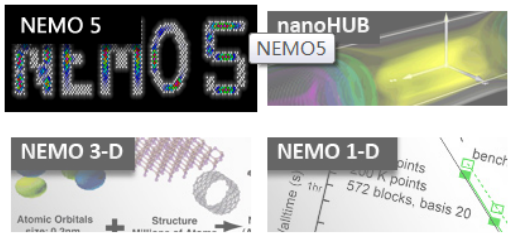
accuracy and computational capability are being improved

Empirical methods, e.g. empirical tight binding (ETB)

- Requires fitting parameters,

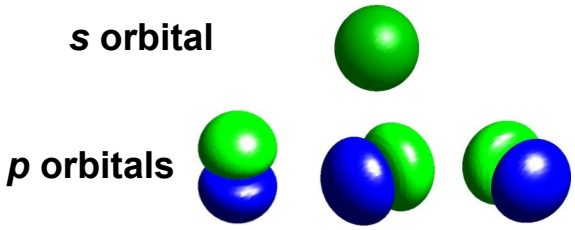
- Have been applied to device level simulations

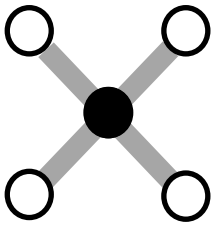
Software



Why are ETB models so efficient?

ETB is a computationally efficient atomistic model





$$H_{s,s} = V_{ss\sigma}$$
$$H_{x,y} = lm\left(V_{pp\sigma} - V_{pp\pi}\right)$$

A few Localized basis functions per atom

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

Hamiltonian Matrix size: $N_{atom}N_{orbitals}$

Short range Interactions

- Nearest neighbors interactions

Sparse Hamiltonian matrix

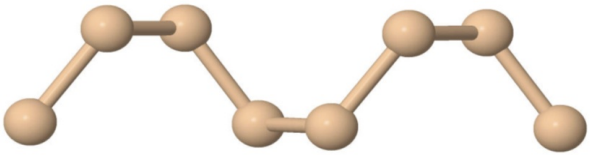
Empirical method

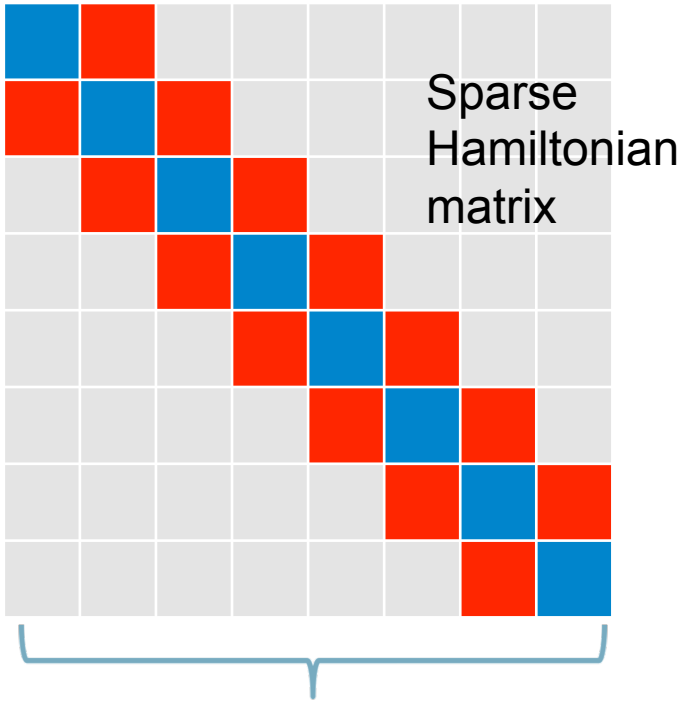
- Slater Koster type formula with **fitting parameters**

Fast Hamiltonian construction

How does ETB Hamiltonian look like?

Tight binding model



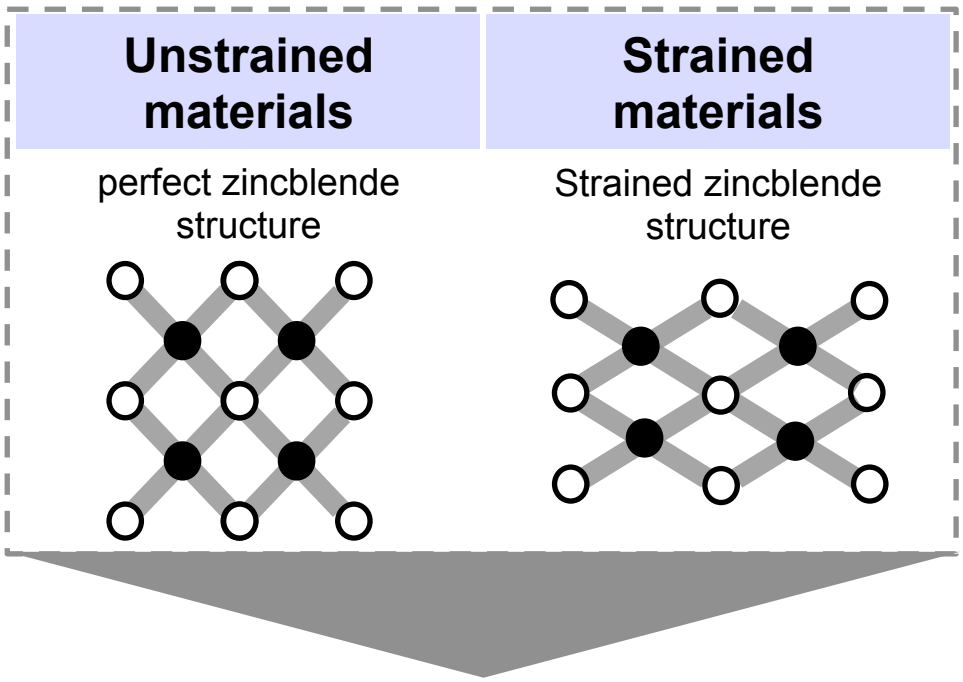


- **Materials → parameters**
  - **Atoms → onsite blocks**
  - **Bonds → interatomic interactions**

How do we get the parameters for the ETB model?

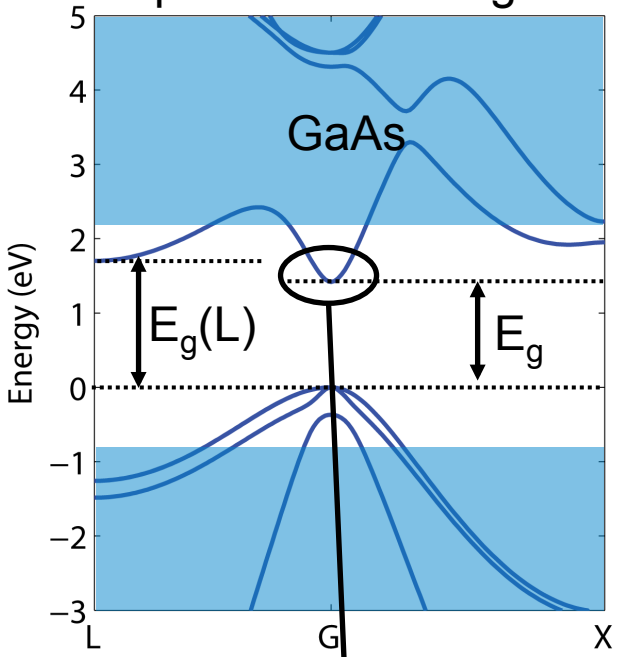
Traditional way of parameterizing ETB models has shortcomings

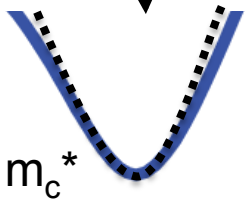
Unstrained materials	Strained materials
perfect zincblende structure	Strained zincblende structure



ETB parameters:
Fit to theoretical or experimental
band structures

Important band edges





Important effective mass

ETB models parameterized by traditional fitting have problems!

Shortcomings of ETB

2 key problems of ETB models parameterized by traditional fitting

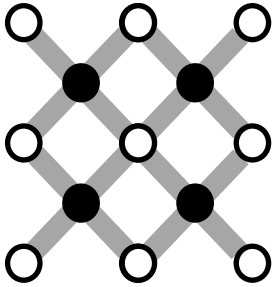
ETB shortcomings

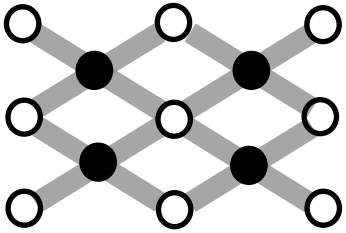
1. Unphysical results in confined structures
2. Ambiguity for heterostructures

More concern about ETB

Ideal/Simple systems → Realistic/Complicated systems

Unstrained materials	Strained materials	Strained nano structures, heterojunctions …
perfect zincblende structure	Strained zincblende structure	nanostructures





ETB parameters:
Fit to theoretical and experimental band structures

Are ETB models good enough for nanostructures?

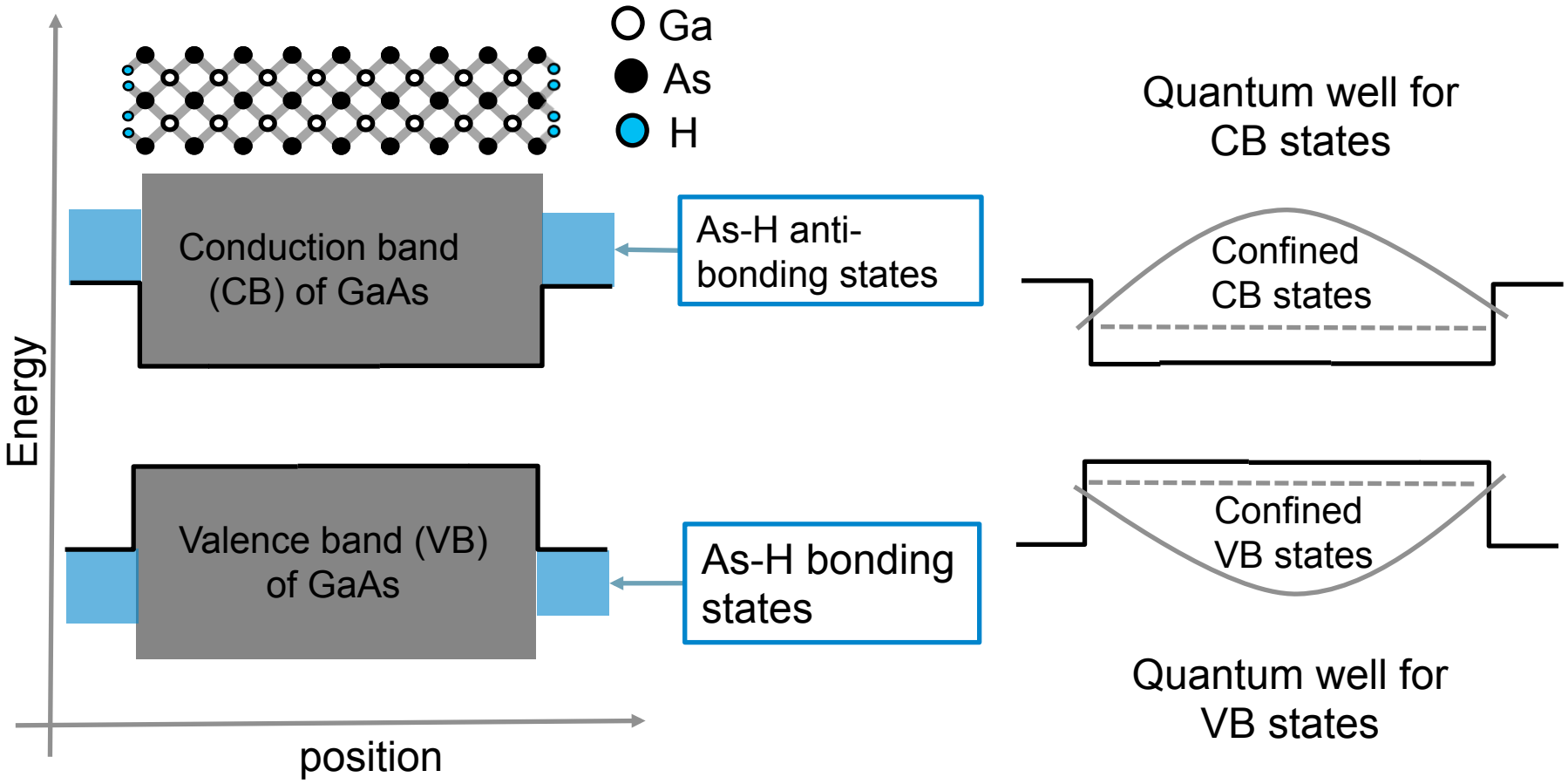
- **Confined structures (Problem 1)**
- **Hetero structures (Problem 2)**

2 key problems of ETB models parameterized by traditional fitting

ETB shortcomings

1. **Unphysical results in confined structures**
2. Ambiguity for heterostructures

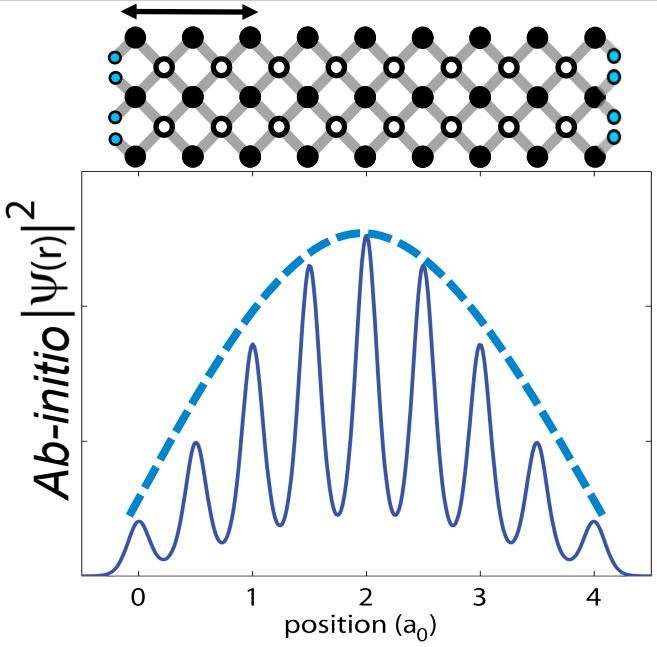
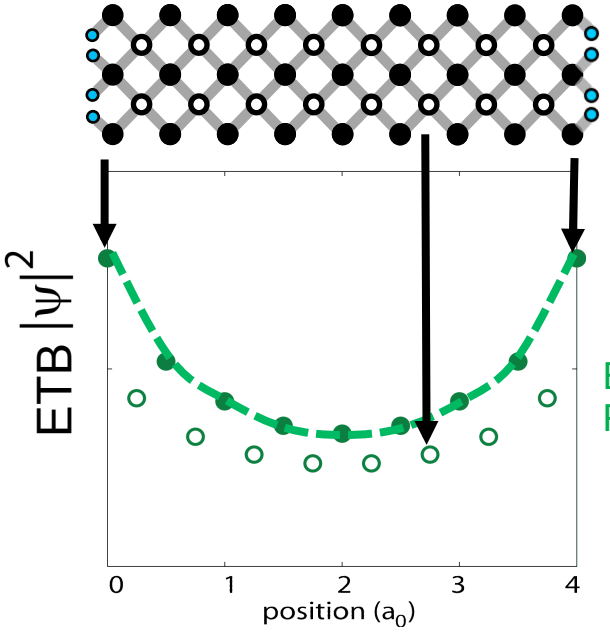
Confined states in H-passivated structures



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

Problem 2 : unphysical results in confined structures.

