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Software for semiconductor nanodevices

NEGF Basis in Multiband Models for Broken-Gap Sb-Based Tunneling Devices

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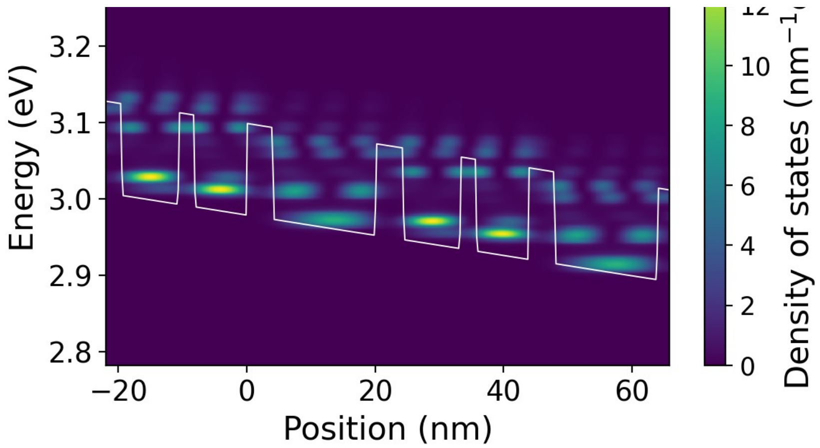
IWCN, June 13, 2023

nextnano products

- Schrodinger-Poisson-drift-diffusion solver (nextnano++)

  Quasi-equilibrium semiclassical transport



Tunneling charge transport

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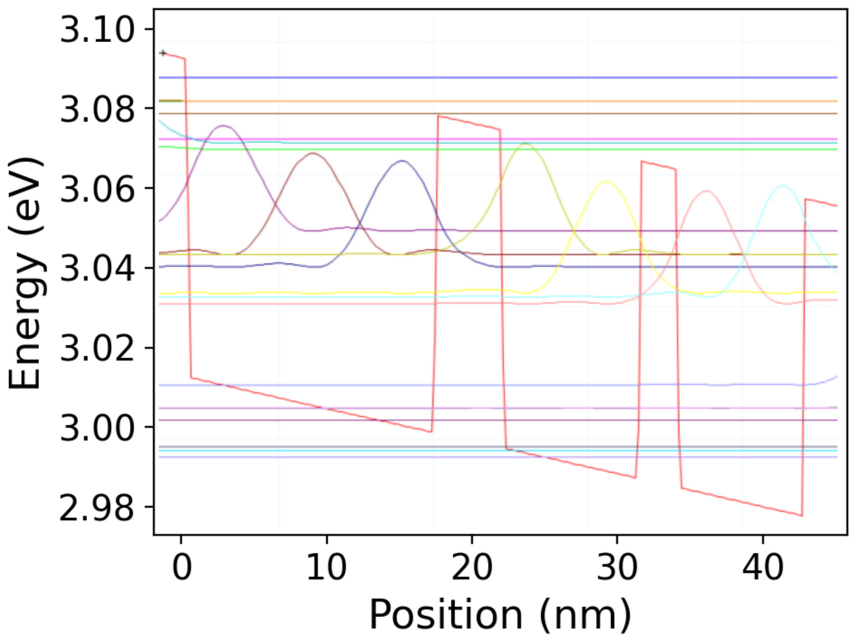
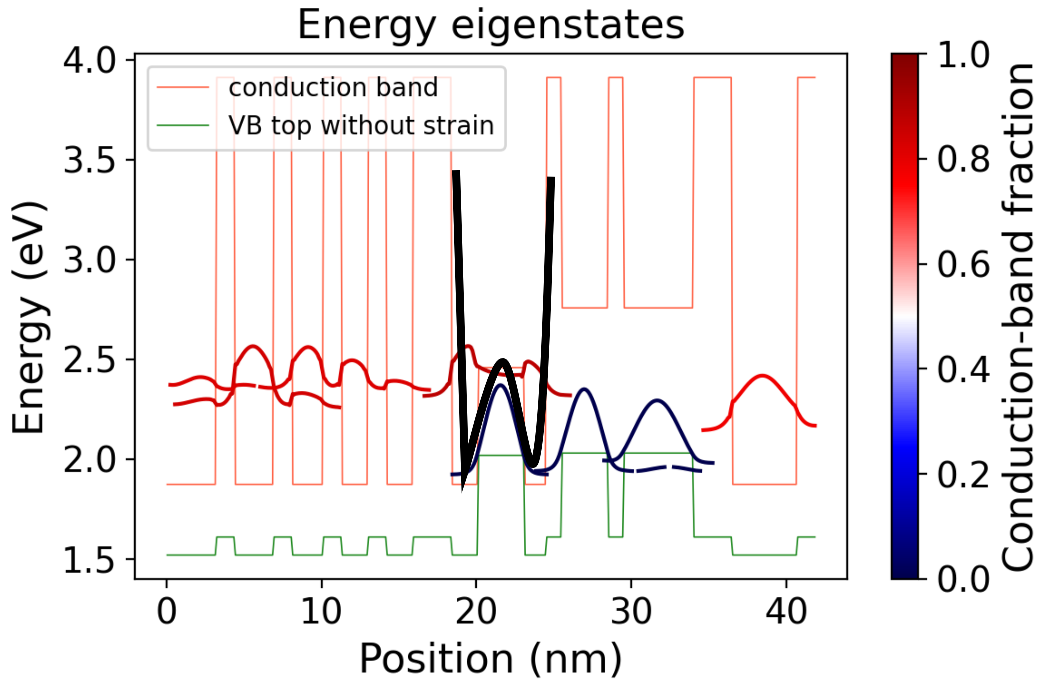
III-Sb broken-gap tunneling devices – photodetector, lasers

Intersubband e.g. QCLs

Interband e.g. ICLs





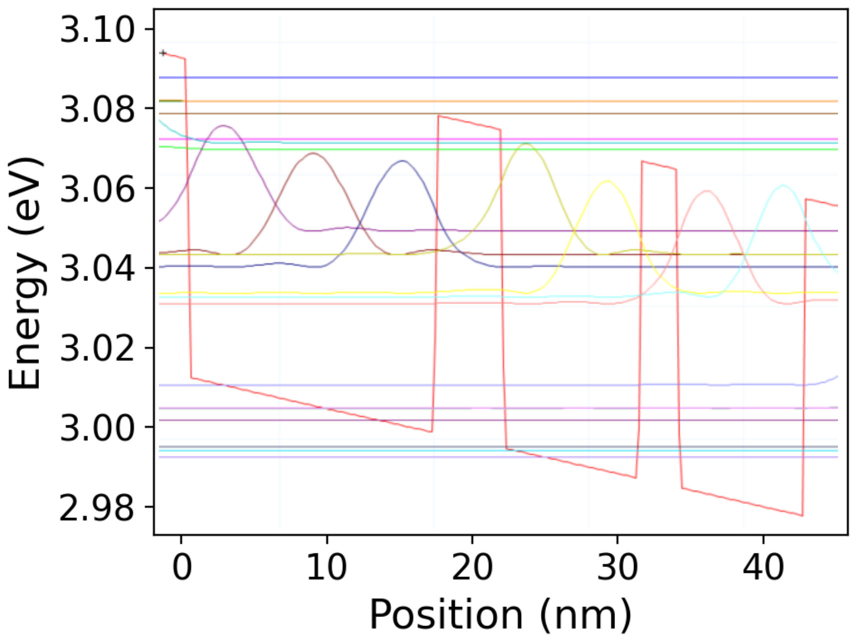
nextnano.NEGF

nextnano.NEGF x (this project)

Tunneling charge transport

III-Sb broken-gap tunneling devices – photodetector, lasers

Intersubband e.g. QCLs



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Interband e.g. ICLs

We will simulate non-equilibrium charge distribution in steady states

nextnano.NEGF x (this project)

Tunneling charge transport

Accuracy

Reduce problem size

$H_0 + H_{scatt}$

- NEGF formalism

  rather than Schrodinger-Poisson

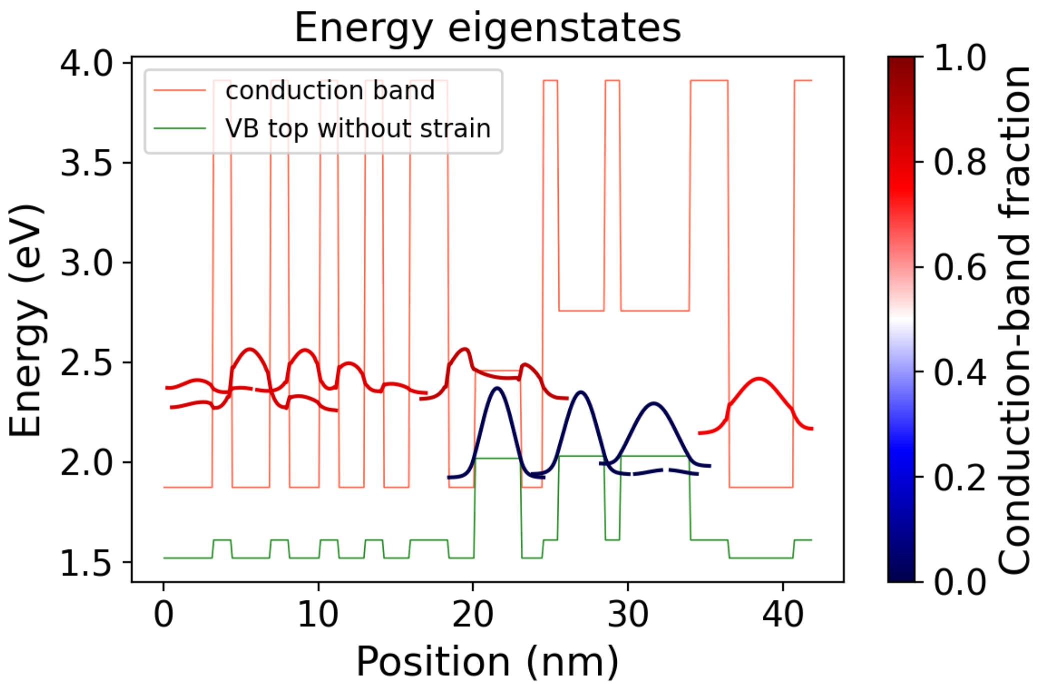
- 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model

  for accurate energy levels & interband coupling

- Consistent Hamiltonian discretization

  Robust against spurious solutions

Interband



Consistent Hamiltonian discretization

8-band k.p — z-dependence

$$\mathcal{H} = \mathcal{H}_{\text{band}} \otimes \mathcal{H}_{\text{spatial}}$$

Discretization = matrix representation of the Hamiltonian in $\mathcal{H}$

Consistent Hamiltonian discretization

8-band k.p — z-dependence

$$\mathcal{H} = \mathcal{H}_{\text{band}} \otimes \mathcal{H}_{\text{spatial}}$$

1. **Heterostructure ←→ bulk**

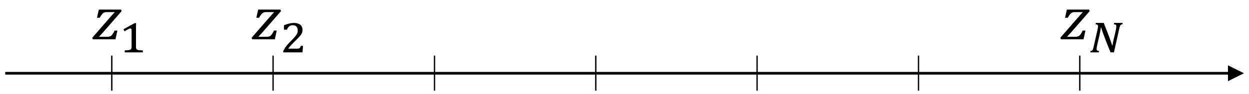
$$\psi_{n\mathbf{k}} = e^{i\mathbf{kr}} u_{n\mathbf{k}}(\mathbf{r})$$

2. Avoid oscillatory solutions and peaks at the interfaces
3. Consistent discretization of the 1st- and 2nd-order derivatives
4. Hamiltonian must be Hermitian!

