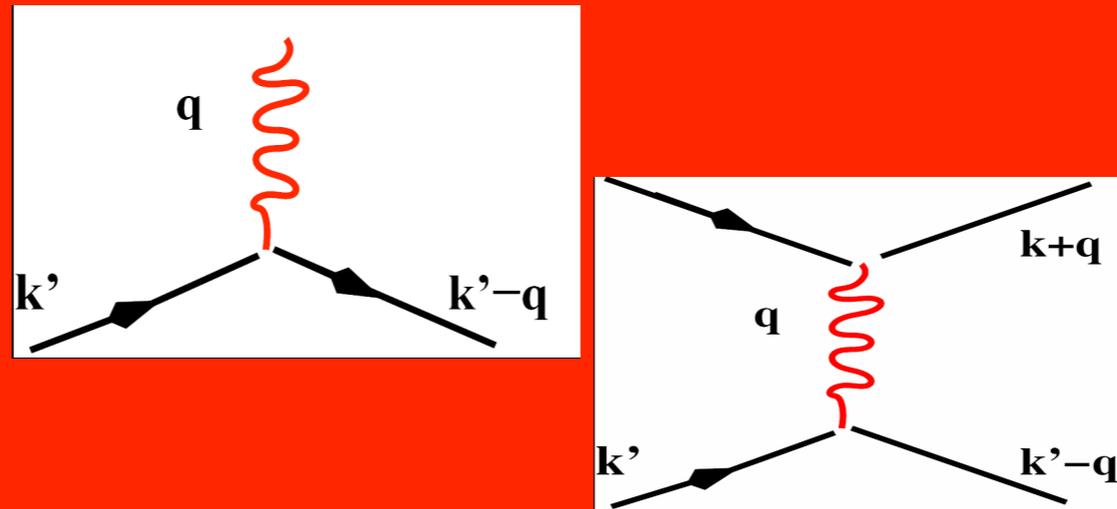


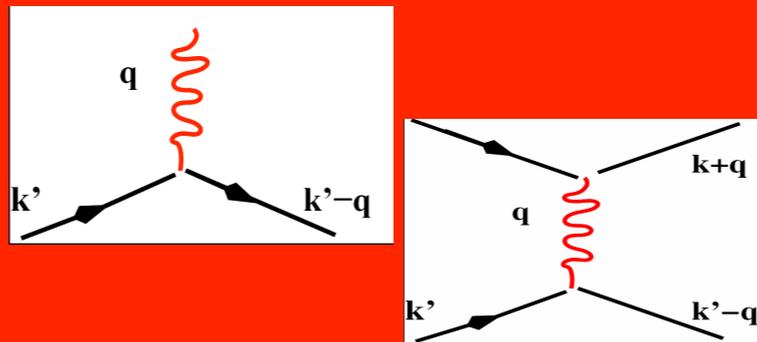
# Minimizing negative and maximizing positive effects of electron scattering



Inès Montaña, M.C. Wanke, C.T. Fuller, and J.L. Reno

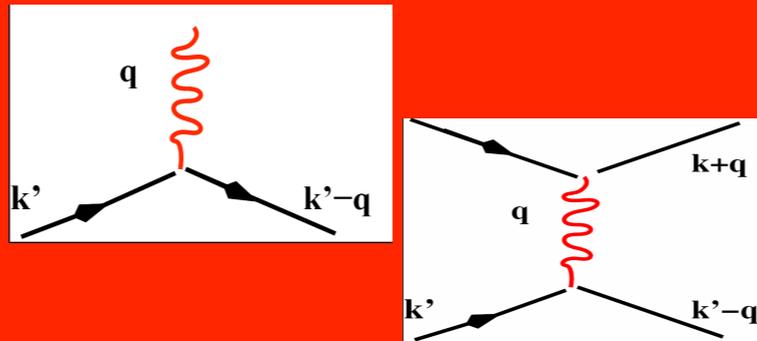
Sandia National Laboratories

Minimizing negative  
and  
maximizing positive  
effects of electron scattering



300–500 nm Photocathodes (???)