Top VB states in a As terminated GaAs UTB

Ab-initio wave function	ETB wave function (existing model/ parameters)
	
➢**Confined states** ➢Explicit passivation	➢ **Un-confined states** ➢ Implicit passivation

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

Existing ETB model/parameters
→ unphysical states in some nanostructures

2 key problems of ETB models parameterized by traditional fitting

ETB shortcomings

1. **Unphysical results in confined structures**
2. Ambiguity for heterostructures

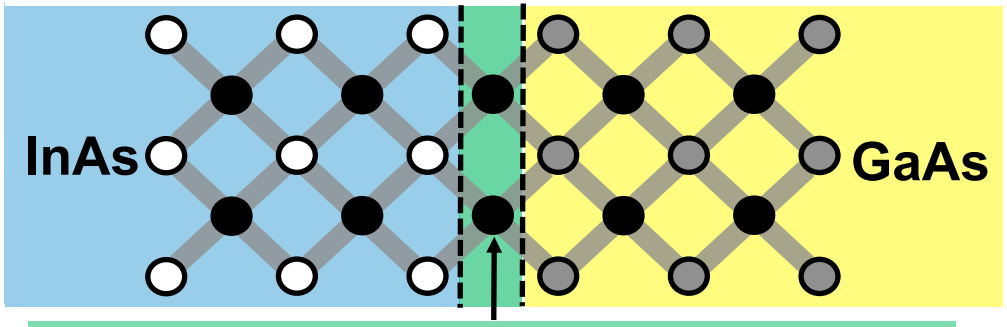
2 key problems of ETB models parameterized by traditional fitting

ETB shortcomings

1. Unphysical results in confined structures
2. **Ambiguity for heterostructures**

Problem 2: (example a) Ambiguity for heterostructures

Assumption 3



Interface As atoms → average of GaAs and InAs

$E_{As}(interface) = (E_{As}(GaAs) + E_{As}(InAs))/2$

based on assumption without validation

$E_{As}(GaAs) \neq E_{As}(InAs)$

$E_{As}(interface)$ = ?

$E_{As}(GaAs)$

$E_{As}(InAs)$

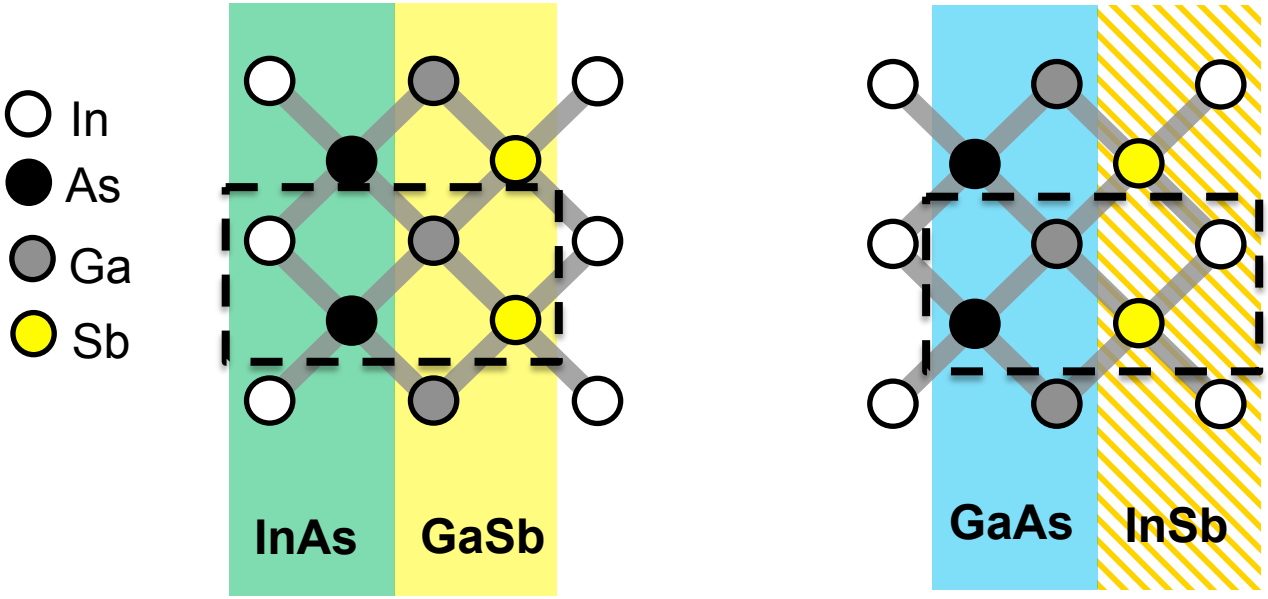
$(E_{As}(GaAs) + E_{As}(InAs))/2$

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

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 and solutions

Problems of traditional ETB

1. Unphysical wave functions in UTBs

2. Ambiguities at material interfaces

Solutions and applications

- Parameterization algorithm from *ab-initio* calculations
- Application to unstrained bulk
- Application to ultra thin bodies (UTBs)

- Environment dependent strain model
- Transferability to interface

Can we solve these problems without losing efficiency?

- Keep number of basis functions
- Keep interaction range (1st nearest neighbors)

ETB model : sp3d5s*+SO with 1st nearest neighbor interactions

Solutions and applications

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Solutions and applications

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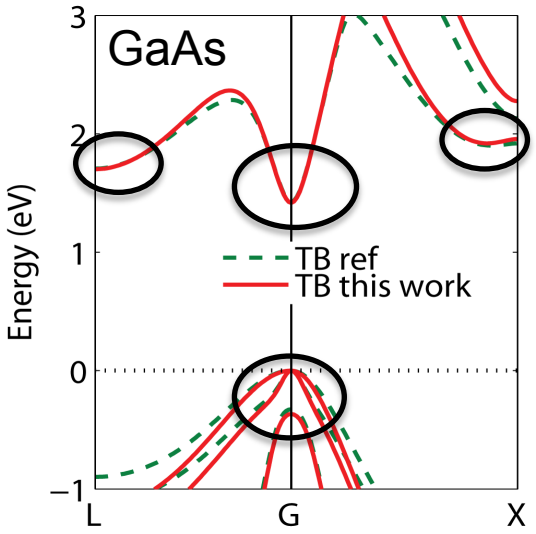
How to improve traditional parameterization?

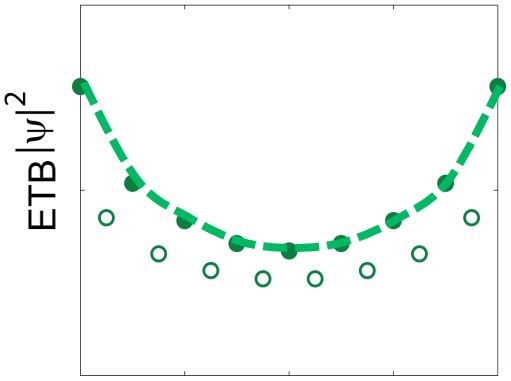
Ambiguous ETB parameters from traditional parameterization

- 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



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



Problematic ETB wave functions → Include wave functions into fitting

How to get good TB parameters? make use of *ab-initio* results

Traditional way	This work
Fitting to experimental band structures.	*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 *ab-initio* wave functions
- ETB wave functions match *ab-initio* ones

Less empirical parameters

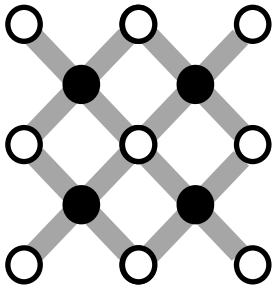
- Efficiency of the ETB model maintained.

How to relate ETB wave functions to *ab-initio* ones?

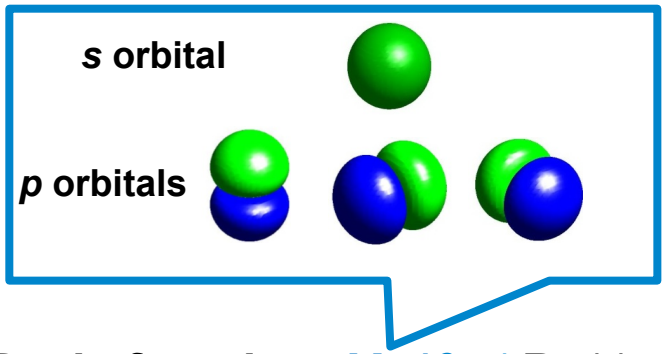
- ETB basis functions

What is missing in the ETB basis function?

Unstrained materials



ETB parameters:
Fit to theoretical or experimental **band structures**



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

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 parameteriztion from *ab-inito* calculations

1. *ab-initio* calculations → $E(k)$, $\varphi(r)$, $H_{ab\text{-}initio}$
2. initial TB basis functions [?] → radial part $R(r)$ only initial TB Hamiltonian H
3. Represent *ab-initio* wave functions on ETB basis functions
4. Solve TB band structures and wave functions
5. Compare the TB band structures and wave functions to *ab-initio* targets;
6. Reconstruct exact TB basis functions.

Iteratively optimize the TB basis functions and Hamiltonian

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.

Y Tan et al. Phys. Rev. B **92**, 085301

Solutions and applications

1. **Parameterization algorithm from *ab-initio* calculations**
2. Application to unstrained bulk
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1. Parameterization algorithm from *ab-initio* calculations
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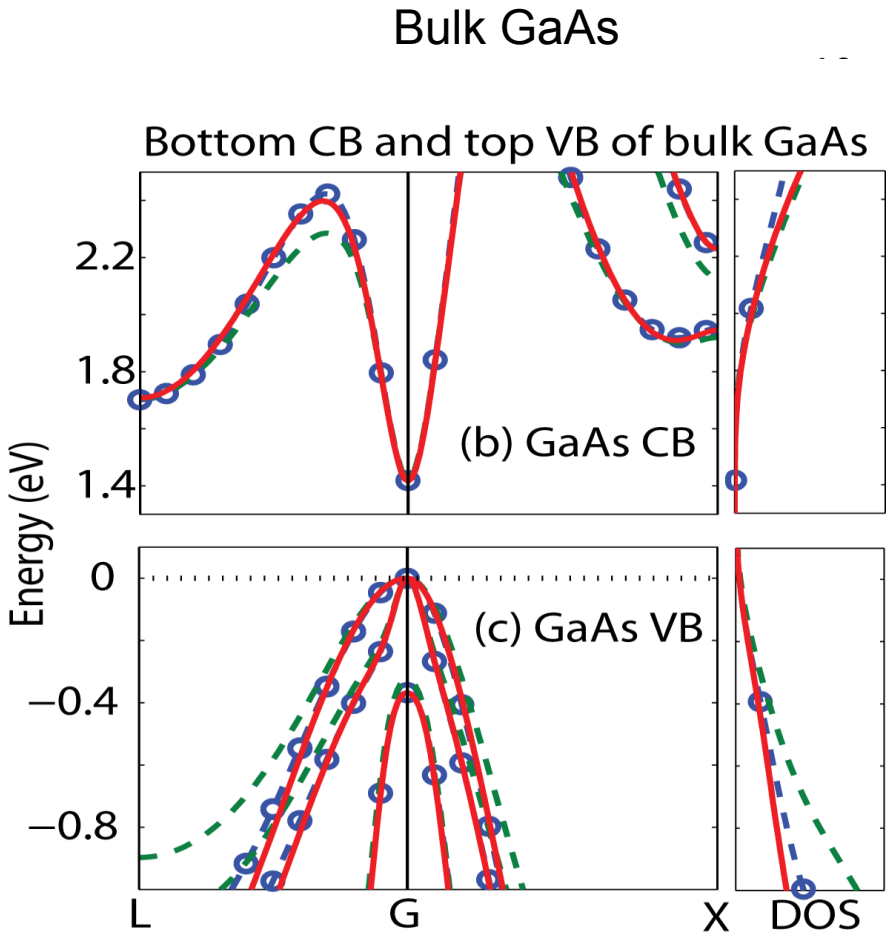
Band structure of bulk GaAs: good agreement between ETB and *ab-initio*

sp3d5s* ETB model + nearest neighbor interactions.

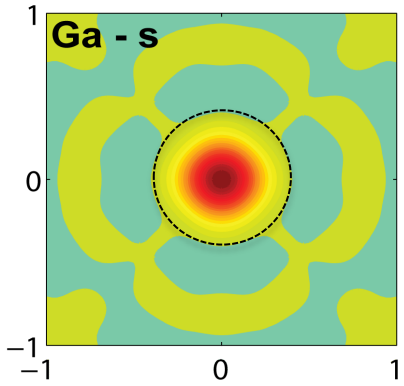
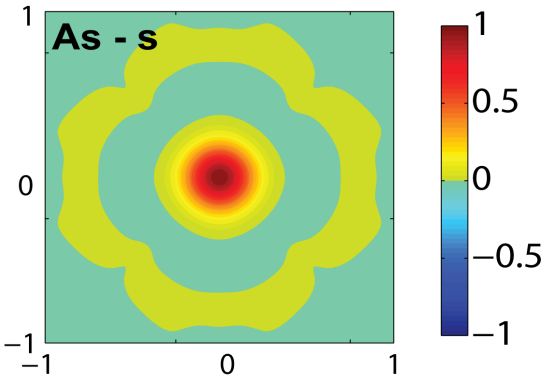
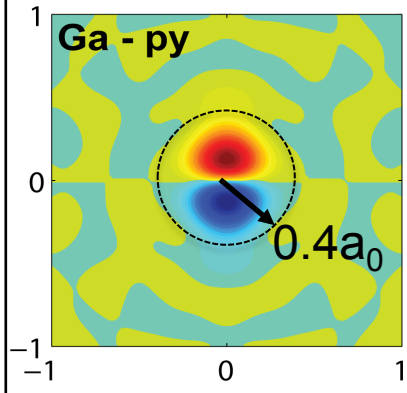
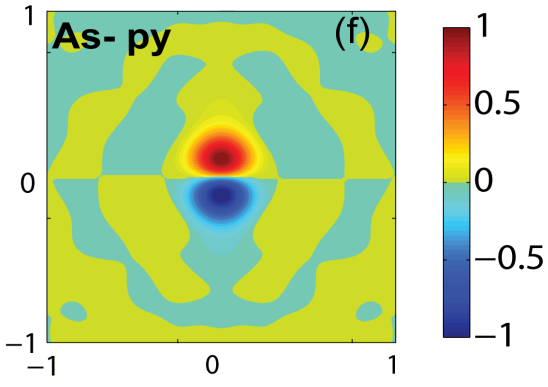
ETB ref : T. Boykin et al. PRB 66, 125207 (2002).



ETB band agree with HSE06 calculations in bulk case

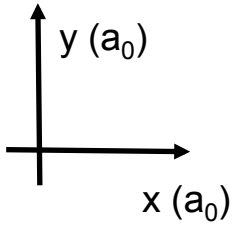
HSE06 is a kind of hybrid functional used in *ab-initio* calculations.