Consistent Hamiltonian discretization

8-band k.p   z-dependence

$$\mathcal{H} = \mathcal{H}_{\mathrm{band}} \otimes \mathcal{H}_{\mathrm{spatial}}$$



1. **Heterostructure ←→ bulk**

$$\psi_{n\mathbf{k}} = e^{i\mathbf{kr}} u_{n\mathbf{k}}(\mathbf{r})$$

2. **Avoid oscillatory solutions and peaks at the interfaces**
   Foreman, PRB (1997)

$$H = H^{(0)} + H^{(L)}\frac{d}{dz} + \frac{d}{dz}H^{(R)} + \frac{d}{dz}H^{(2)}\frac{d}{dz}$$

3. Consistent discretization of the 1st- and 2nd-order derivatives

4. Hamiltonian must be Hermitian!

Consistent Hamiltonian discretization

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$$\mathcal{H} = \mathcal{H}_{\mathrm{band}} \otimes \mathcal{H}_{\mathrm{spatial}}$$

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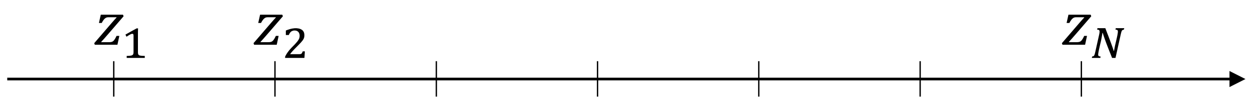

$$\psi_{n\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

$$H = H^{(0)} + H^{(L)}\frac{d}{dz} + \frac{d}{dz}H^{(R)} + \frac{d}{dz}H^{(2)}\frac{d}{dz}$$

$$\hat{\mathrm{d}}_{\mathrm{F}}\gamma f(z)\Big|_i = \frac{1}{h}(\gamma_{i+1}f_{i+1} - \gamma_i f_i),$$

$$\gamma\hat{\mathrm{d}}_{\mathrm{F}} f(z)\Big|_i = \frac{1}{h}\gamma_i(f_{i+1} - f_i),$$

$$\hat{\mathrm{d}}_{\mathrm{B}}\gamma f(z)\Big|_i = \frac{1}{h}(\gamma_i f_i - \gamma_{i-1}f_{i-1}),$$

$$\gamma\hat{\mathrm{d}}_{\mathrm{B}} f(z)\Big|_i = \frac{1}{h}\gamma_i(f_i - f_{i-1}),$$

Consistent Hamiltonian discretization

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8-band k.p z-dependence

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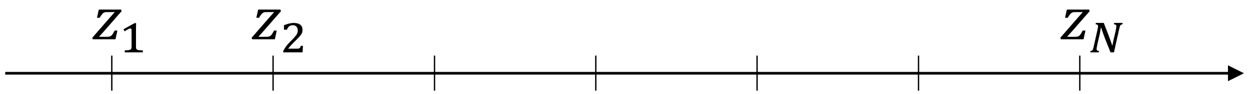

1. **Heterostructure ←→ bulk**

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   Foreman, PRB (1997)

$$H = H^{(0)} + H^{(L)}\frac{d}{dz} + \frac{d}{dz}H^{(R)} + \frac{d}{dz}H^{(2)}\frac{d}{dz}$$

3. **Consistent discretization of the 1st- and 2nd-order derivatives**
   Frensley *et al.*, arXiv (2014)

$$\hat{\mathrm{d}}_{\mathrm{F}}\gamma f(z)\Big|_i = \frac{1}{h}(\gamma_{i+1}f_{i+1} - \gamma_i f_i),$$
$$\gamma\hat{\mathrm{d}}_{\mathrm{F}} f(z)\Big|_i = \frac{1}{h}\gamma_i(f_{i+1} - f_i),$$
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$$\gamma\hat{\mathrm{d}}_{\mathrm{B}} f(z)\Big|_i = \frac{1}{h}\gamma_i(f_i - f_{i-1}),$$

4. **Hamiltonian must be Hermitian!**

Implemented

Transition energy in W-shaped QW

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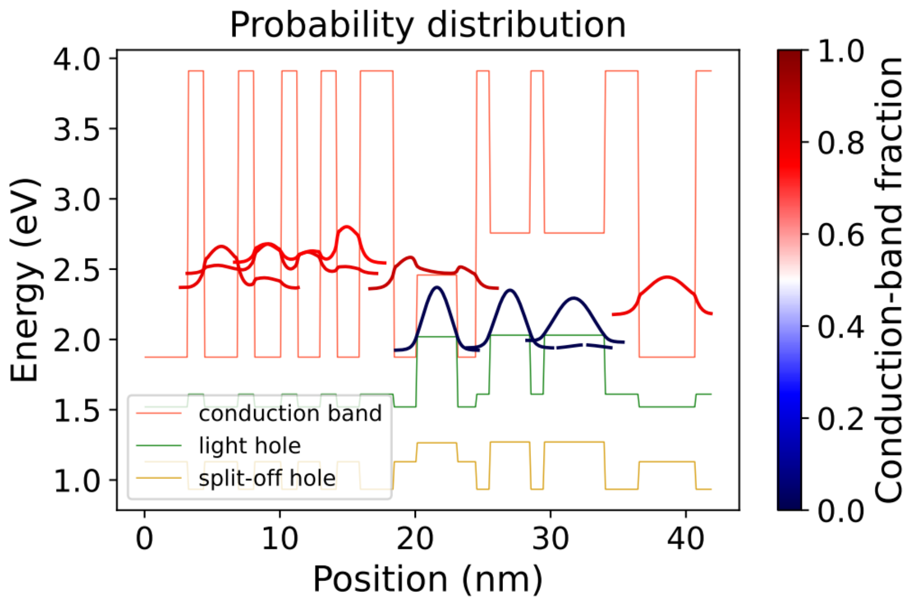
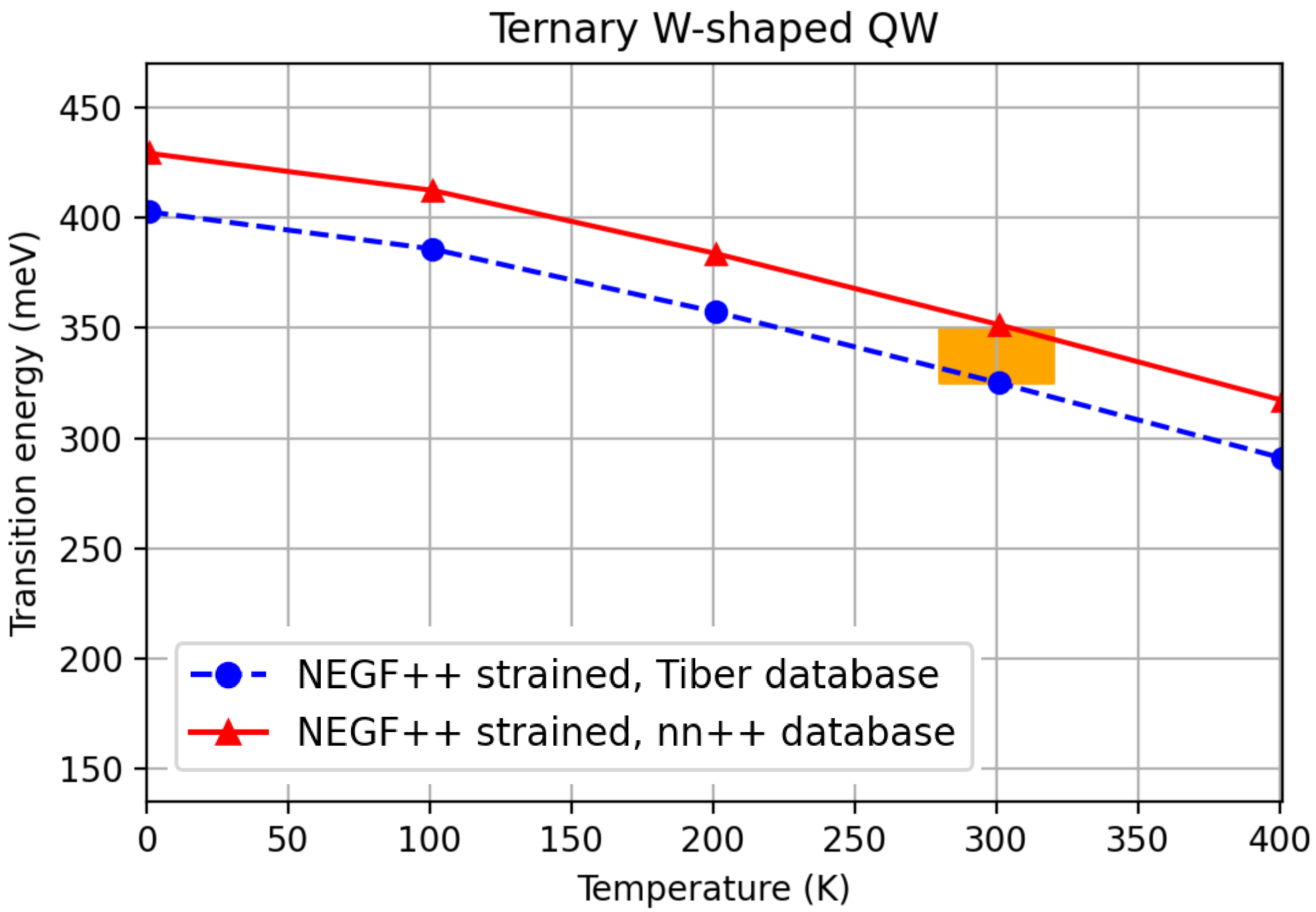
Measurement:
325 – 350 meV (3.6 - 3.9 µm)
Vurgaftman, *et al.*, Nat. Comm. (2012)