ETB Basis functions for GaAs

	Ga	As
s orbitals 		
p orbitals 		

ETB basis functions:

- Have the feature of sp(d) orbitals
- Highly localized (within $0.4a_0$)



Highly localized ETB basis functions are obtained

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

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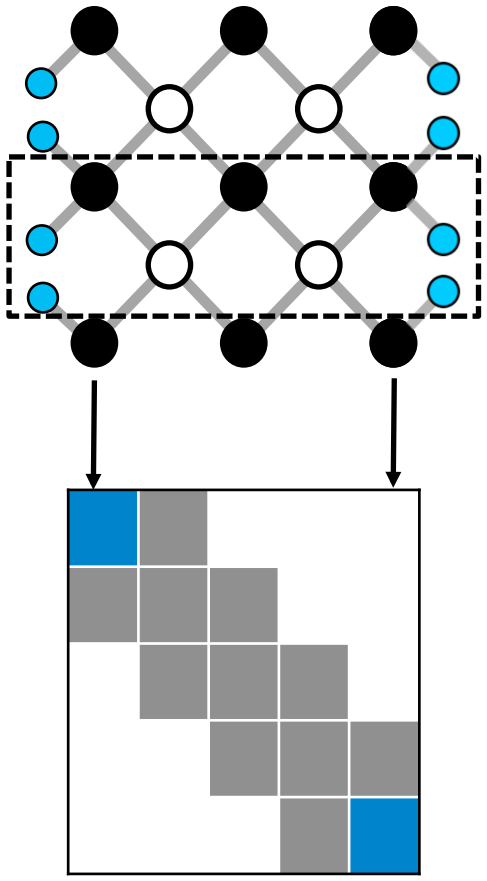
ETB models for passivated UTBs

Implicit passivation model

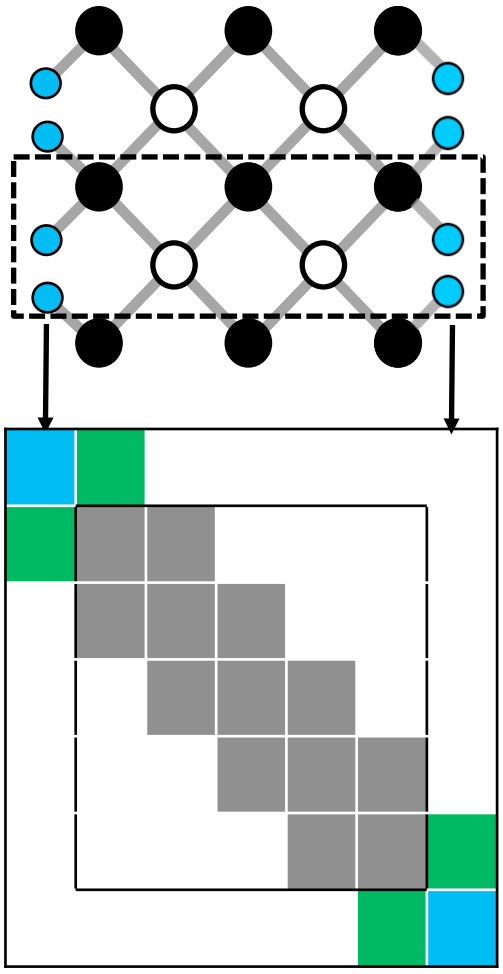


As
Ga
H

Surface As Onsite

Universal parameters

Explicit passivation model



As
Ga
H

Onsites (H)

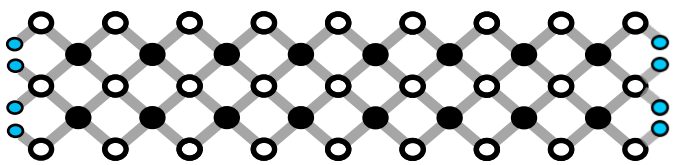
Coupling (H-As)

Extra fitting parameters

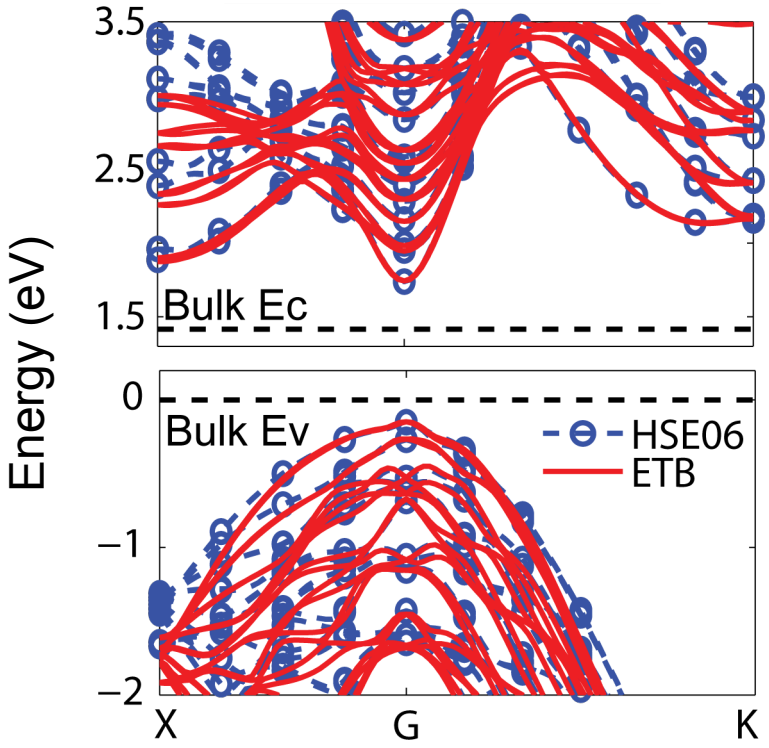
Previous work: implicit passivation model
This work: explicit passivation model

As terminated GaAs UTB: Band structures

GaAs UTBs



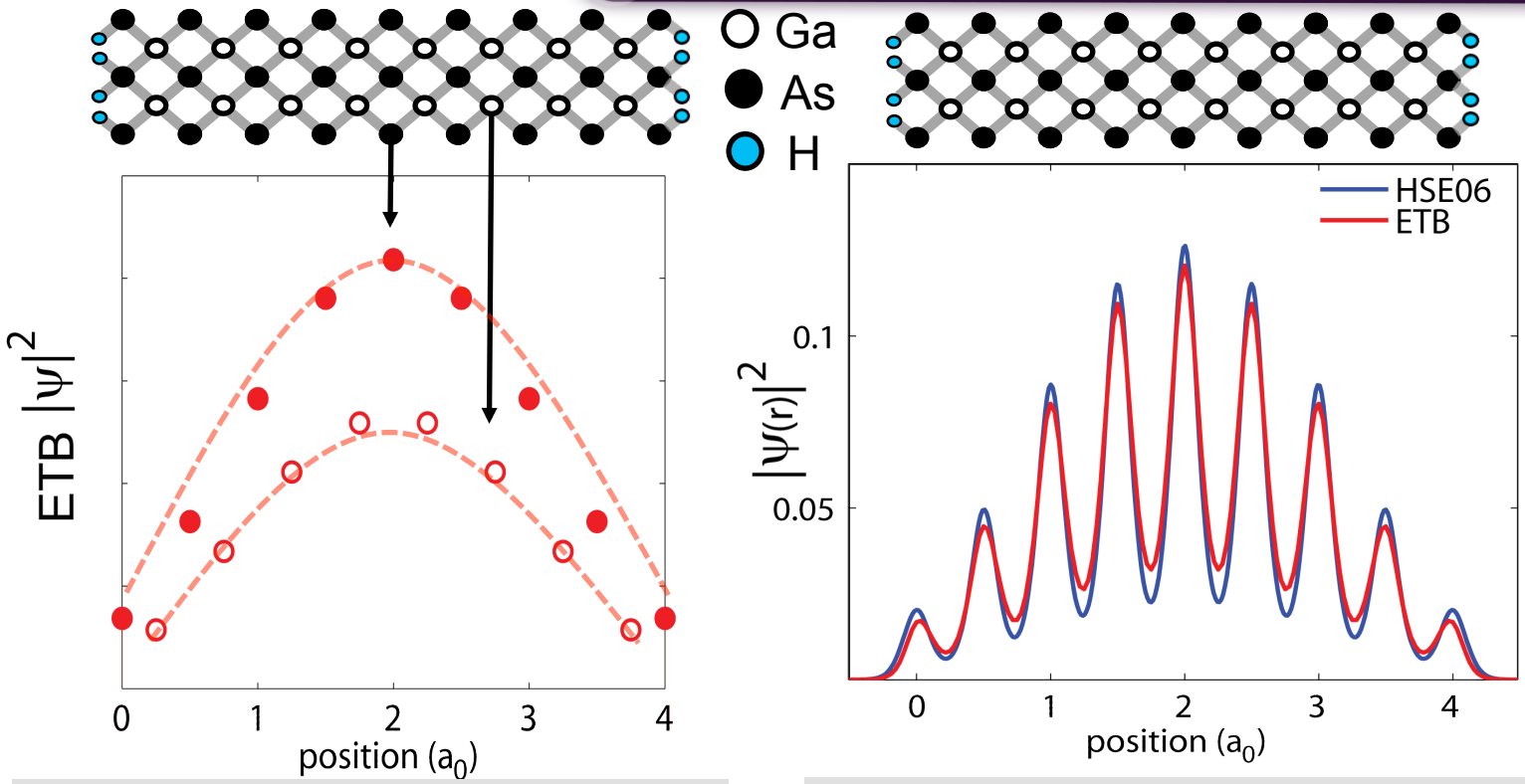
Ga
As
H



- 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:

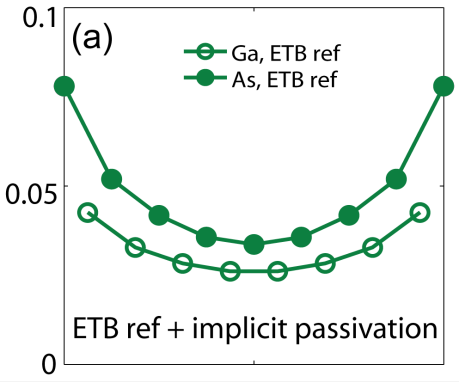
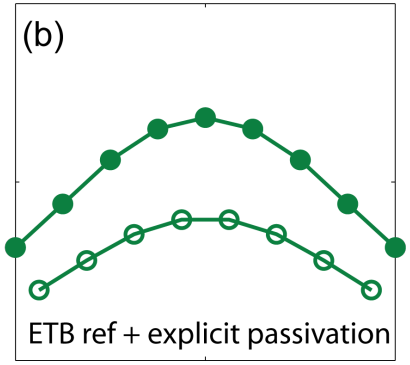
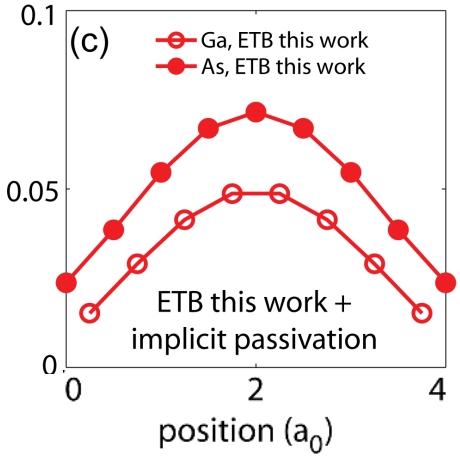
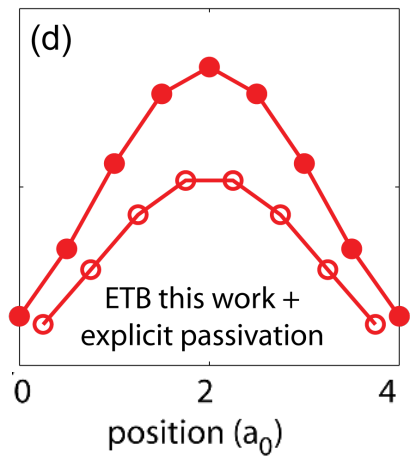
- Continuous
- Subatomic resolution can be achieved

Realspace ETB wave function match HSE06 wave functions well.

What's the problem of previous results?

More confined states

More confined states

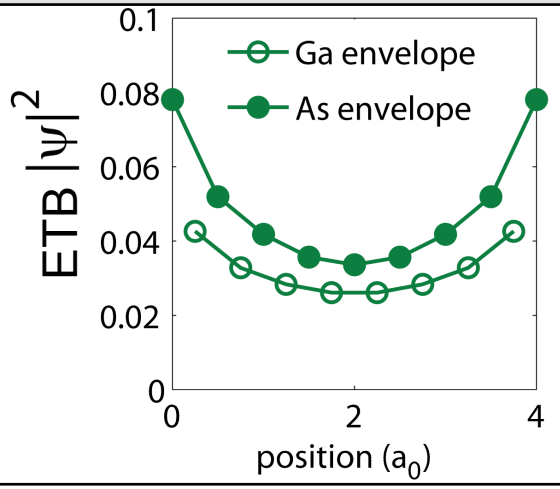
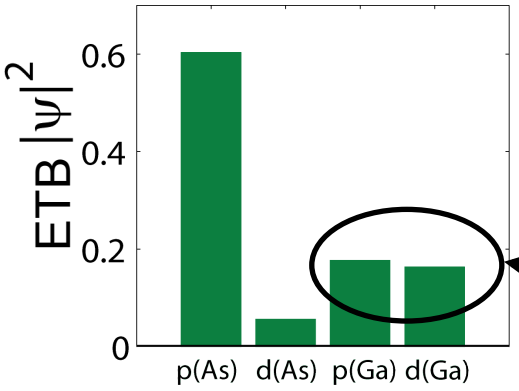
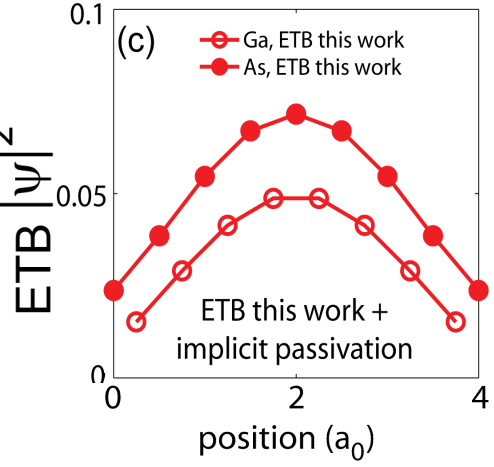
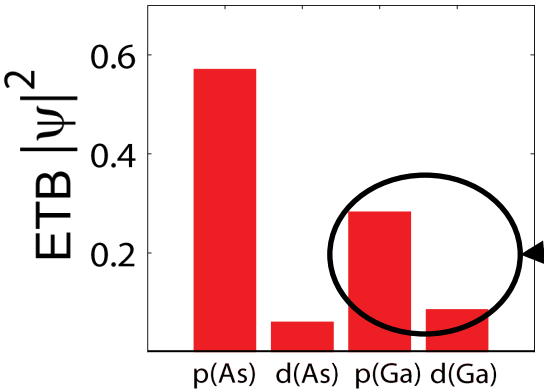
	Implicit passivation	Explicit passivation
Previous parameters		
parameters by this work		

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

What property does the new parameters improve?

Explicit passivation model and better ETB parameters → more physical VB states

Problem of the previous parameters: d-orbitals contribute too much

	UTB wave functions	Bulk wave functions
Previous parameters		
Parameters In this work		

d-orbital contribute too much.