Tunneling charge transport

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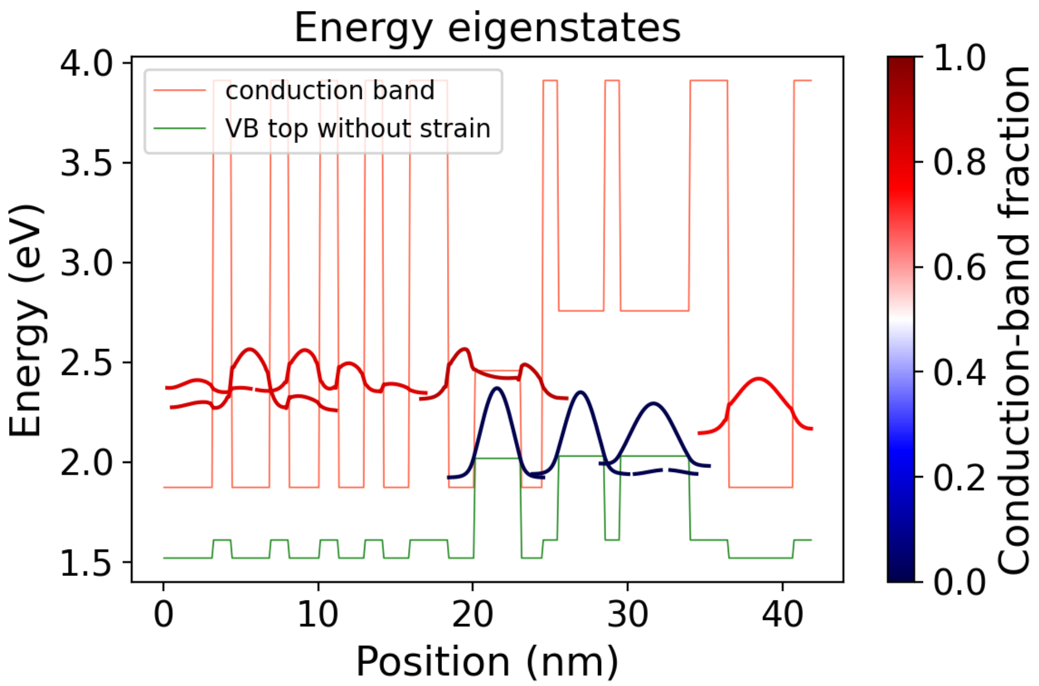
Accuracy

Reduce
problem size

Interband



Tunneling charge transport

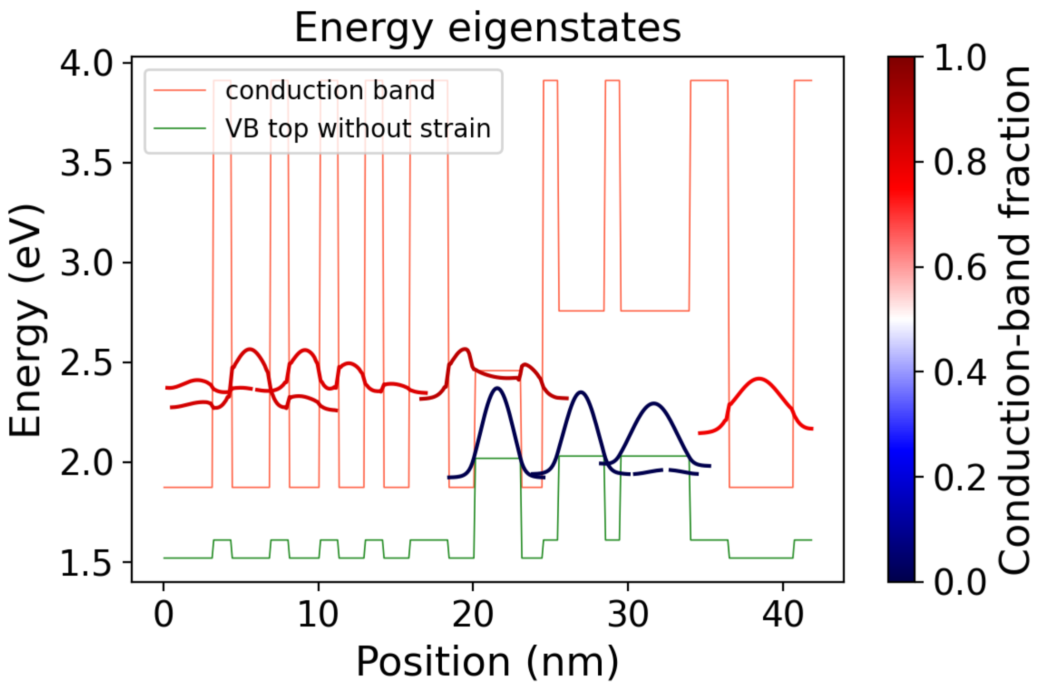
Accuracy

Reduce problem size

$$G^{<}(\boldsymbol{r}_1, \boldsymbol{r}_2; t_2 - t_1)$$

- Solve 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model
- Position eigenstates basis

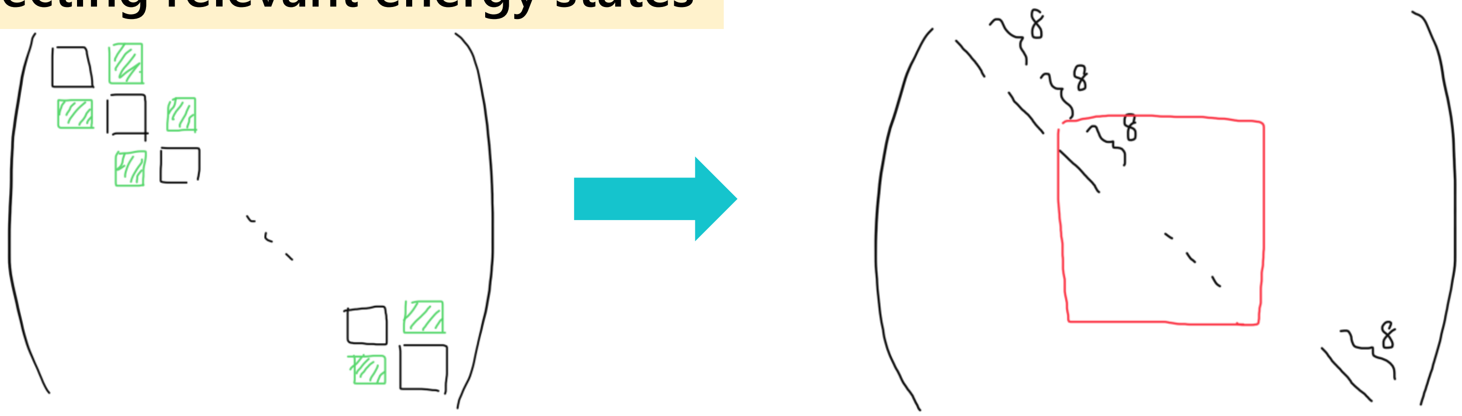
Interband



Reduced Real Space basis

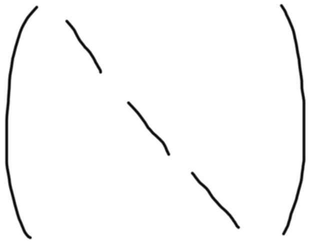
1. Reduce size by selecting relevant energy states

$H_0 =$

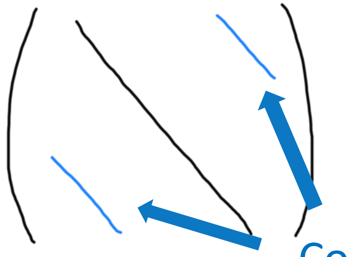


2. Diagonalize reduced position operator

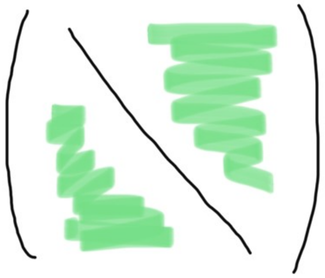
$PH_0P =$



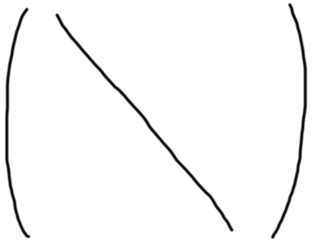
$U^\dagger PH_0PU =$



$PzP =$



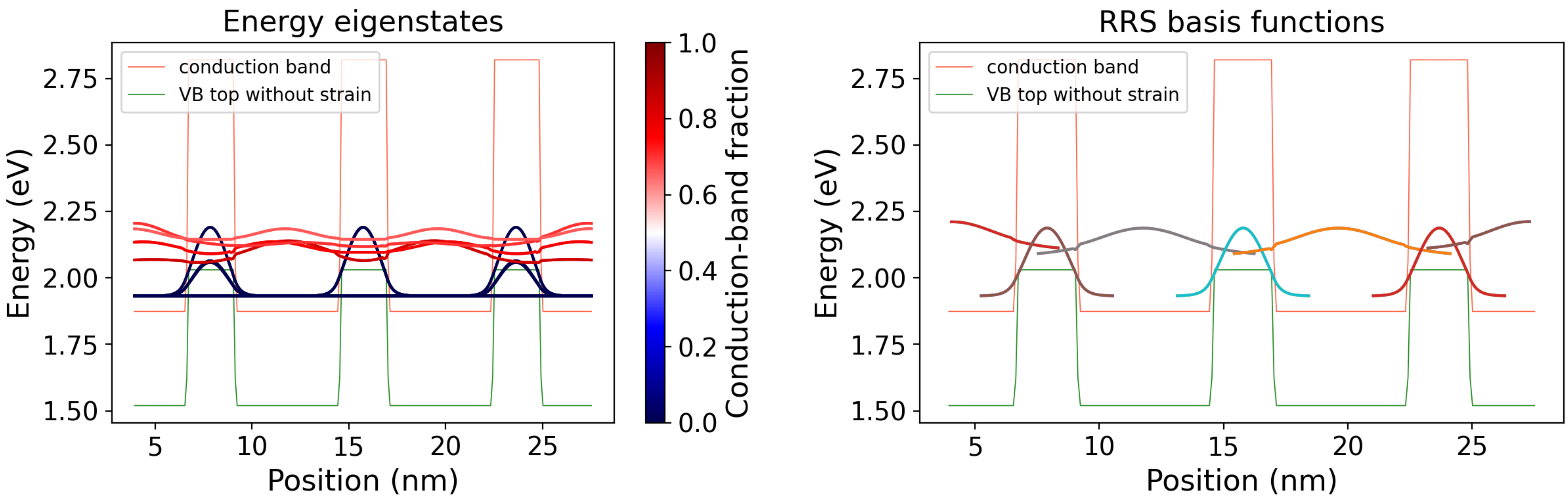
$U^\dagger PzPU =$



Position eigenbasis

Reduced Real Space basis

InAs/GaSb SLs



Basis set ready for NEGF

Summary

III-Sb broken-gap tunneling devices – photodetector, lasers

Accuracy

- NEGF for non-equilibrium charge distribution
- 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ solutions to account for interband coupling & nonparabolicity
- Consistent discretization of differential operators

Reduce problem size

- Position eigenstates reflecting interband coupling

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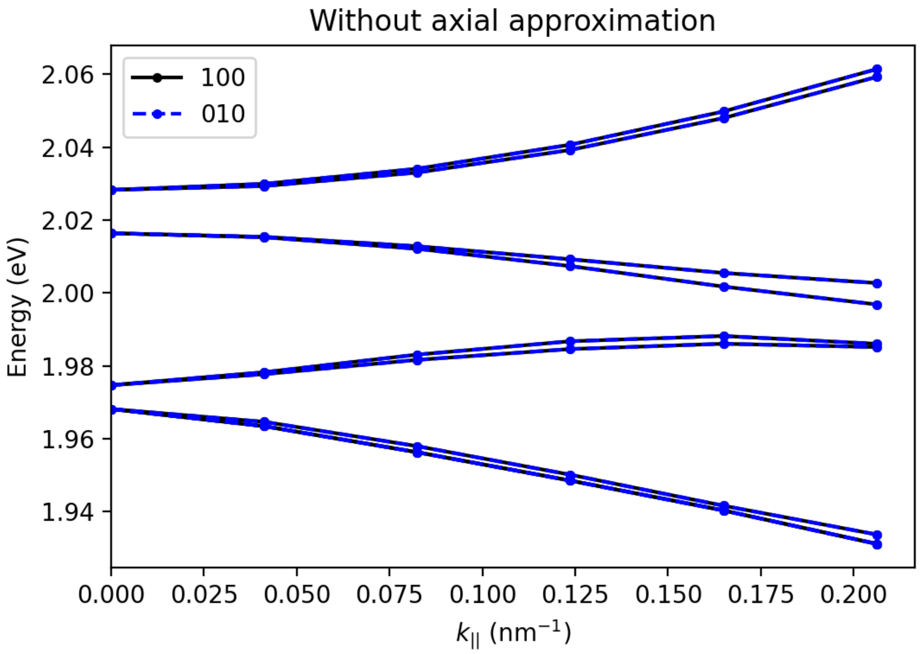
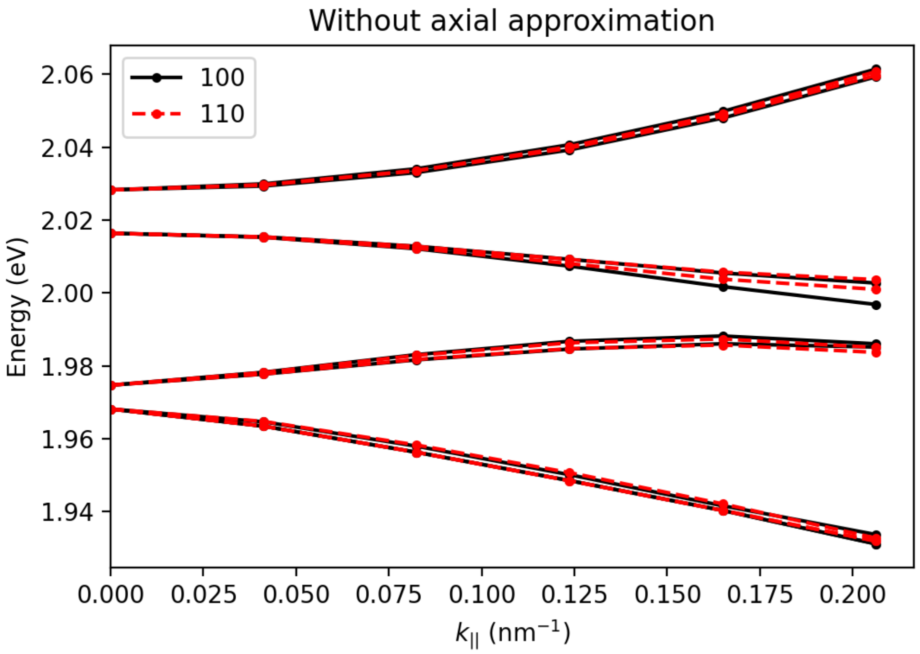
Quantum Semiconductor Technologies exploiting Antimony

MSCA-ITN-2020 Funding Scheme from the European Union's Horizon 2020 programme under Grant agreement ID: 956548

In-plane anisotropy

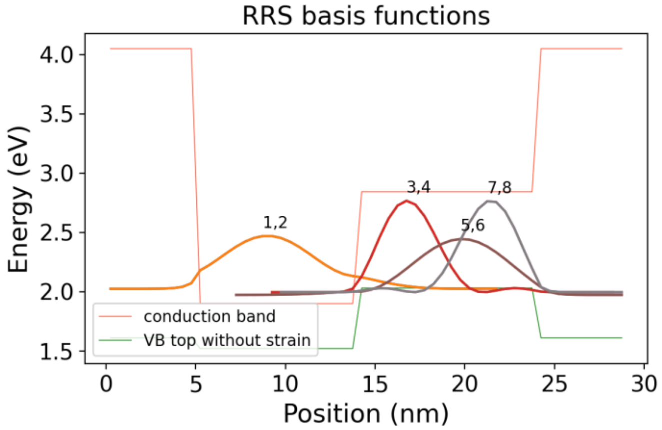
- Unlike nonparabolicity, in-plane anisotropy isn't significant.



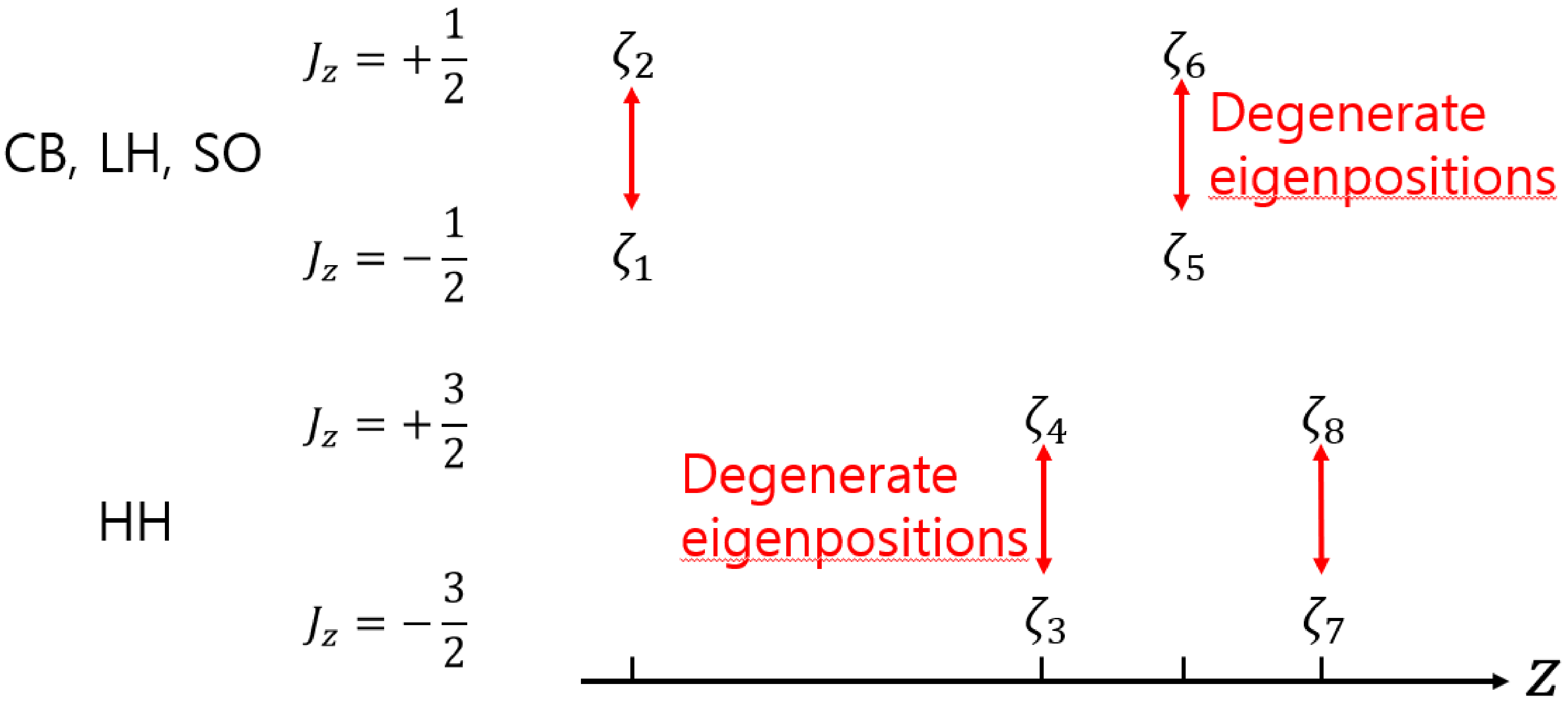


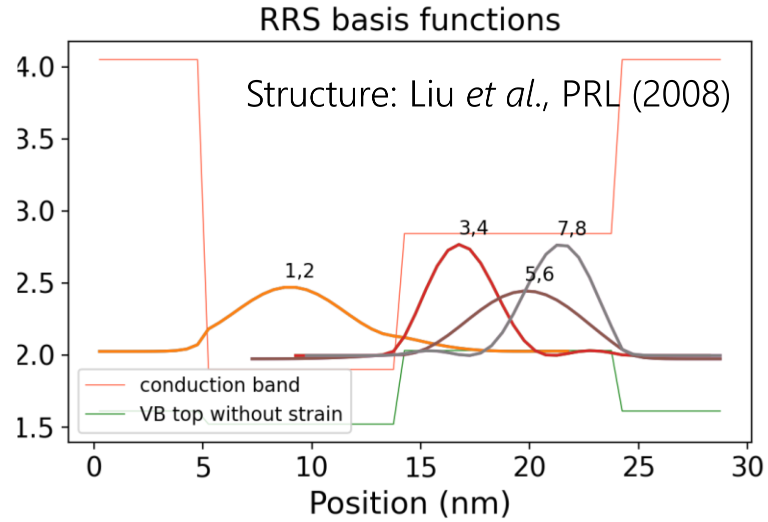
AlSb/InAs/GaSb/AlSb

Structure: Liu *et al.*, PRL (2008)