Fitting of ETB wave functions constraint the d contribution

New parameters have better quality
→ Wave function is properly controled

Summary

- Tight binding parameter obtained from *ab-initio* calculations has better transferability;
- TB model with nearest neighbor interactions can work for unstrained bulk and UTBs.
- 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
5. Transferability to interface

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

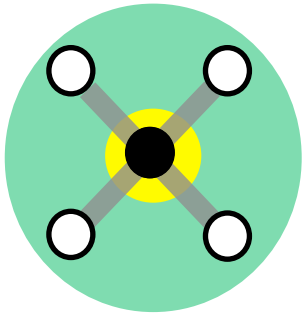
Environment dependent ETB model

	Traditional ETB model	Environment dependent ETB model (this work)
Onsite blocks	Atom + material	Atom + environment
Interatomic interaction blocks	Bond + material	Bond + environment

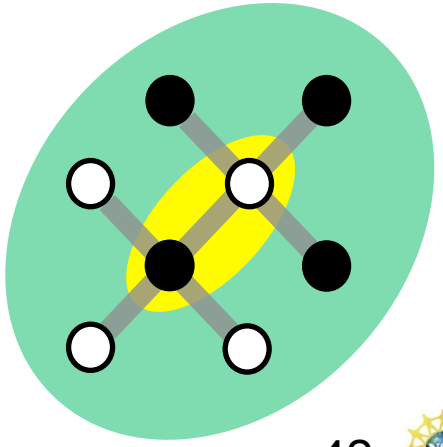
Ga and As atom in GaAs material

Ga-As bond in GaAs material

Ga atom and its environment

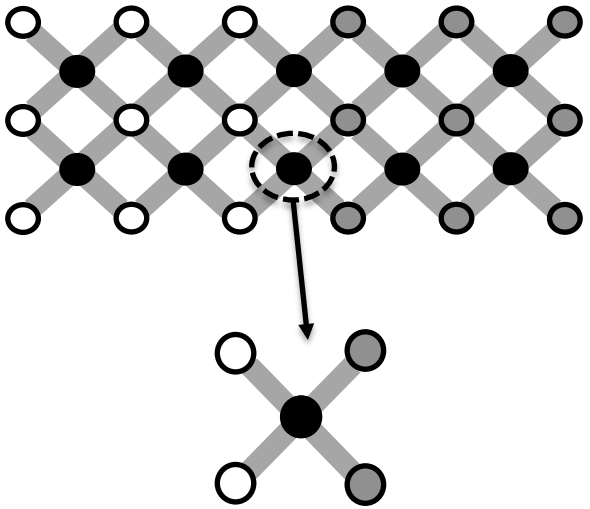
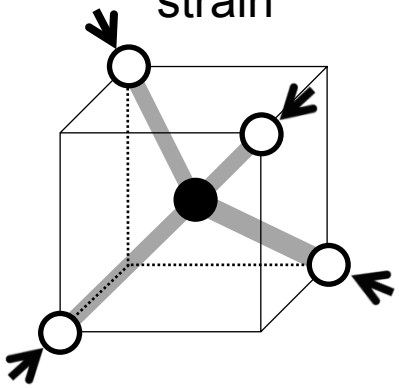
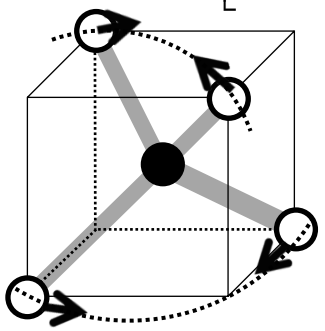


Ga-As bond and its environment



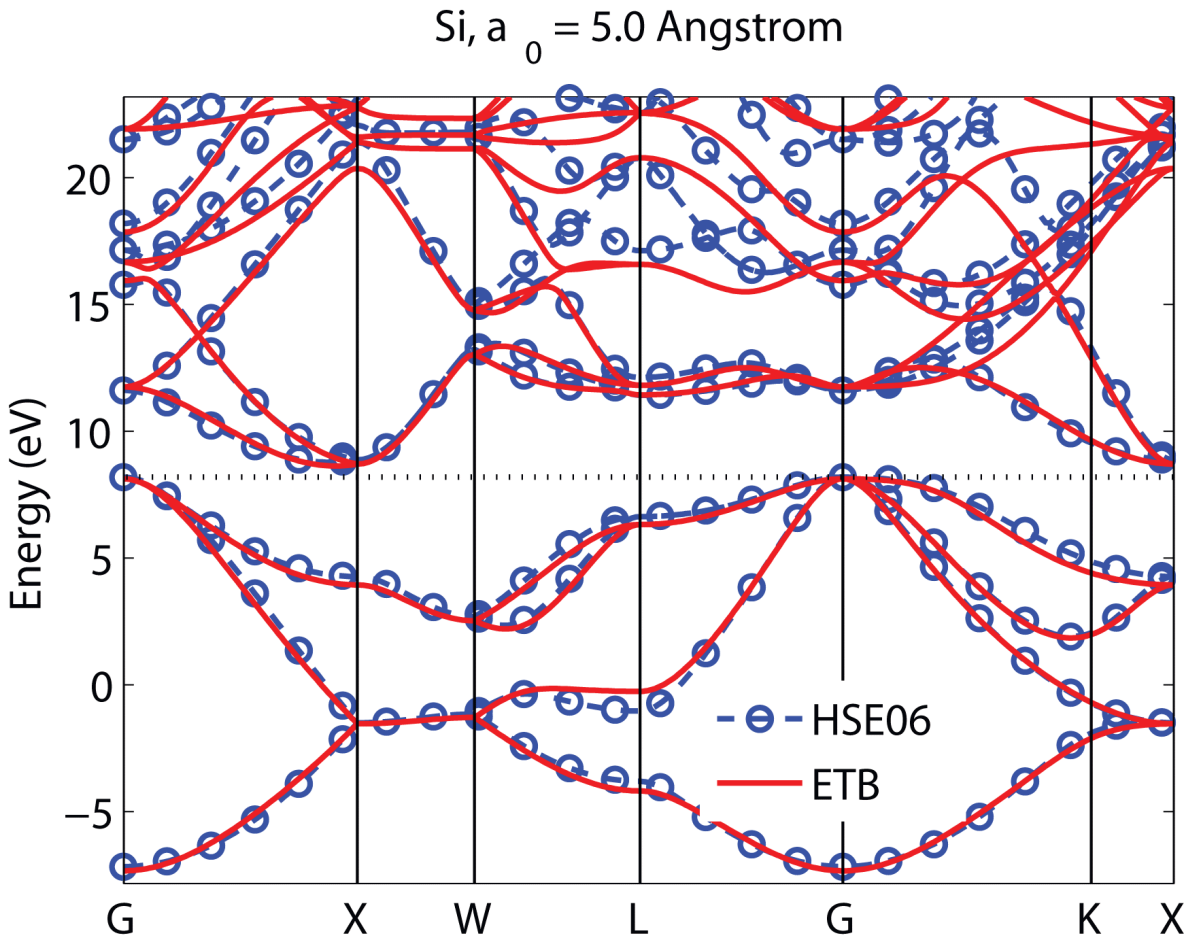
What is the environment?

Environments:
(the status of neighbors)

Atom types of neighbors	Bond lengths	Bond angles
	Hydrostatic strain 	strains $\begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & -2\varepsilon \end{bmatrix}$ 

ETB model in this work
→ Environment dependent Hamiltonian
- strains
- Interfaces

Si under hydrostatic strain

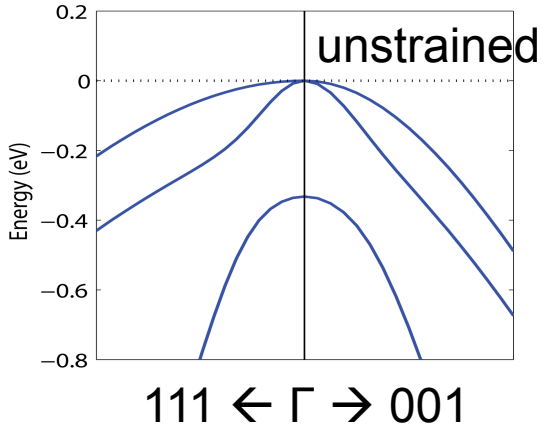


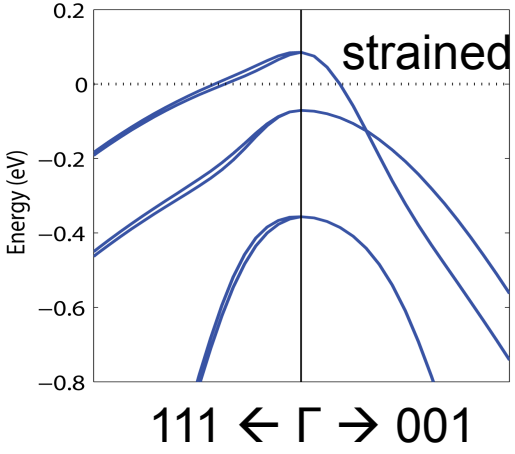
With hydrostatic strain:

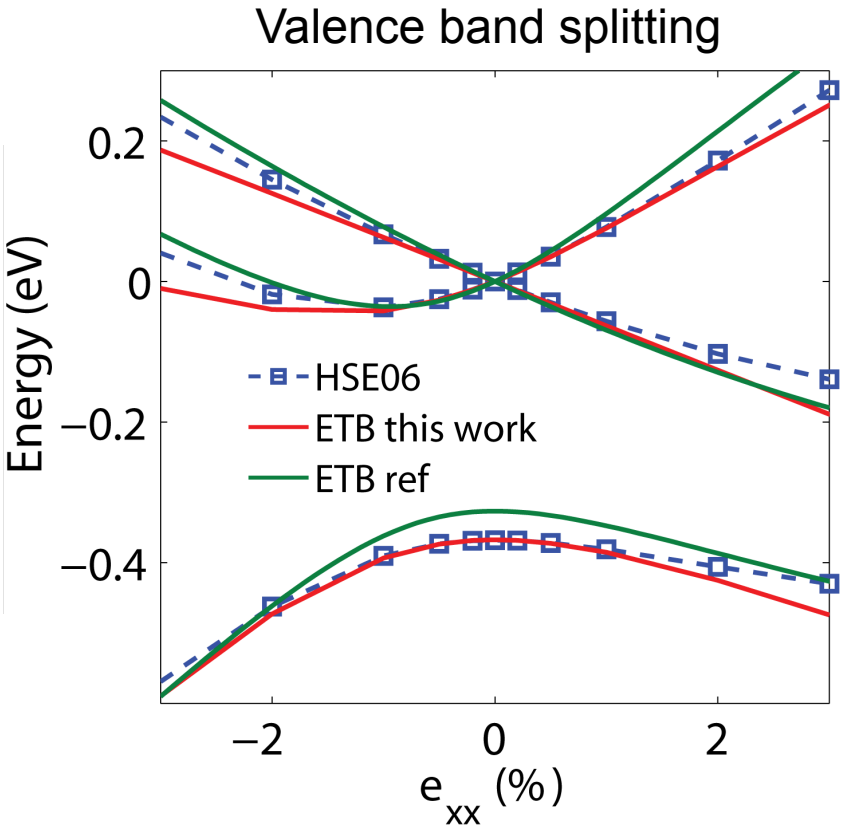
- Band gaps will change;
- Indirect gap → direct gap.

The TB model in this work can be applied to hydrostatic strain cases

Strained effect to valence bands





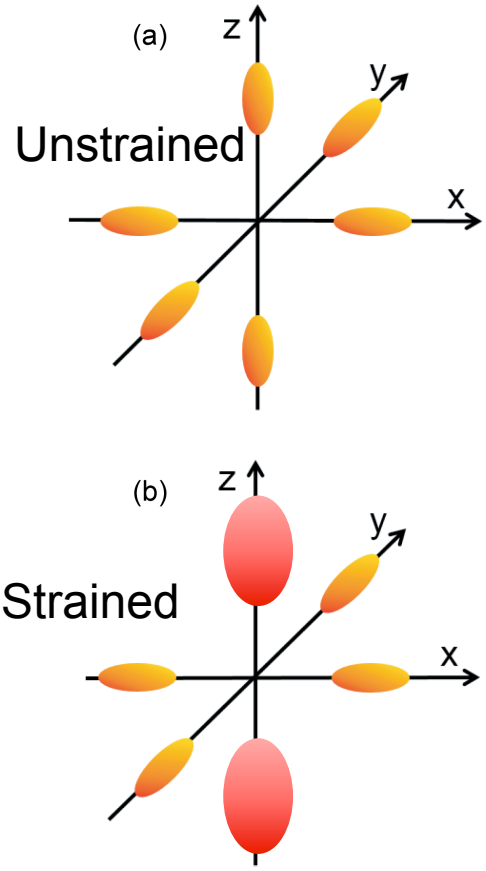


$$\begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & -2\varepsilon \end{bmatrix}$$

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

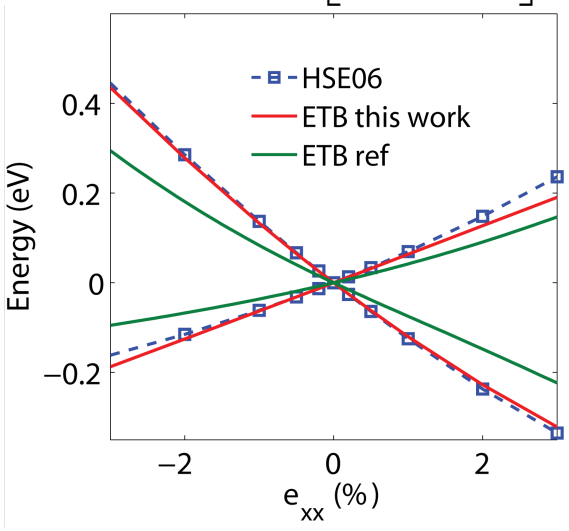
ETB model in this work reproduce the strain valence bands.