Degeneracy & coupling in Reduced Real Space





Degeneracy & coupling in Reduced Real Space

CB, LH, SO

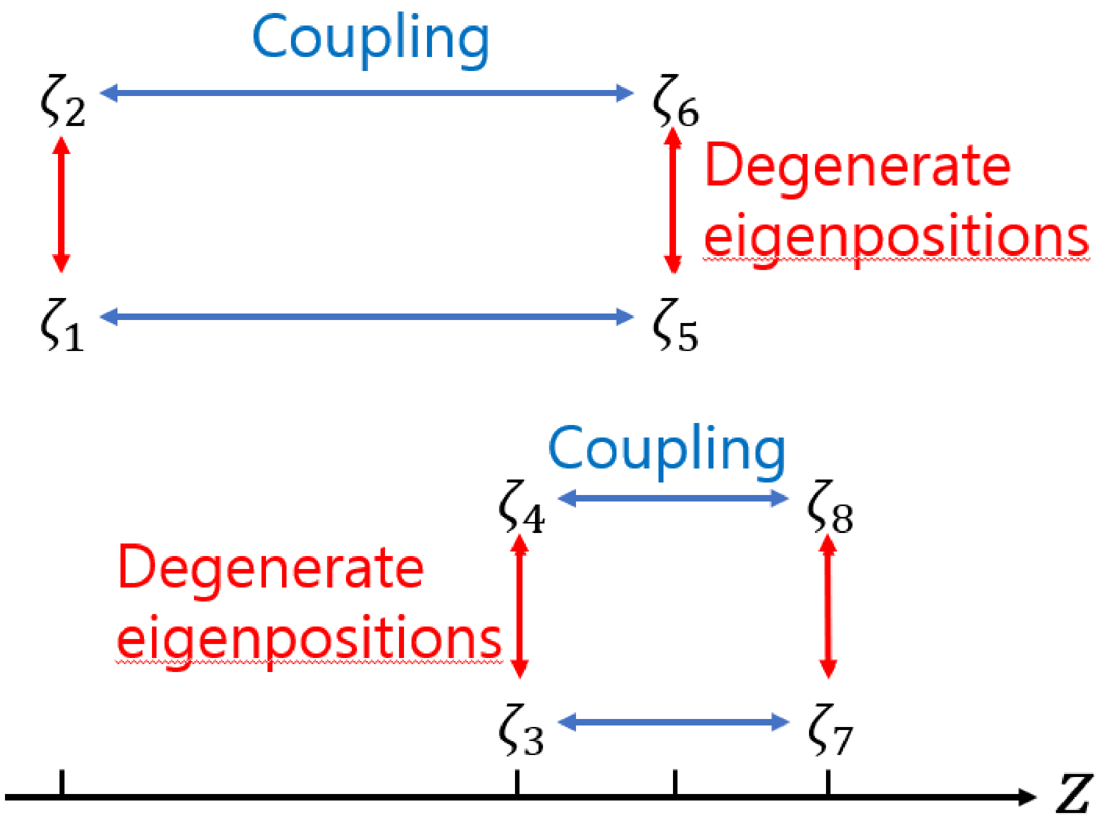
$J_z = +\frac{1}{2}$

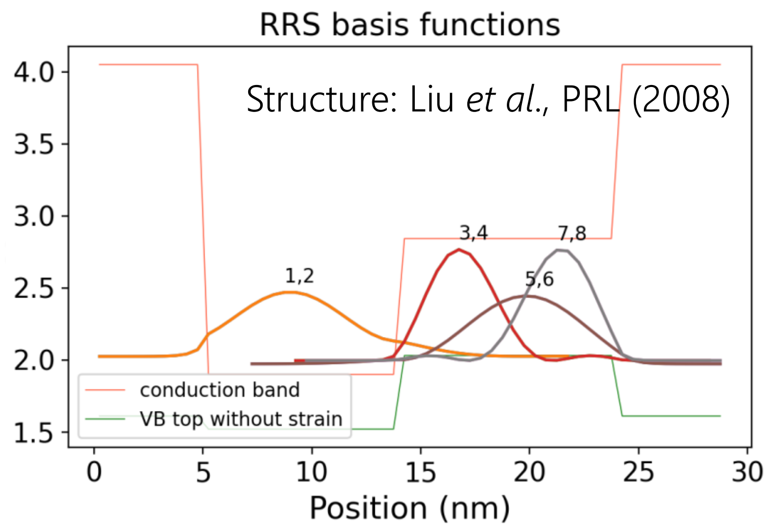
$J_z = -\frac{1}{2}$

HH

$J_z = +\frac{3}{2}$

$J_z = -\frac{3}{2}$





Degeneracy & coupling in Reduced Real Space

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$J_z = +\frac{1}{2}$

CB, LH, SO

$J_z = -\frac{1}{2}$

$J_z = +\frac{3}{2}$

HH

$J_z = -\frac{3}{2}$

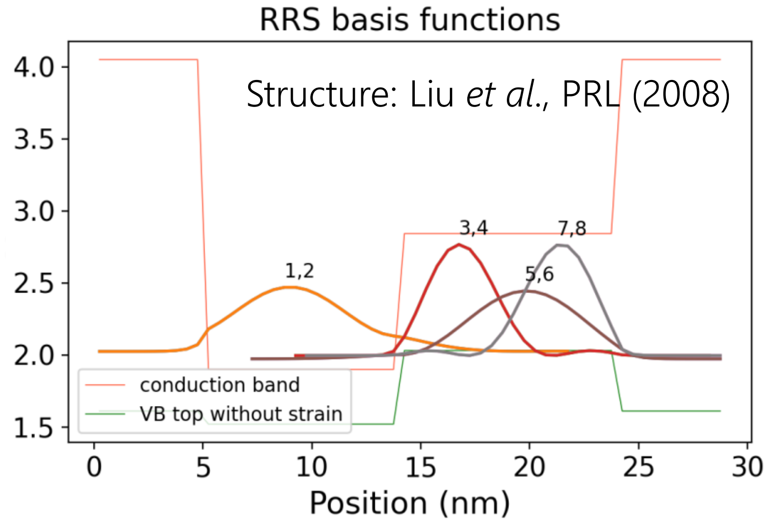
Coupling

$\zeta_2 \leftrightarrow \zeta_6$

Coupling

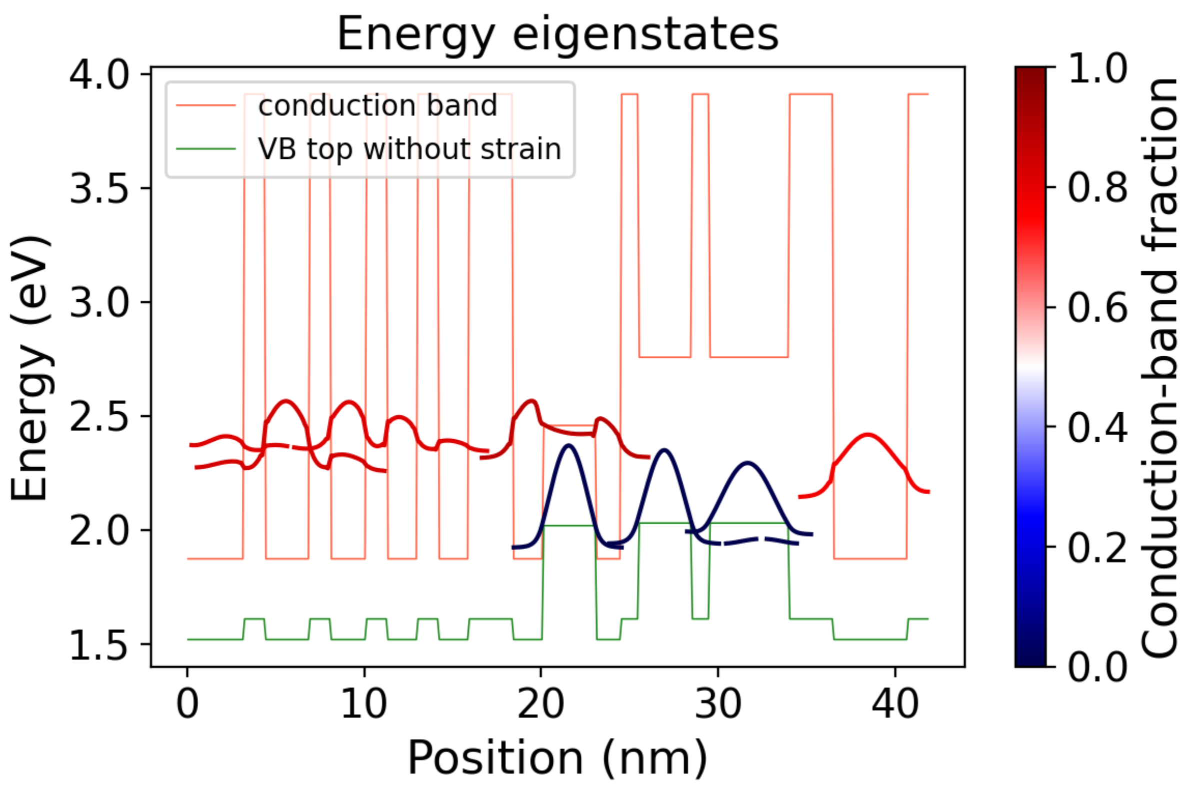
$\zeta_4 \leftrightarrow \zeta_8$

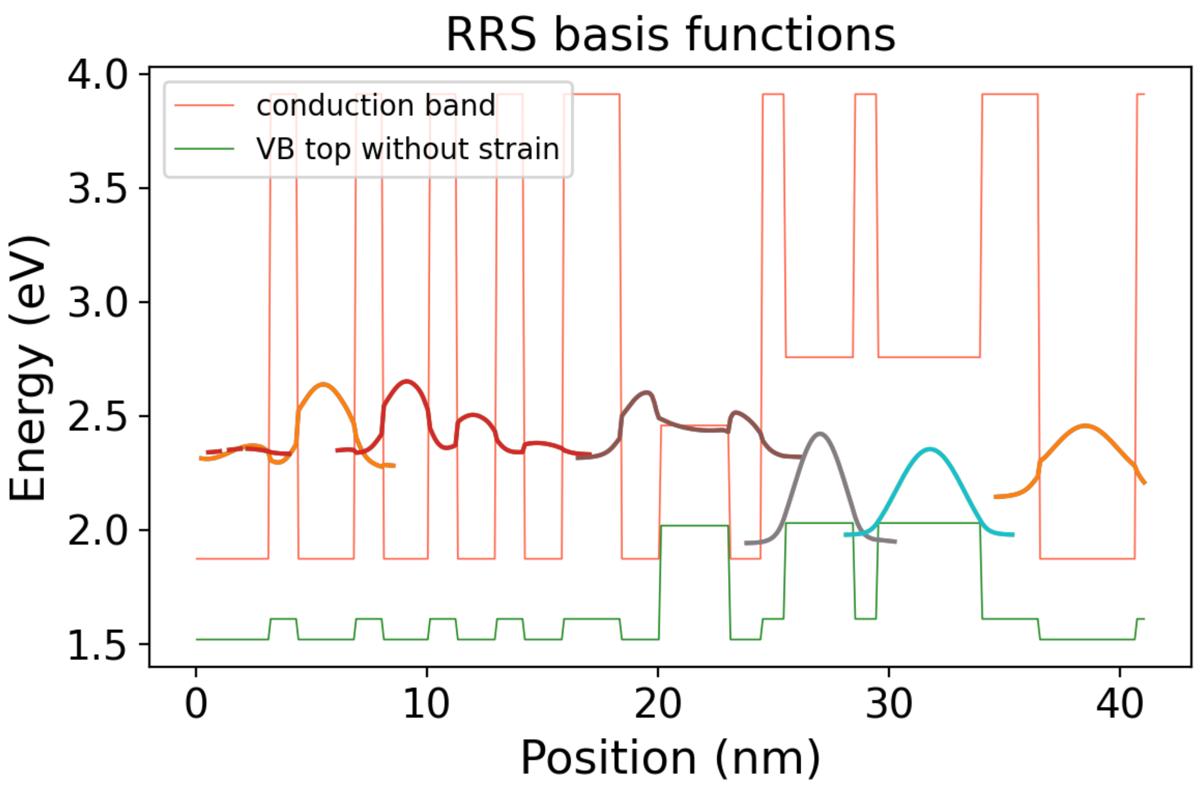
z



Reduced Real Space basis

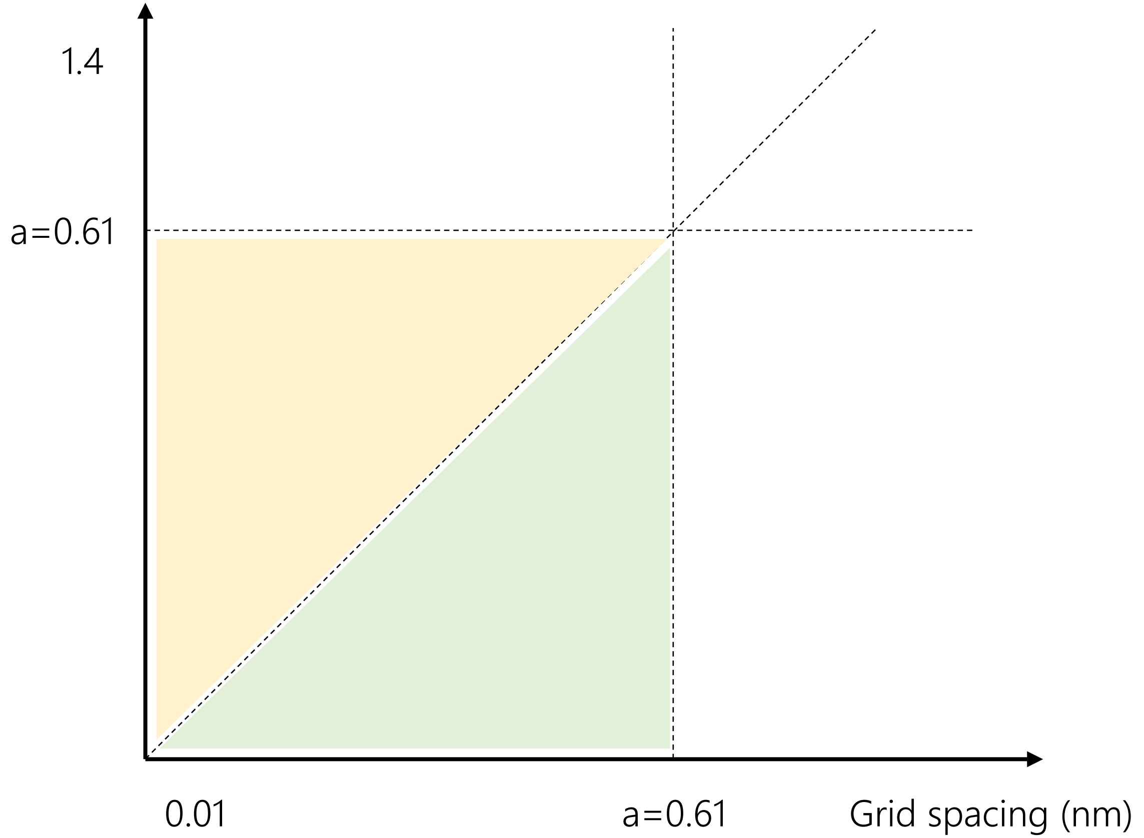
InAs/GaInSb ICLs



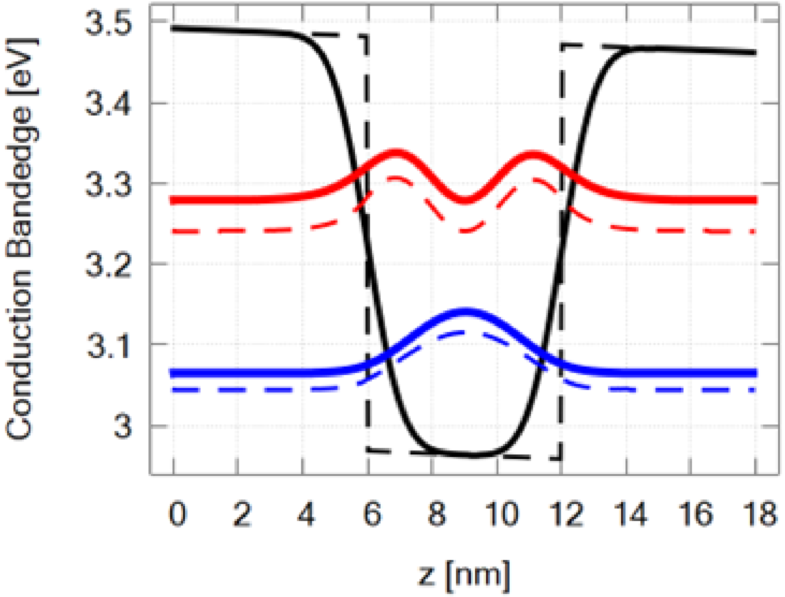


Structure: Vurgaftman *et al.*, Nat. Comm. (2012)

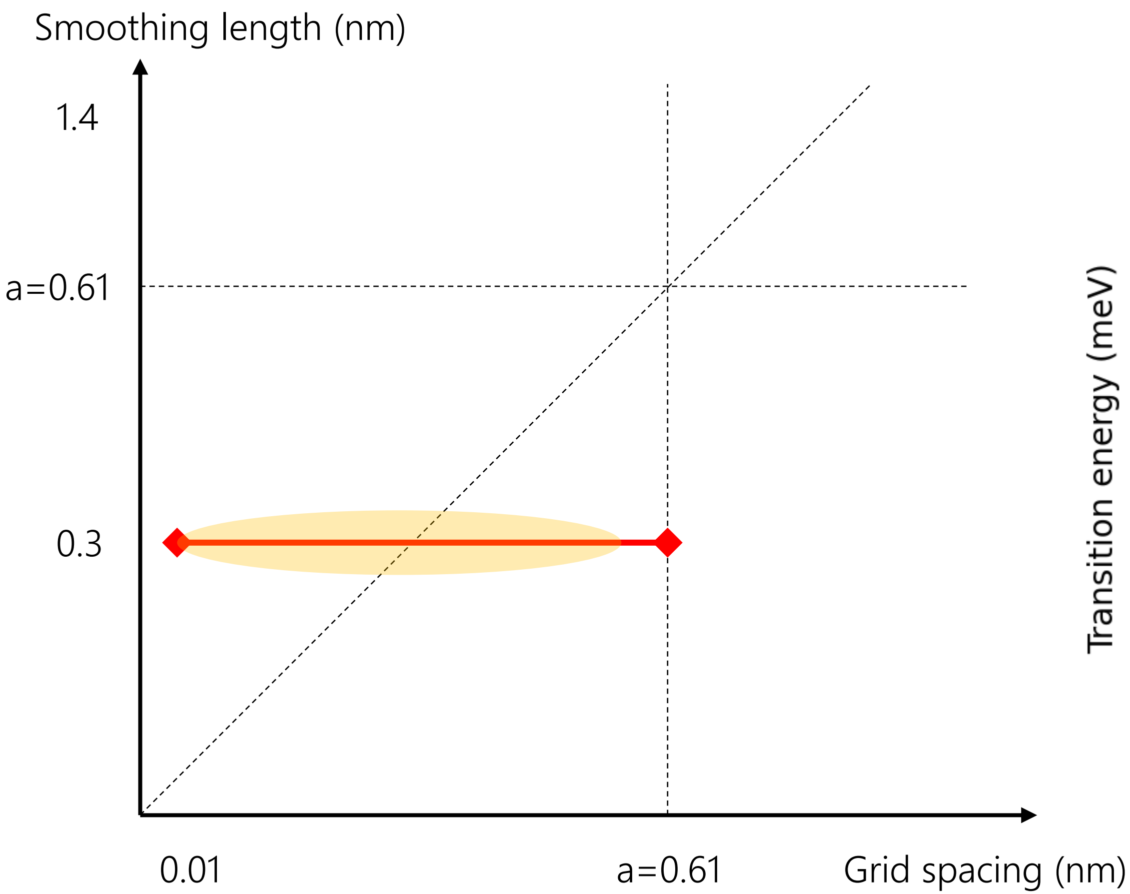
Transition energy in W-shaped QW

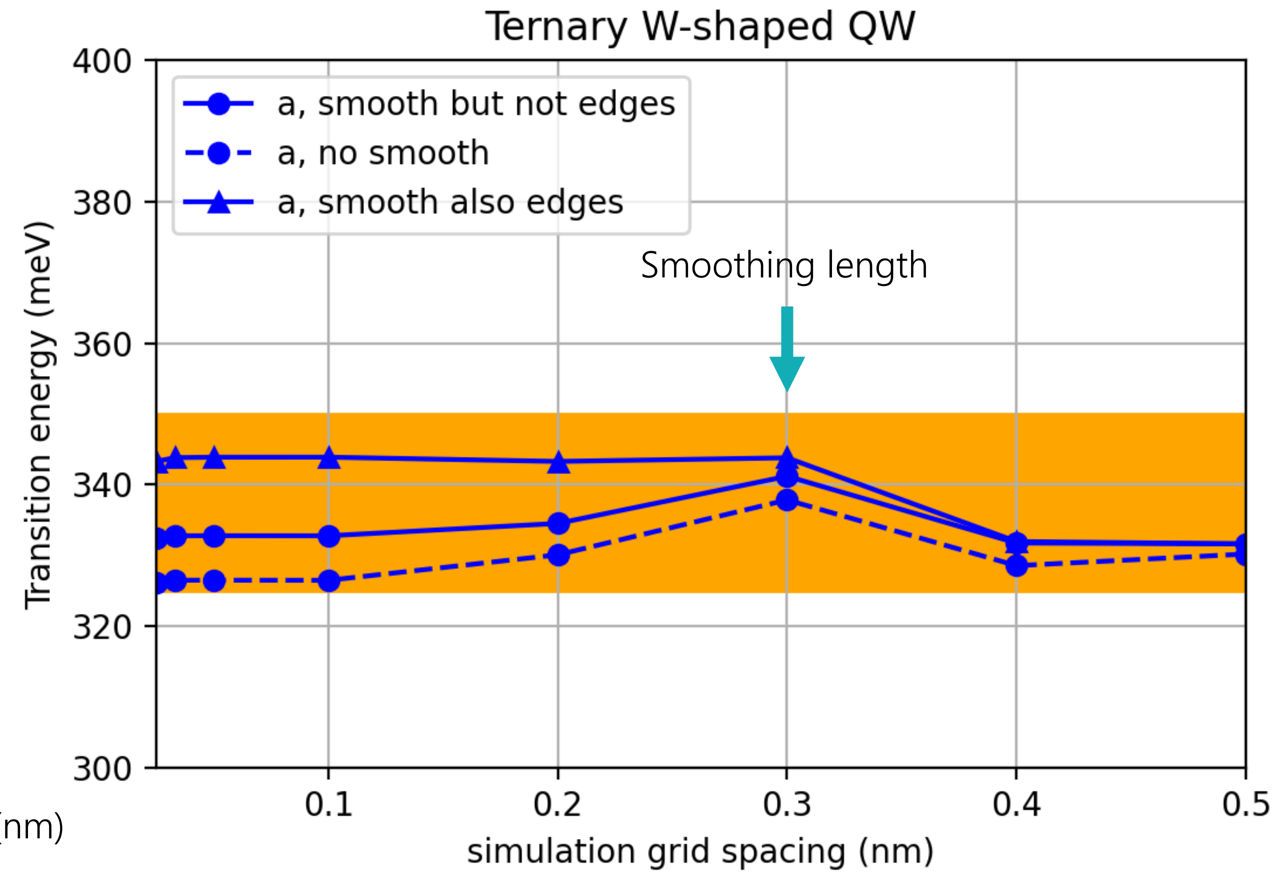


Smoothing of material parameters



Transition energy in W-shaped QW





Transition energy in W-shaped QW