Strained effect to conduction bands (X valleys)

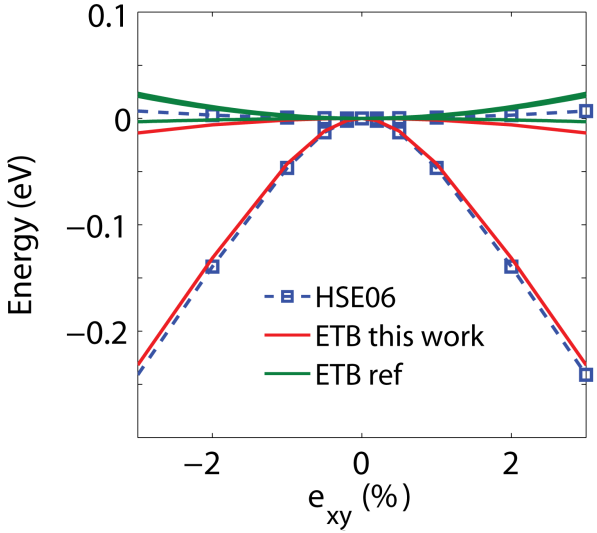


Band edge of X valleys

diagonal strain $\begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & -2\varepsilon \end{bmatrix}$



Off-diagonal strain $\begin{bmatrix} & \varepsilon & \\ \varepsilon & & \\ & & \end{bmatrix}$



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

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

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

Solutions and applications

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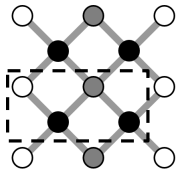
4. **Environment dependent strain model**
5. Transferability to interface

Solutions and applications

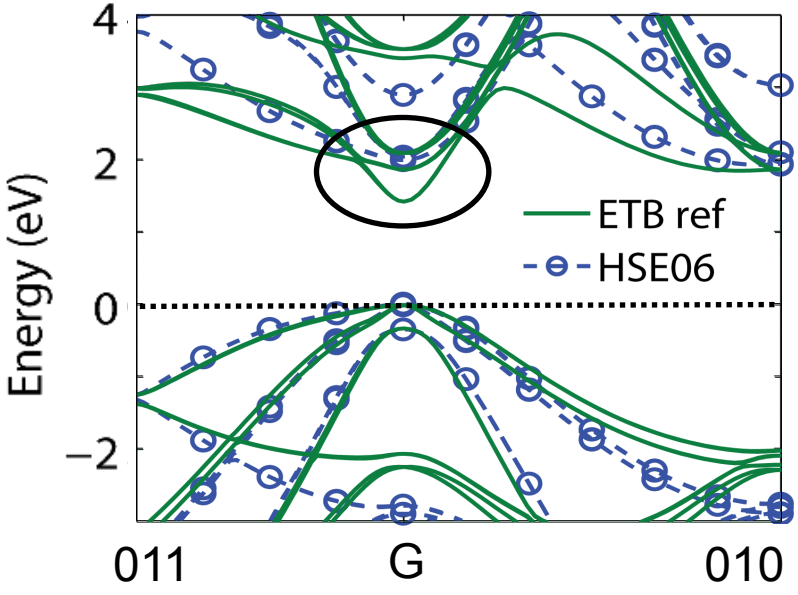
1. Parameterization algorithm from *ab-initio* calculations
2. Application to unstrained bulk
3. Application to ultra thin bodies (UTBs)
4. Environment dependent strain model
5. **Transferability to interface**

Strained GaAs/AlAs superlattices

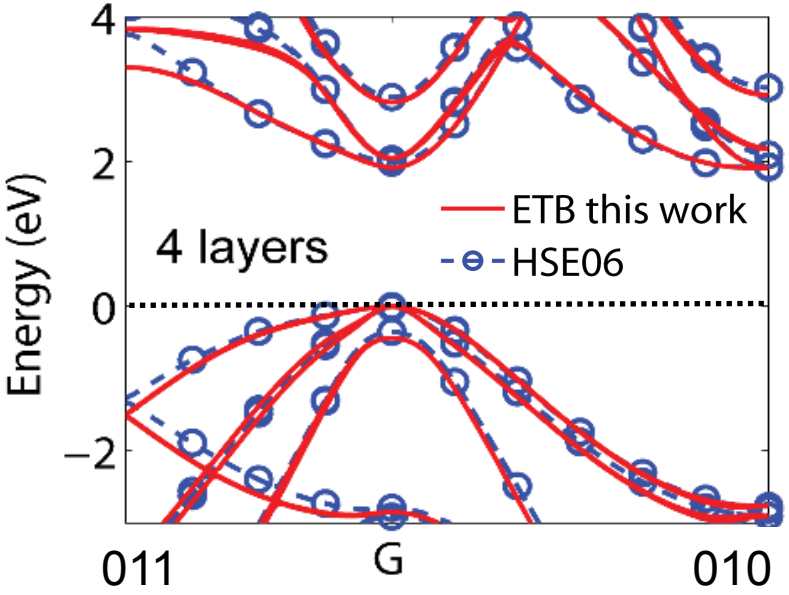


As
Ga
Al

Existing ETB



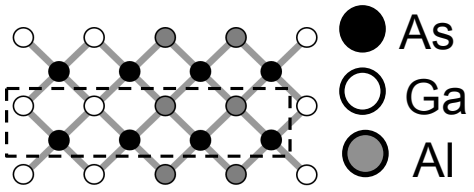
ETB This work



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

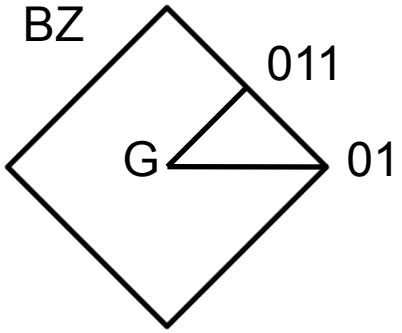
Existing ETB model shows significant differences in a GaAs/ AlAs superlattice

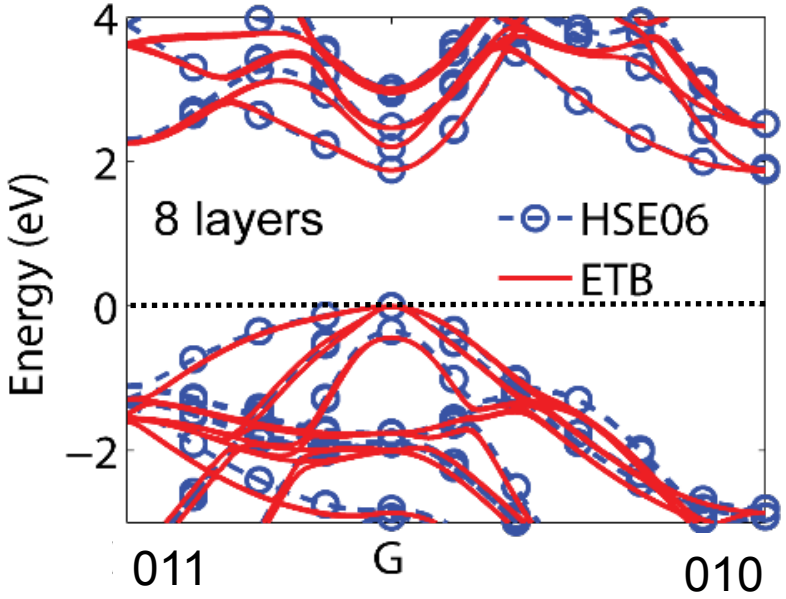
Strained GaAs/AlAs superlattices



ETB calculations in this work :

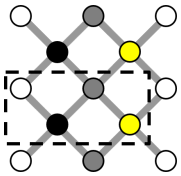
- sp3d5s* +SO
- 1st nearest neighbor interaction
- Negligible built-in potential





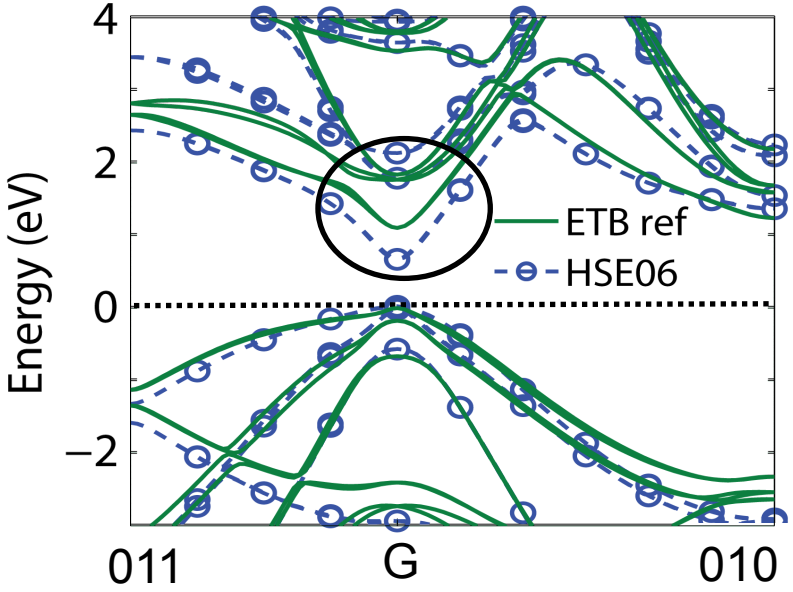
ETB in this work can accurately calculate band structure of GaAs/AlAs superlattices

Strained InAs/GaSb superlattices:

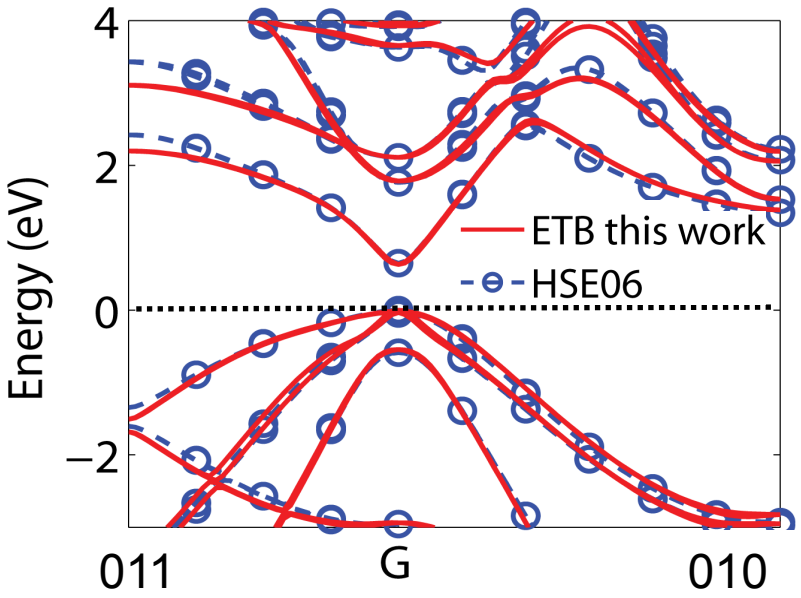


As
In
Ga
Sb

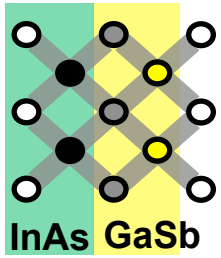
Existing ETB



ETB This work

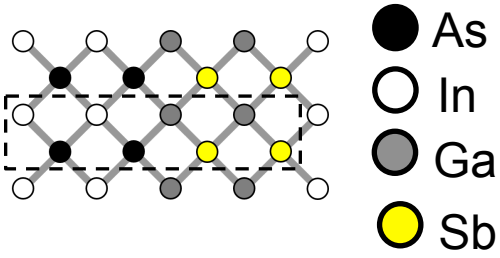


ETB ref : J. Jancu, et al. PRB, 57, 6393 (1998).

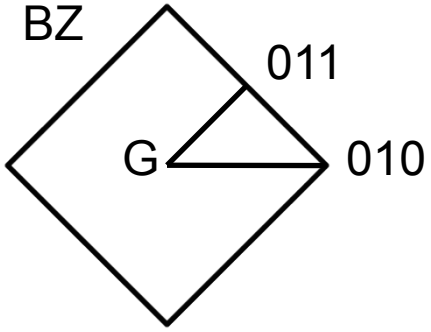


Existing ETB model shows significant differences in a InAs/GaSb superlattice

Strained InAs/GaSb superlattices



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



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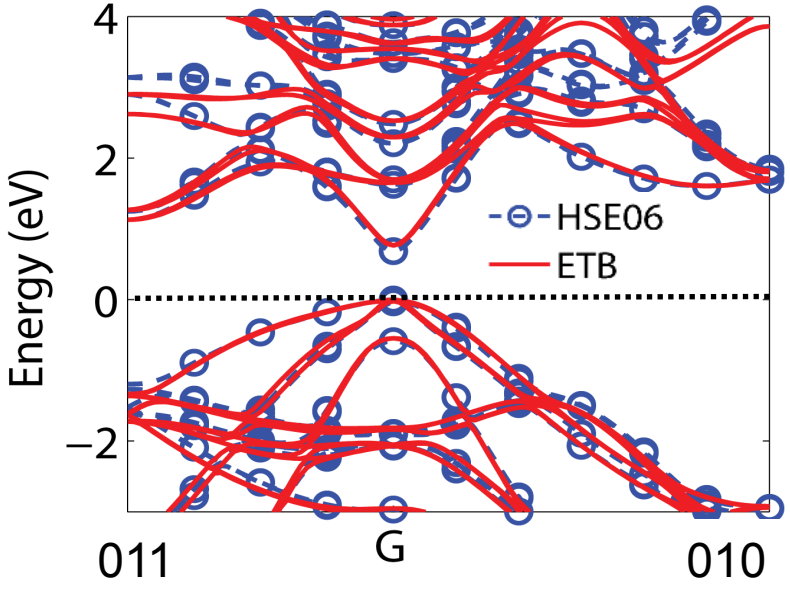
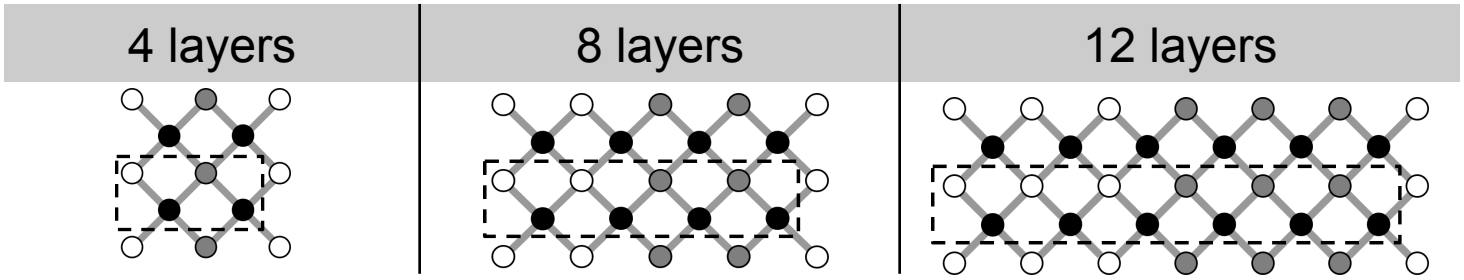
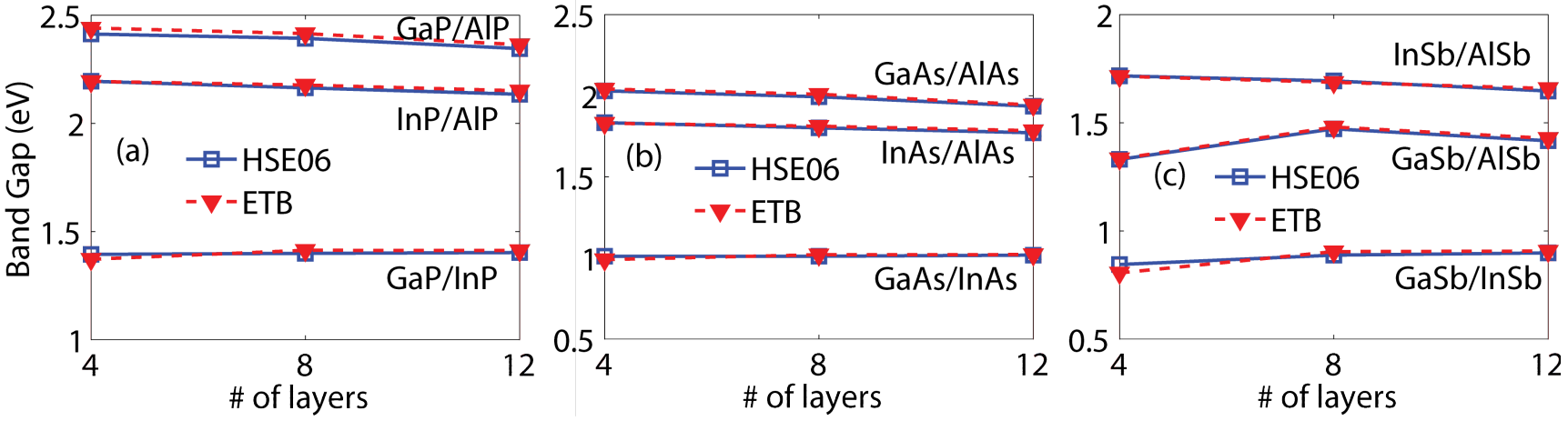


ETB in this work can accurately calculate band structure of InAs/GaSb superlattices

More superlattices: superlattices with common anions

Superlattices with common **anions**





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

Summary & Outlook

Summary

- 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.