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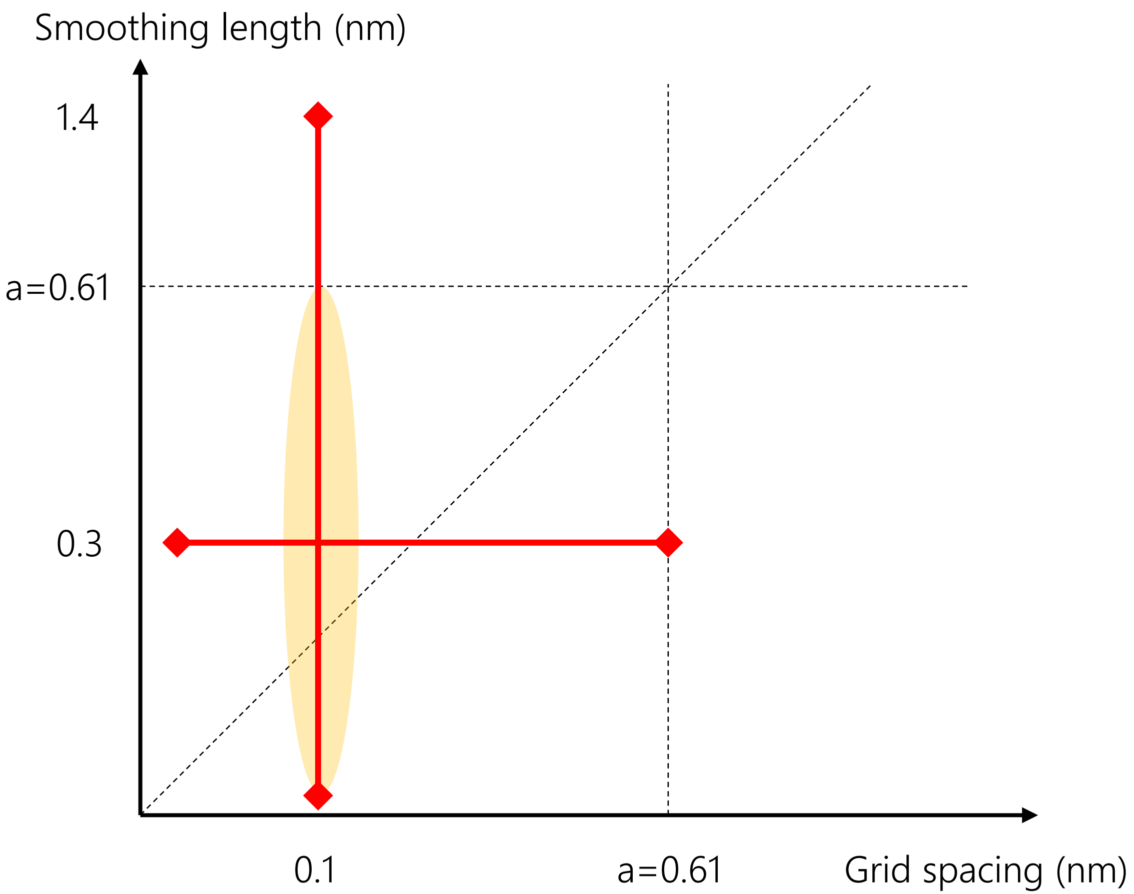
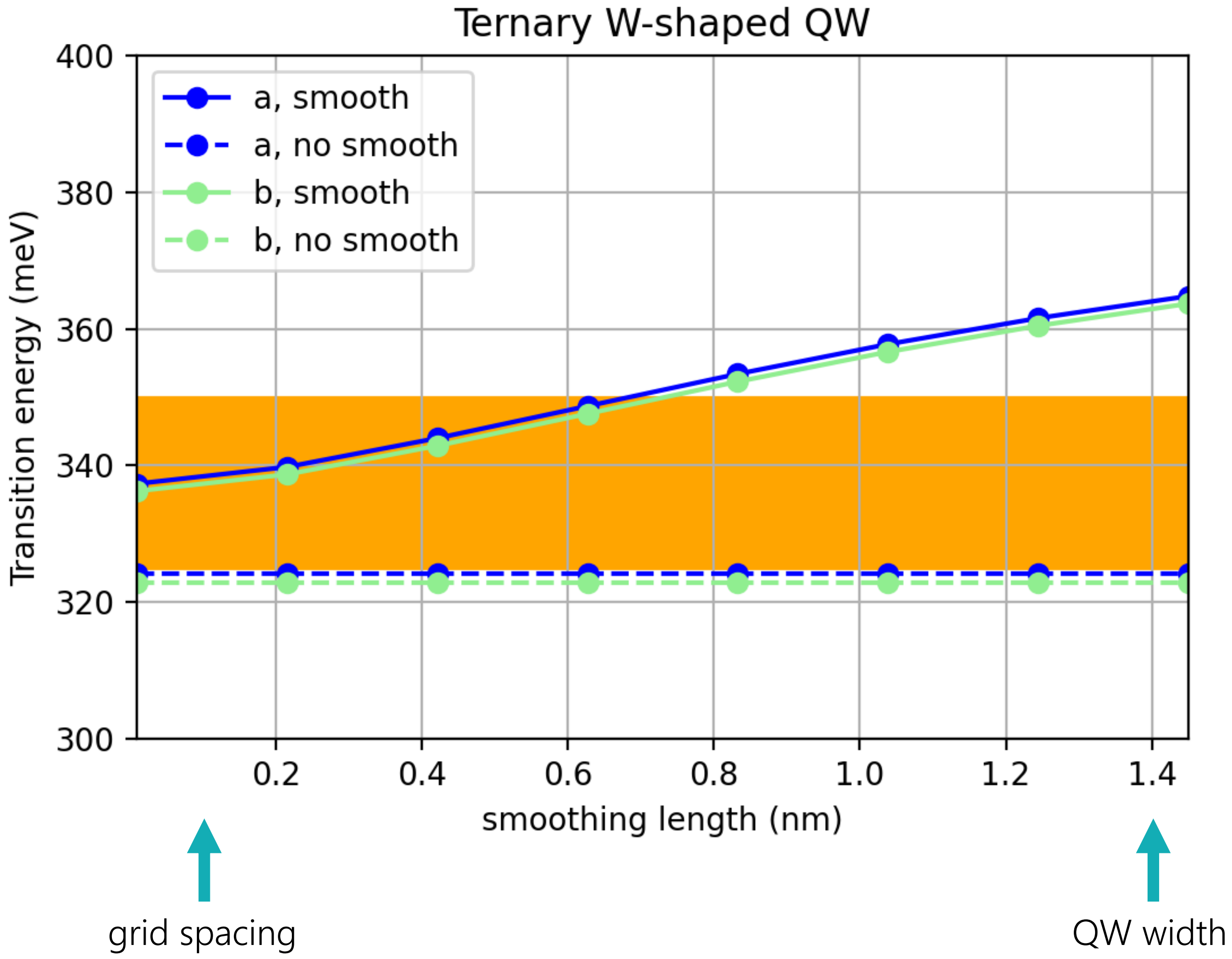
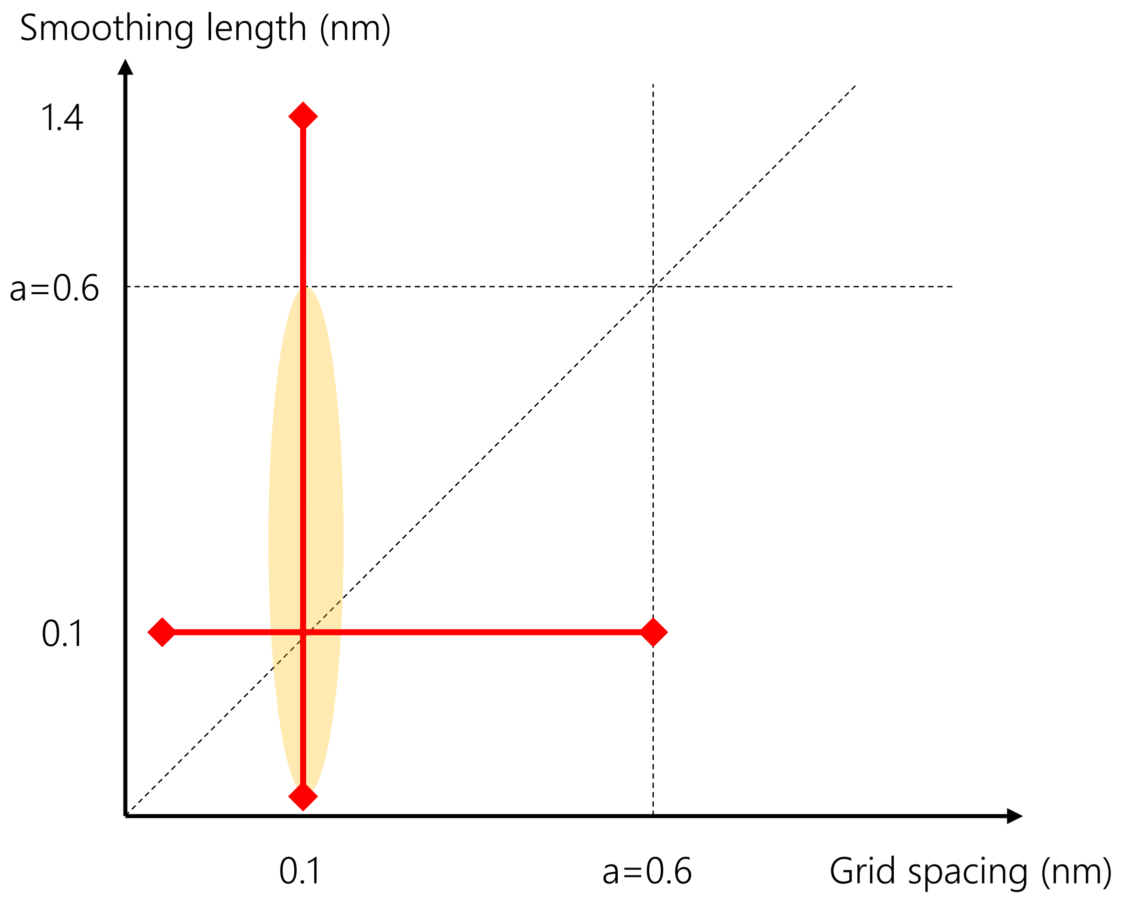
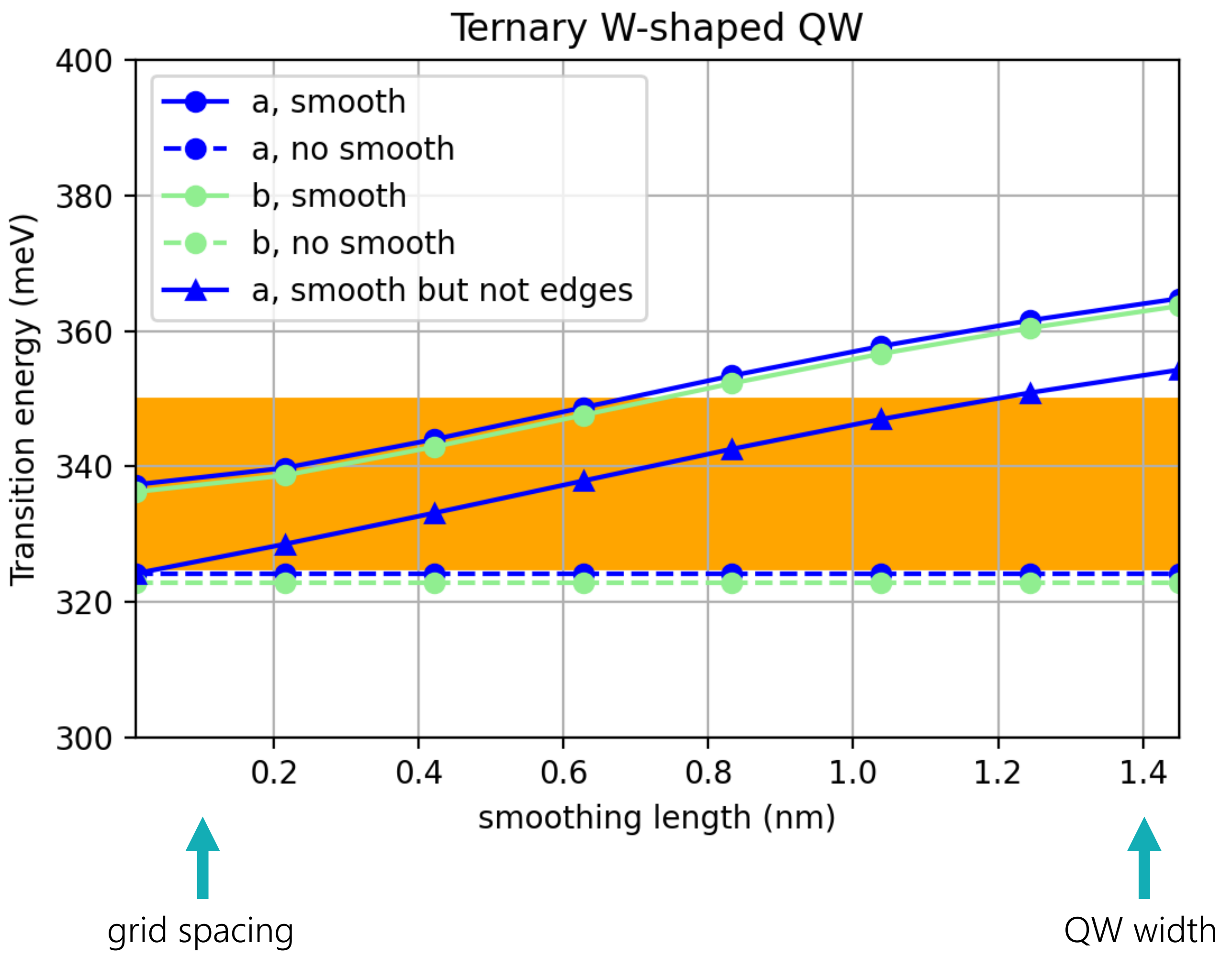