Room temperature ETB parameters

Motivation:

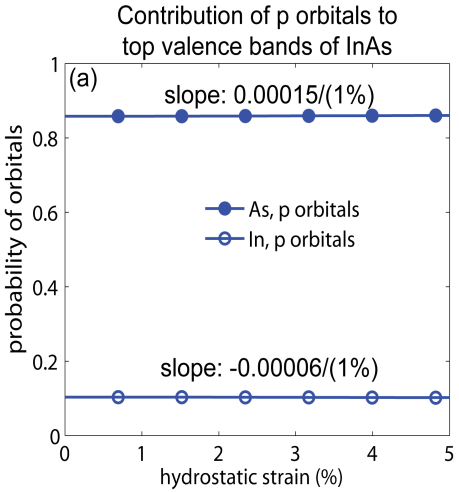
- *Ab-initio* calculations usually assume zero temperature.
- But device simulations require room temperature tight binding parameters.

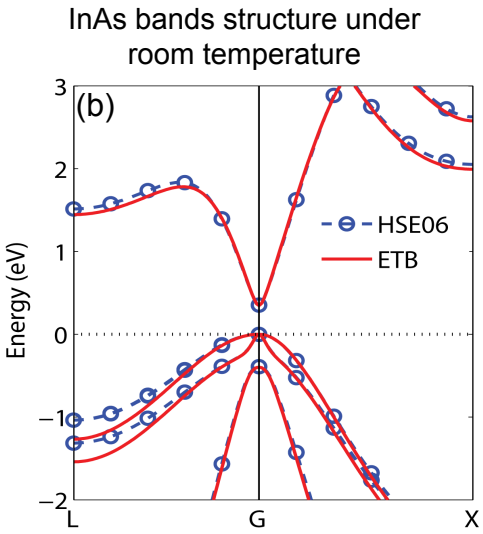
Approach:

- 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 f device level simulation is required.
- Extract TB parameters from DFT results (DFT energy bands & eigenfunctions)

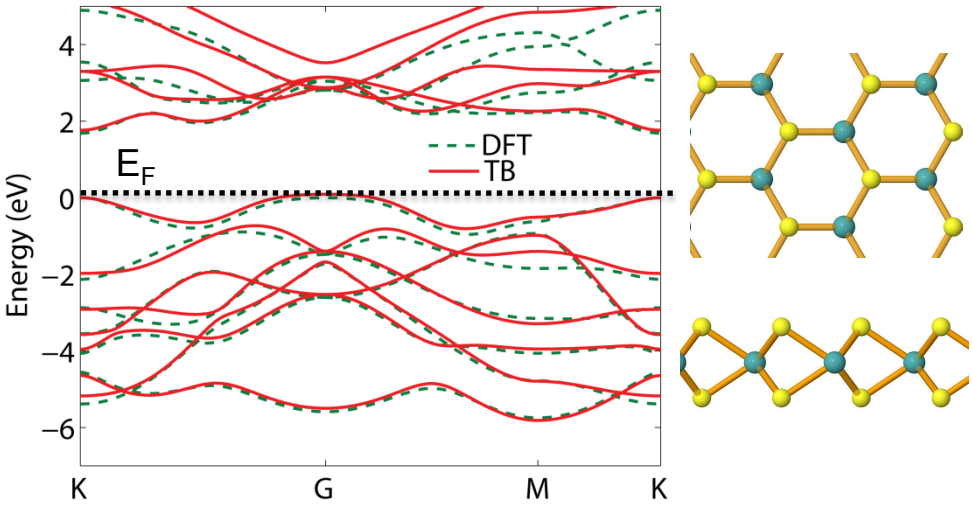
Approach:

- Basis transformation:
  Plane waves → localized orbitals
- TB model: orthogonal TB model with 1st N 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;

Single layer MoS_2 band structure



Impact:

TB parameters for TMDs are obtained, device level calculations of TMD transistors are enabled.

Tight binding model for black phosphorus

Objective:

- Existing four-band tight binding model underestimates band splitting → might affect charge distribution especially if scattering exists.

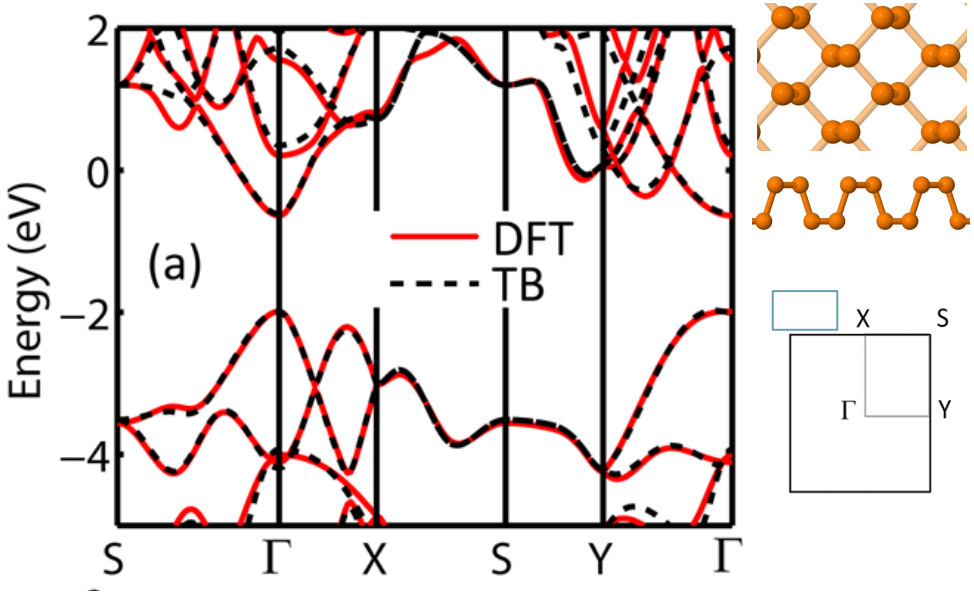
Method:

- 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.

Band structure



Impact:

- Atomistic modeling for black Phosphorus transistors are enabled.

Passivation applied to Si/SiO_2 interface

Objective:

- Investigate the Si UTB/SiO_2 interface and evaluate the normally used hydrogen atom passivation treatment.

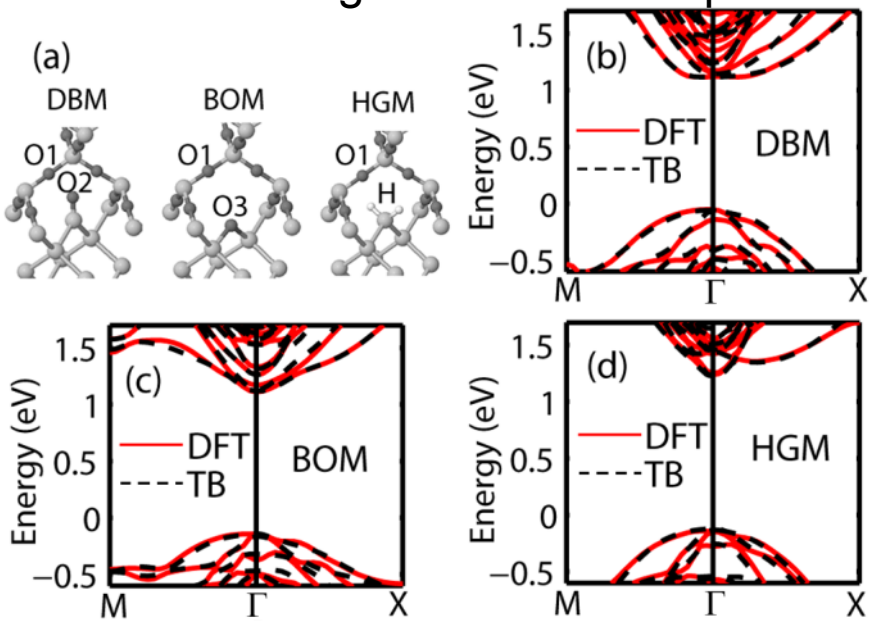
Method:

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

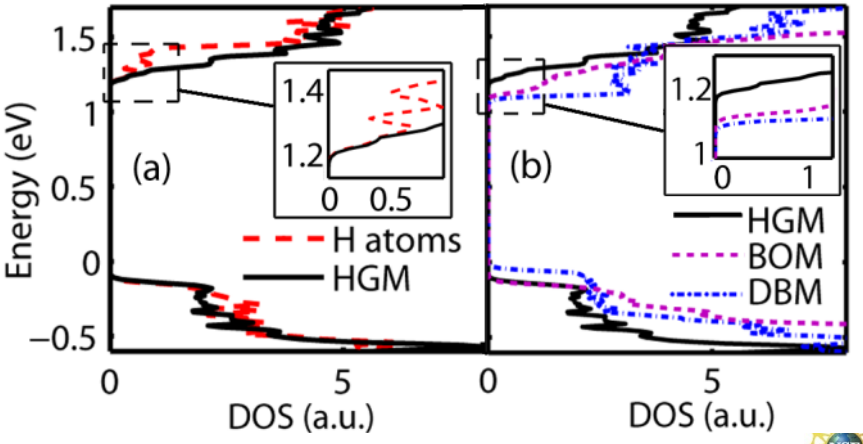
Impact:

- 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.

oxidation configurations and dispersions



DOS for the oxidation configurations

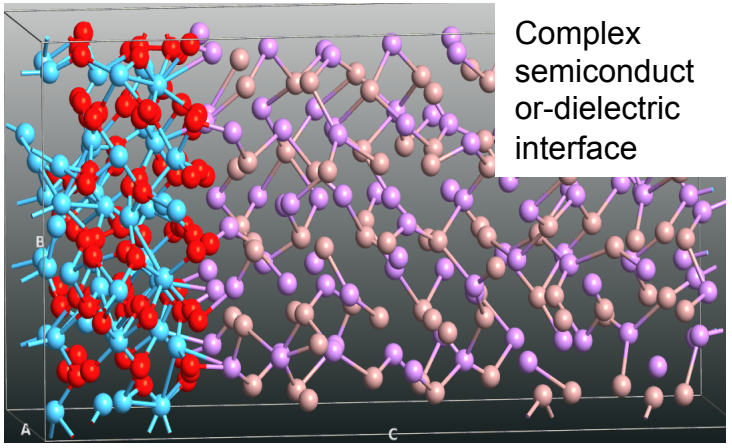


PURDUE UNIVERSITY

Extended Hückel Fitting Based on *ab-initio* mapping

InAs Parameterization

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

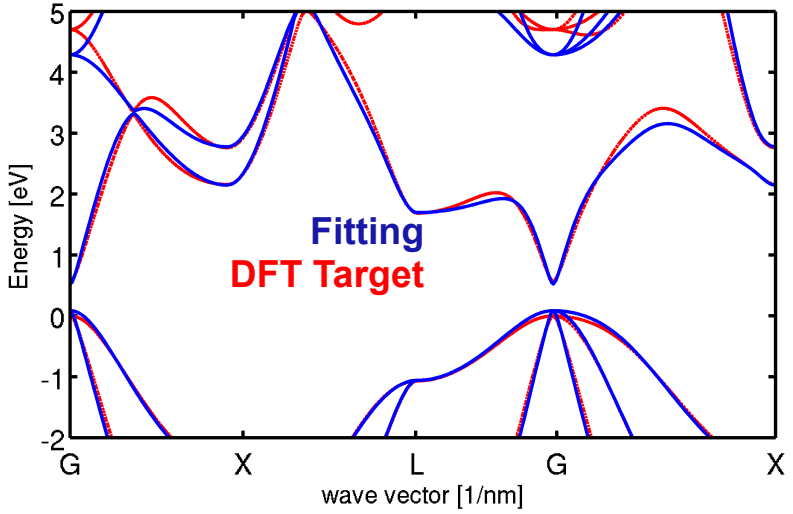


Complex semiconduct or-dielectric interface

HfO2, InAs interface. Strain, rearrangement requires high transferability

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



Mapping of *ab-initio* to Tight Binding for MgO

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:

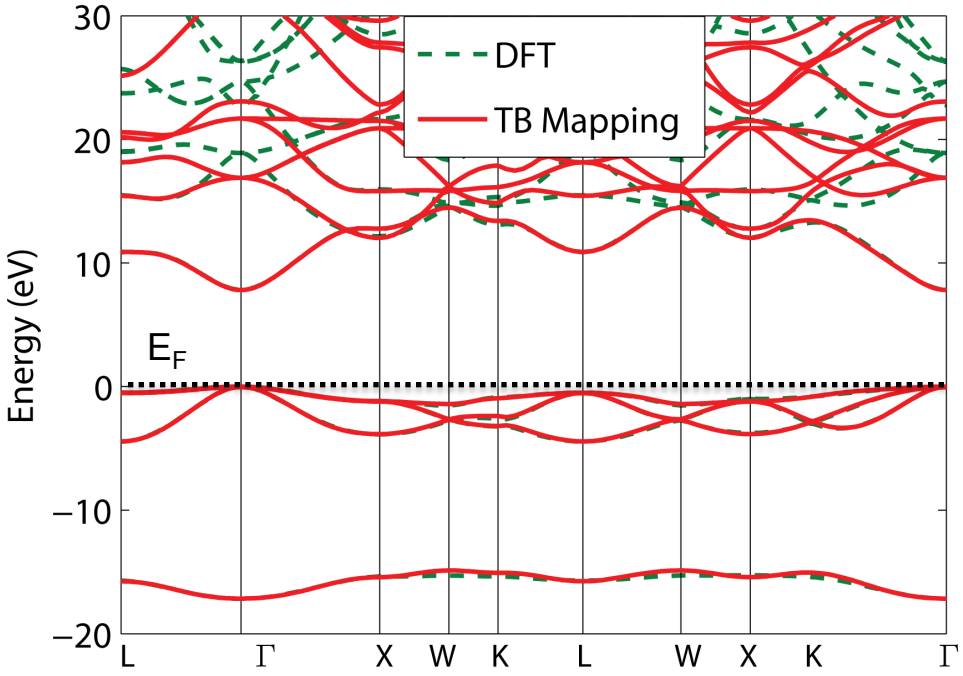
- Low rank approximation:

$$H_{DFT} \rightarrow H_{TB}$$

- constraint:
  - 2st 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.

Mapping of *ab-initio* to Tight Binding for SmSe

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:

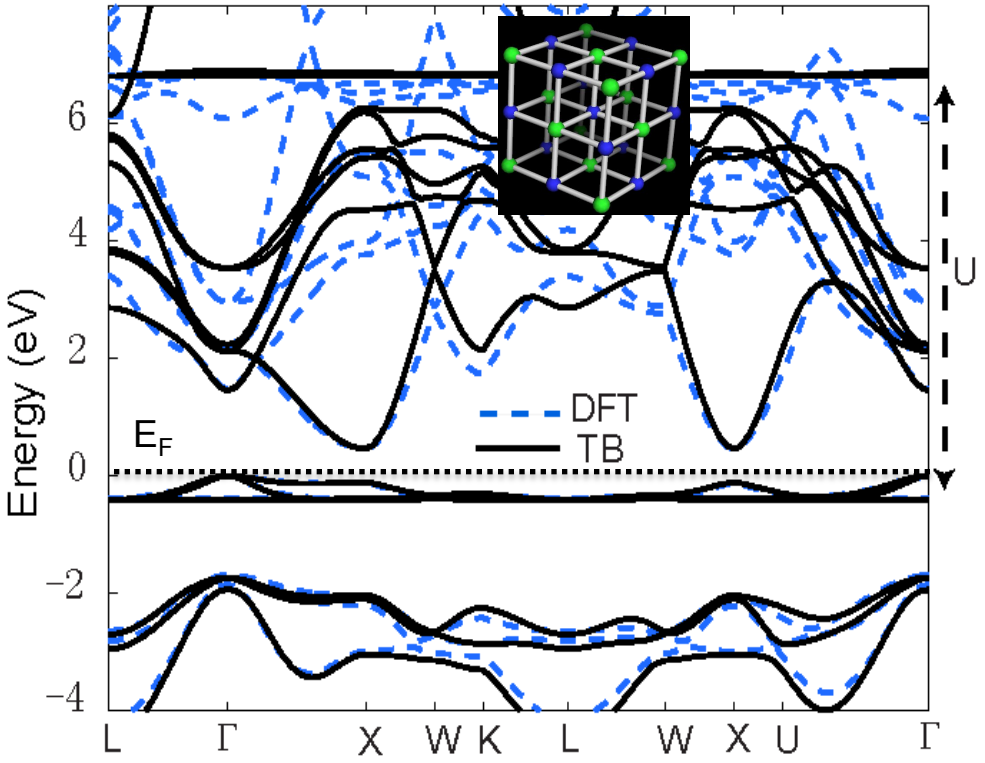
- Low rank approximation:

$$H_{DFT} \rightarrow H_{TB}$$

- 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;

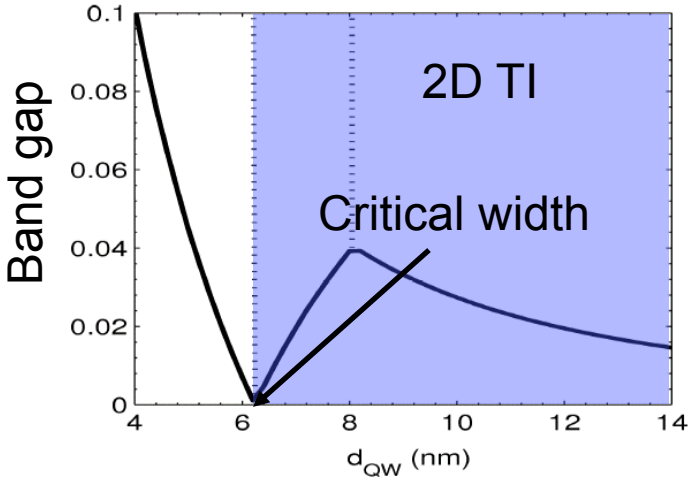


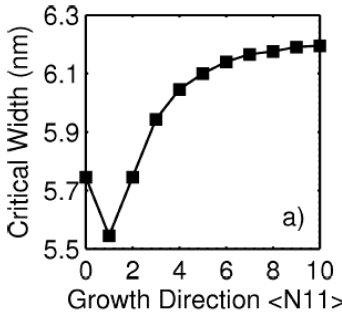
Impact:

TB parameters for complicated material SmSe are obtained, device level calculations of SmSe based piezoelectronic Transistor are enabled.

Design principles for HgTe based Topological Insulator Devices

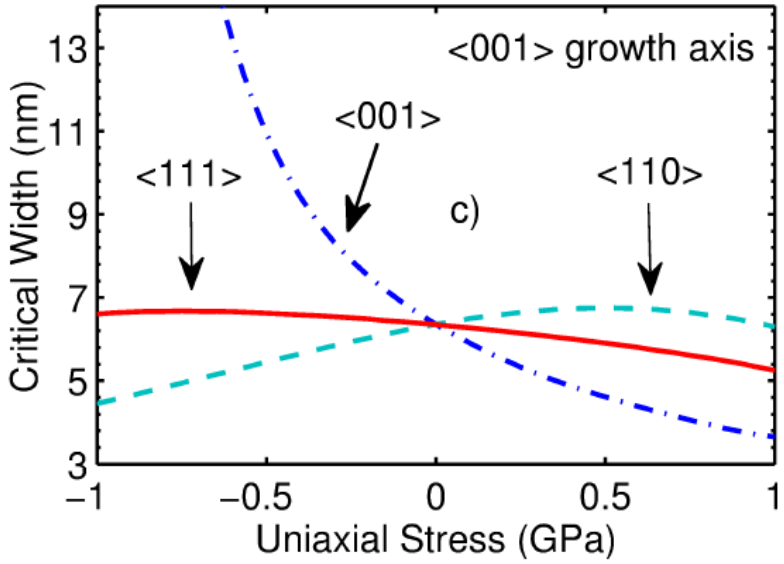
Motivation:
Topological insulators like (CdTe/ HgTe/CdTe QW) are new group of materials.
The behavior of topological insulator in device environment is not clear.





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.



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NCN Staff members:
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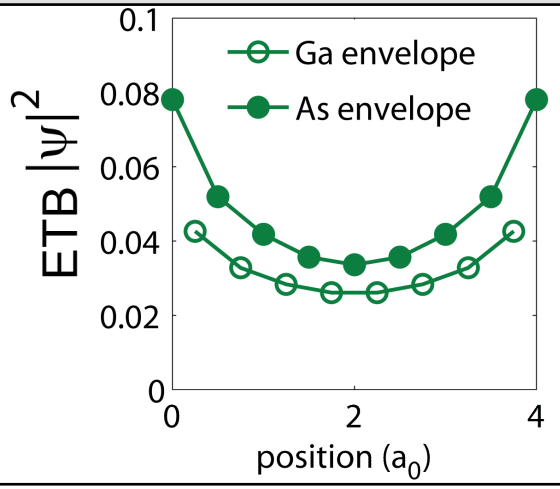
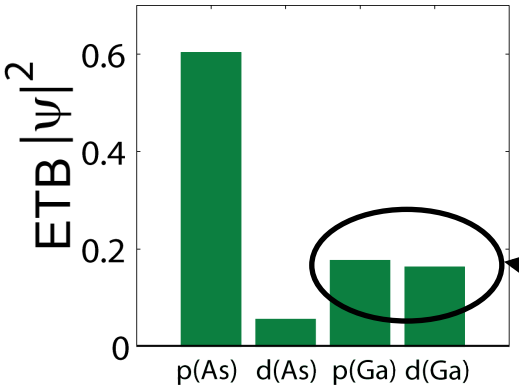
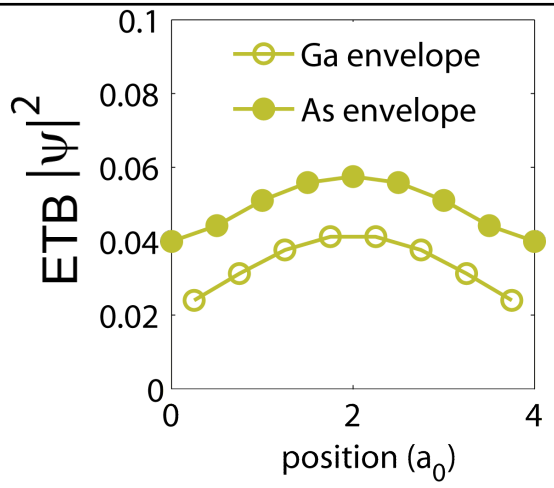
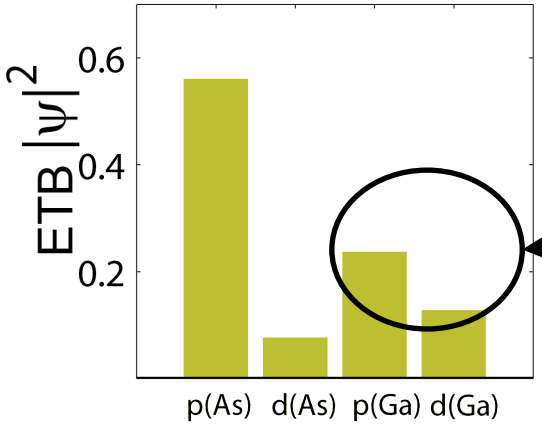
Thank you!

Related Publication list

- **Y. Tan**, M. Povolotskyi, T. Kubis, T. Boykin, G. Klimeck, 'Transferable tight binding model for strained group IV and III-V heterostructures' to be submitted to Phys. Rev. B
- **Y. Tan**, M. Povolotskyi, T. Kubis, T. B. Boykin, G. Klimeck, 'Tight Binding analysis of Si and GaAs ultra-scaled transistors with subatomic wave-function resolution' Phys. Rev. B 92, 085301 (2015)
- **Y. Tan**, M. Povolotskyi, T. Kubis, Y. He, Z. Jiang, G. Klimeck, T. B. Boykin, 'Empirical tight binding parameters for GaAs and MgO with explicit basis through DFT mapping', Journal of Computational Electronics 12 (1), 56-60 (2013)
- Y. He, **Y. Tan**, Z. Jiang, M. Povolotskyi, G. Klimeck, T. Kubis, 'Surface Passivation in Empirical Tight Binding', submitted to IEEE Trans. Elect. Dev.
- Z. Jiang, M. Kuroda, **Y. Tan**, D. Newns, M. Povolotskyi, T. Boykin, T. Kubis, G. Klimeck, G. Martyna, 'Electron transport in nano-scaled piezoelectronic devices', Applied Physics Letters 102 (19), 193501 (2013)
- H. Ilatikhameneh, **Y. Tan**, B. Novakovic, G. Klimeck, R. Rahman, J. Appenzeller, 'Tunnel Field-Effect Transistors in 2D Transition Metal Dichalcogenide Materials', IEEE Journal on Exploratory Solid-State Computational Devices and Circuits, 1,12,(2015)
- P. Sengupta, T. Kubis, **Y. Tan**, M. Povolotskyi, G. Klimeck, 'Design principles for HgTe based topological insulator devices', Journal of Applied Physics 114 (4), 043702 (2013)
- Y. Hsueh, H. Büch, **Y. Tan**, Y. Wang, L. Hollenberg, G. Klimeck, M. Simmons, and R. Rahman, "Spin-Lattice Relaxation Times of Single Donors and Donor Clusters in Silicon", Phys. Rev. Lett. 113, 246406 (2014)
- F. Chen, L. Jauregui, **Y. Tan**, M. Manfra, G. Klimeck, Y. Chen, T. Kubis, 'In-surface confinement of topological insulator nanowire surface states', Appl. Phys. Lett. 107, 121605 (2015)

Backup slides

Problem of the previous parameters

	UTB wave functions	Bulk wave functions
Previous parameters		
Modified Parameters		

d-orbital contribute too much.

Smaller d contribution due to modified parameters

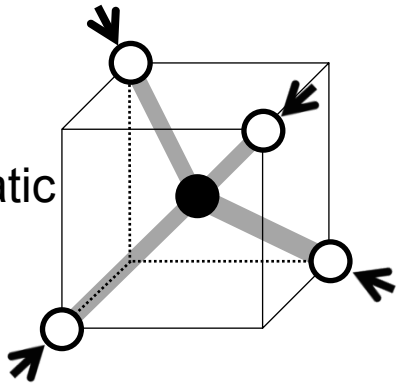
Smaller d-contribution due to modified parameters also eliminate unphysical states

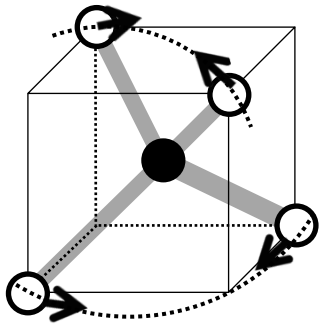
strain ETB model: Strain targets

Special distorted systems considered in fitting:

- Four kinds of atom displacements
- Assume no missing nearest neighbor

Hydrostatic strain

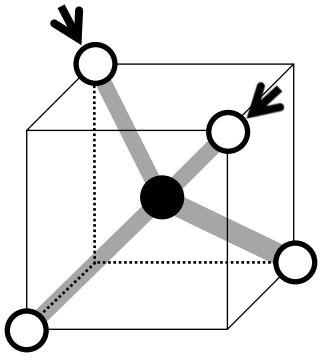


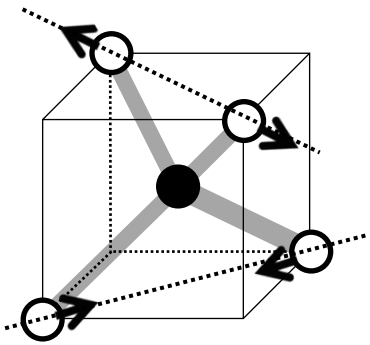


Diagonal strains

$$\begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & -2\varepsilon \end{bmatrix}$$

two bond lengths change

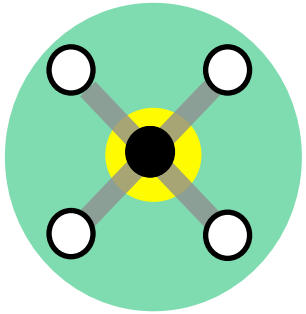




Off-diagonal strains

$$\begin{bmatrix} & \varepsilon & \\ \varepsilon & & \\ & & \end{bmatrix}$$

Environment ETB model

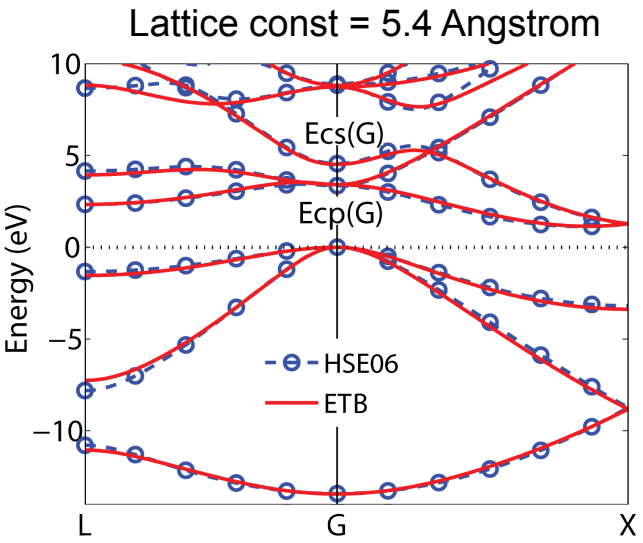


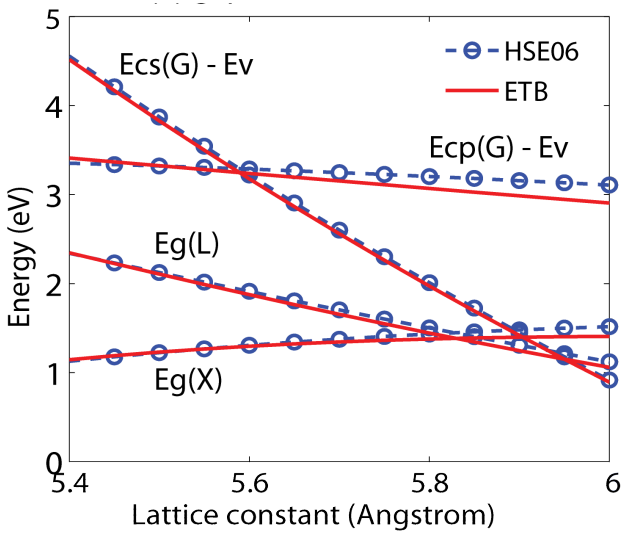
Onsite element:

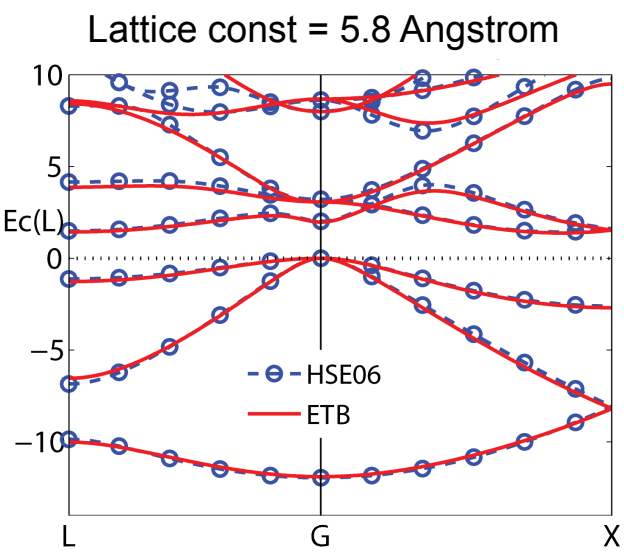
$$H^{(0)}_{\alpha_i,\alpha_i} = E_{\alpha_i} + \sum_{j\in \mathrm{NNs}} I_{\alpha_i,j}(d_{ij}) + \sum_{j\in \mathrm{NNs}} O_{i,j}(d_{ij}),$$

Environment dependent terms:
Sum over nearest neighbors

Si under hydrostatic strain







With hydrostatic strain:

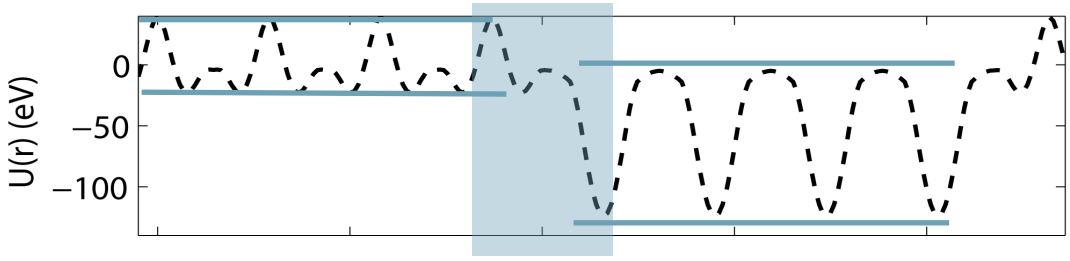
- Band gaps will change;
- Gap of X, L and Γ points change at different ratio;
- Transition from indirect gap to direct gap happens;

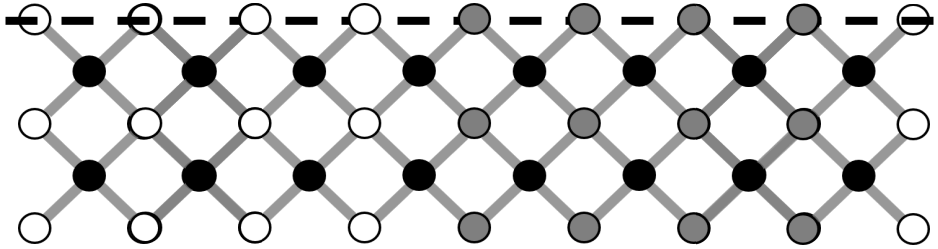
The TB model in this work can be applied to hydrostatic strain cases

Challenge: Application to heterostructures

What is proper interaction radius of TB model?

Observation: Ab-initio potential at IIIV interface varies over the range of first nearest neighbor



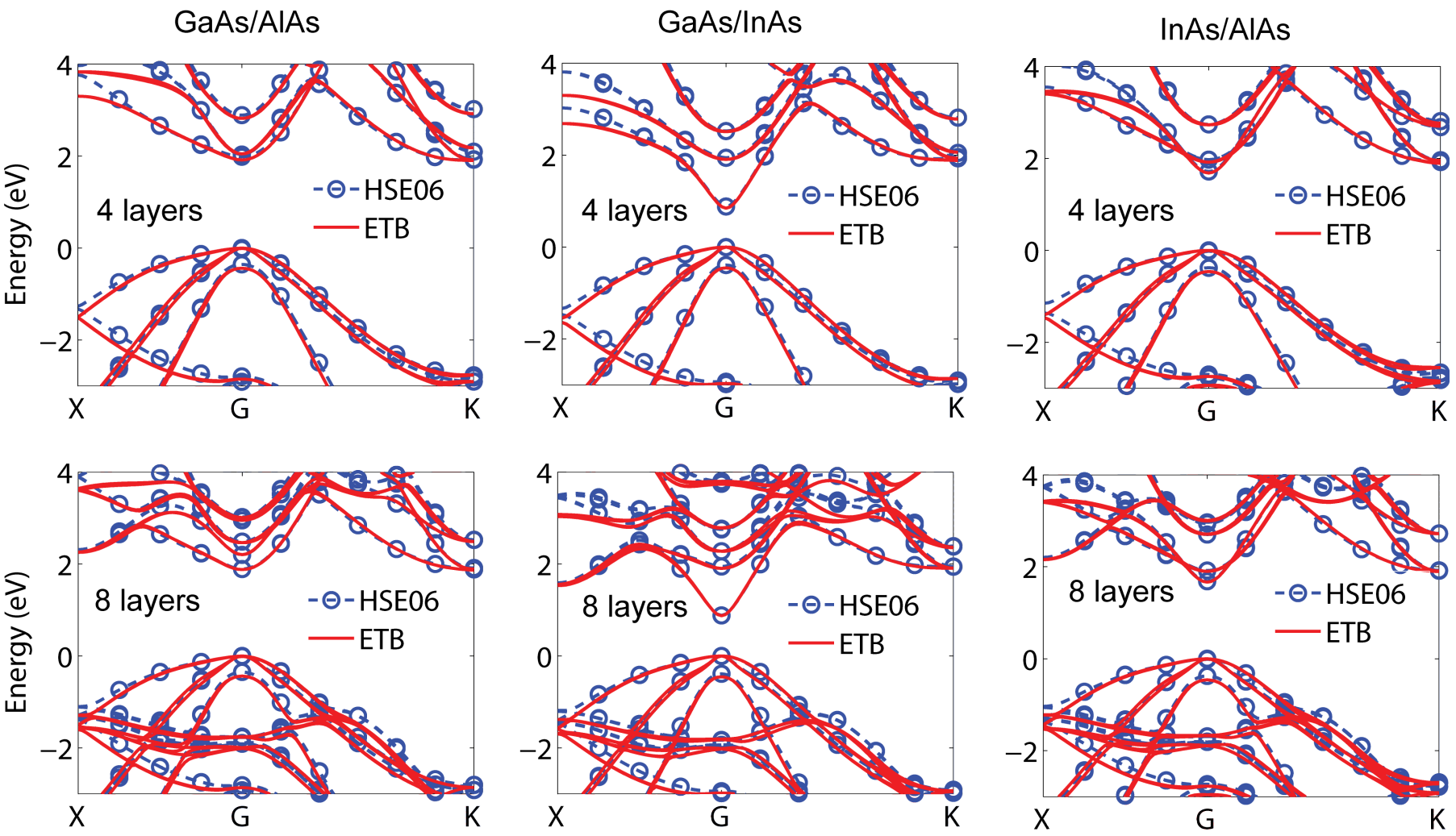


ab-initio local potential of GaAs/InAs superlattice

Is 1st nearest neighbor interaction enough for IIIV hetero structures?

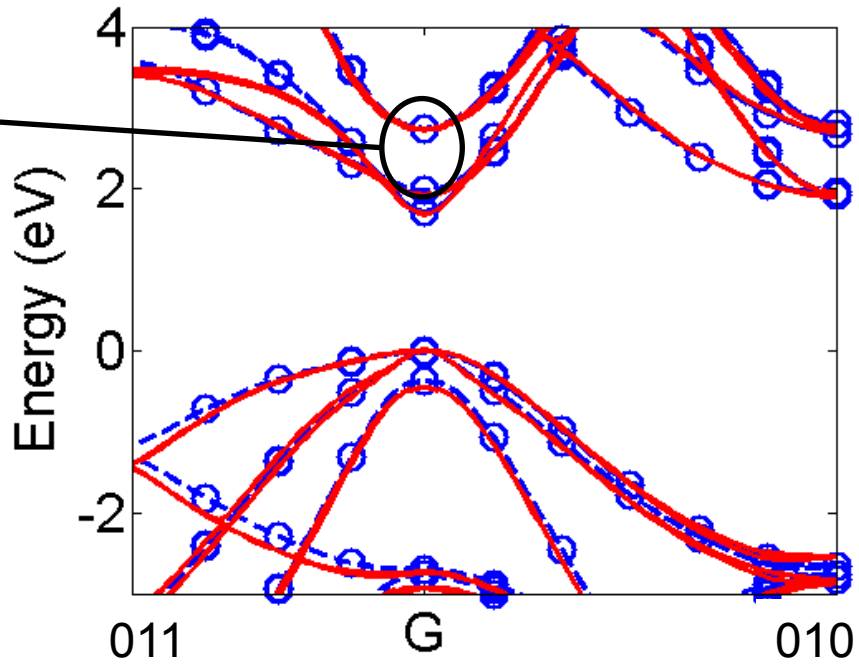
72

Superlattice band structure of Xas/YAs

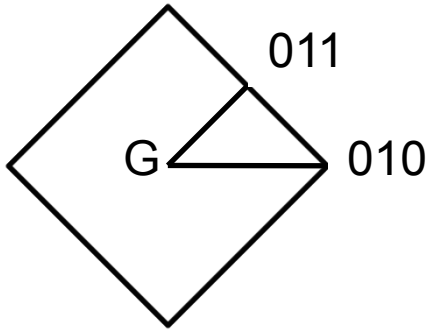


More on AlAs/InAs superlattices

Folded bands originate from X valleys

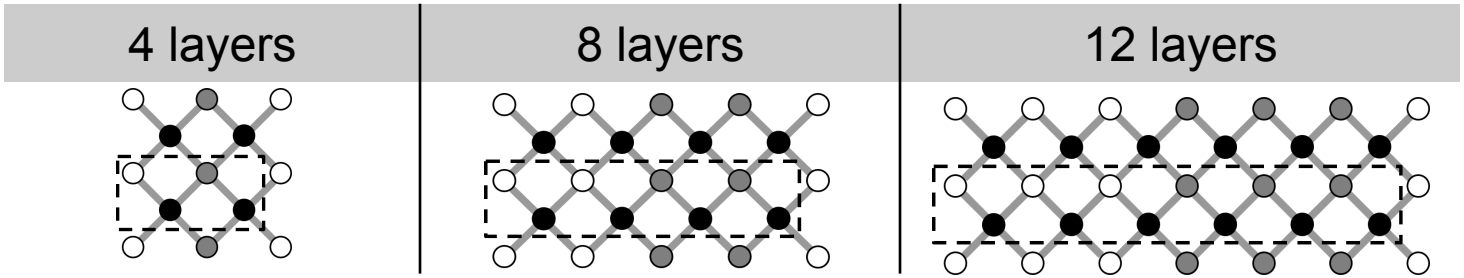


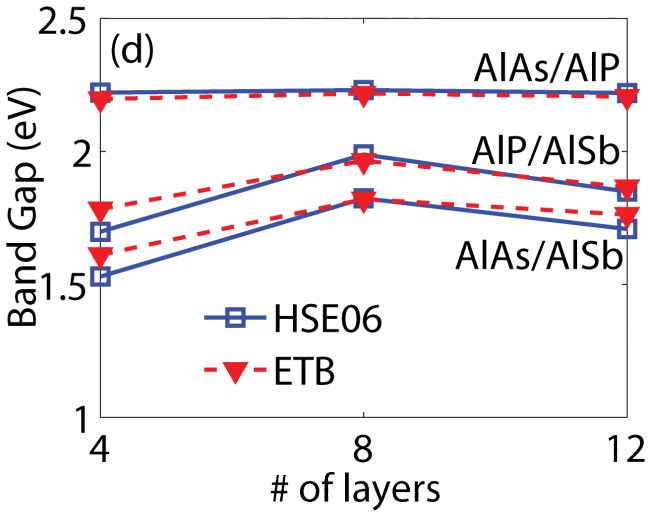
Lowest few conduction bands originate from Γ and X valleys in the fcc BZ

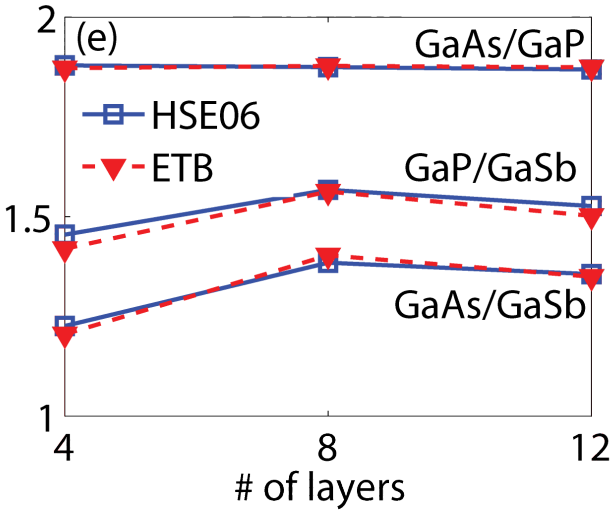


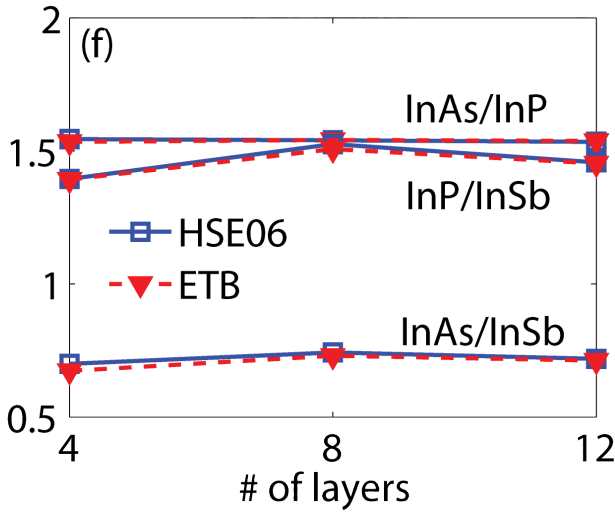
More superlattices: superlattices with common cations

Superlattices with common **cations**









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

InAs/GaSb Superlattice

Type III superlattice? →
confinement opens the band gap