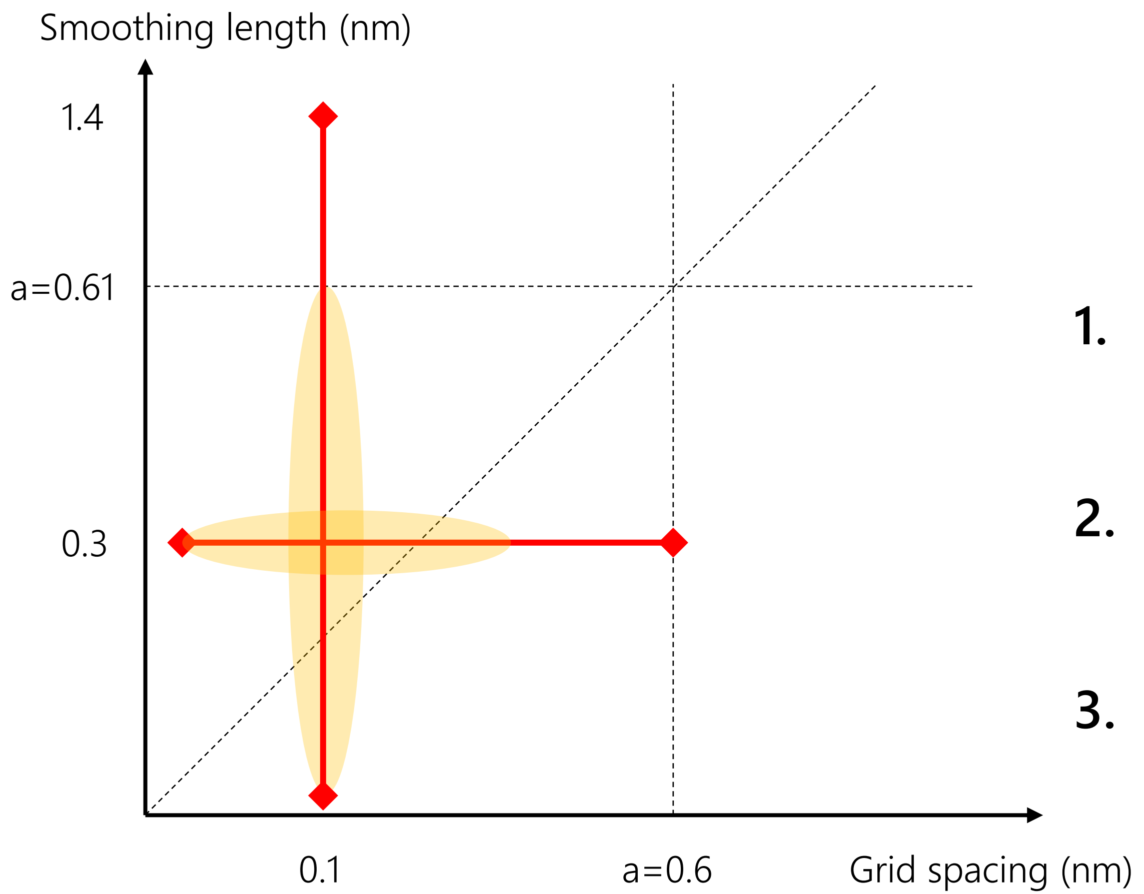


Validity of bandedge smoothing





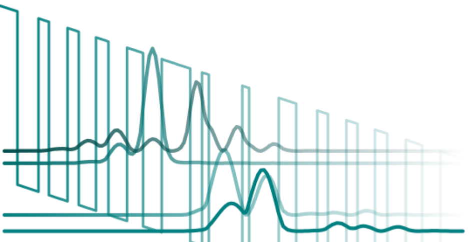
Transition energy in W-shaped QW



1. **If kept < lattice const., numerical parameters do not change results significantly.**

2. **Choice of (a) or (b) does not affect results significantly if numerical parameters < lattice const.**

3. **Small smoothing seems necessary (and justifiable) to avoid jump of wave functions at the material interface.**



Note: bandedge calculation

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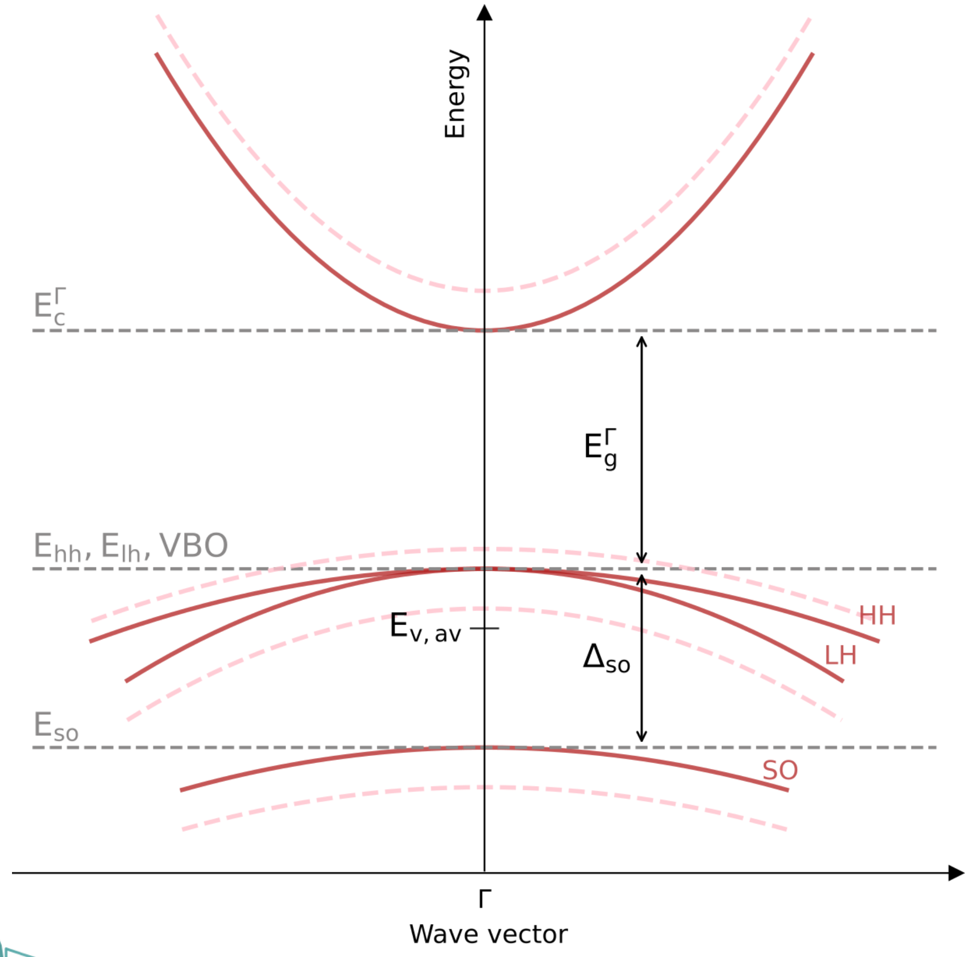

Option 1 (nn3, nn++, nnNEGF):

$$E_c = E_{\mathrm{v,av}} + E_g(T) + \Delta_{\mathrm{SO}}/3$$

Option 2 (nnNEGF):

$$E_{\mathrm{hh,lh}} = E_c - E_g(T)$$

$$E_{\mathrm{SO}} = E_c - E_g(T) - \Delta_{\mathrm{SO}}$$

Option 3 (nn3):

$E_{\mathrm{v,av}}$ and E_c given in database

Ec in the database is for T=0K.
However, Varshni correction is applied to Ec in the code.