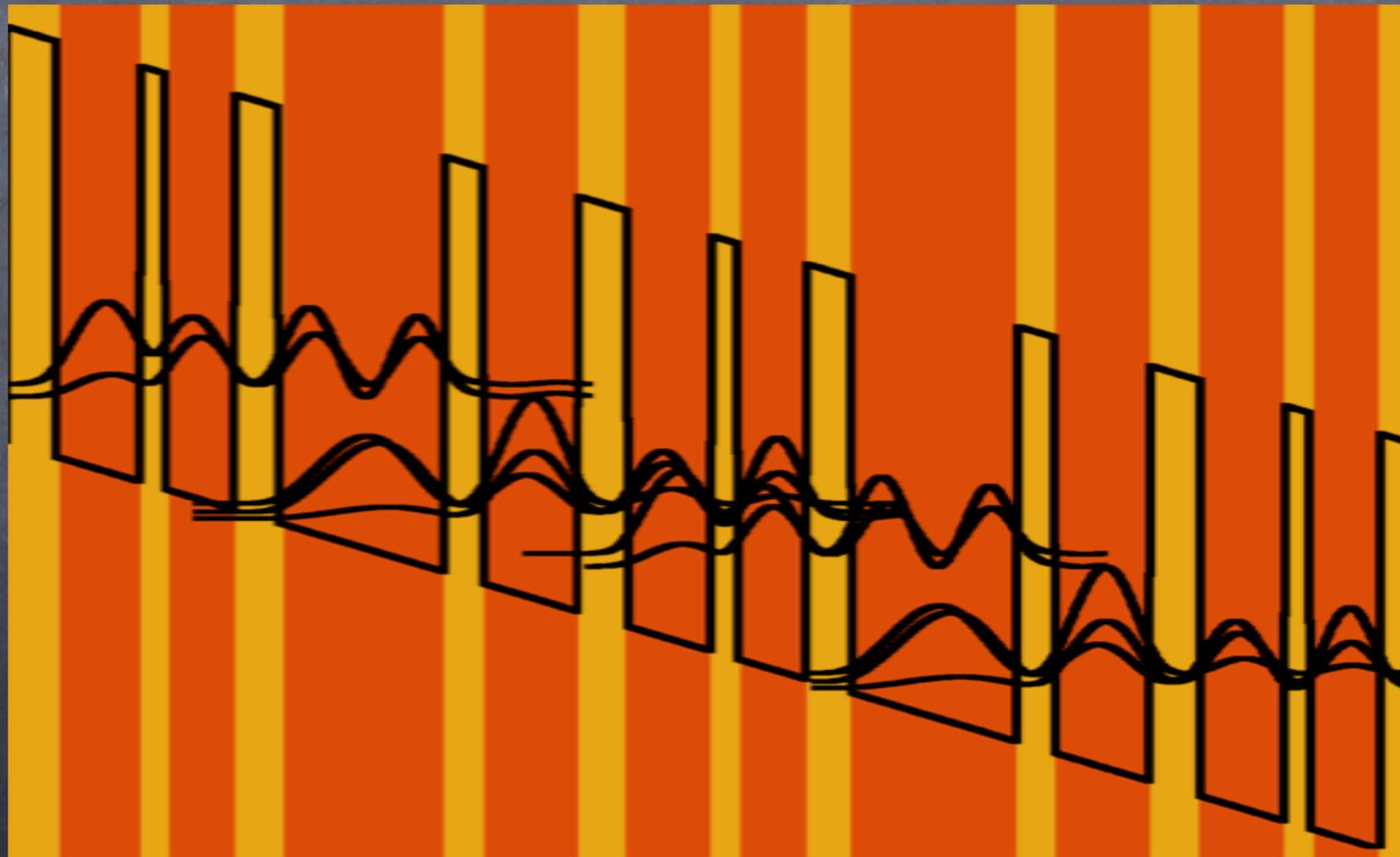
Minimizing negative  
and  
maximizing positive  
effects of electron scattering



Quantum Cascade Lasers !!!

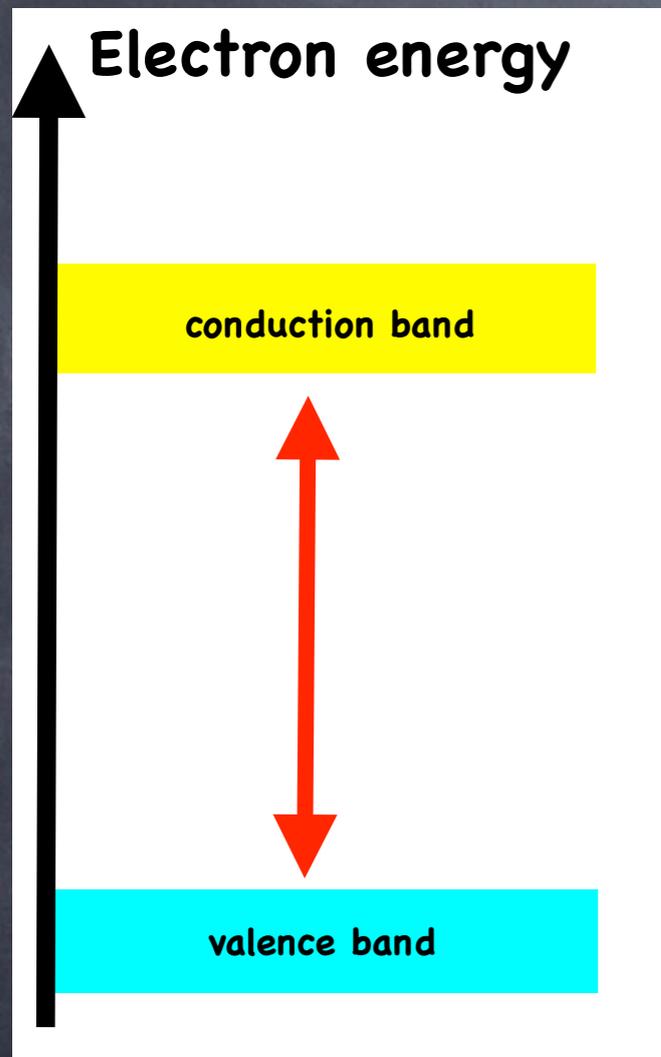
300–500 nm Photocathodes (???)

Quantum Cascade Laser: "Engineered collection of quantum wells with discrete eigenstates"

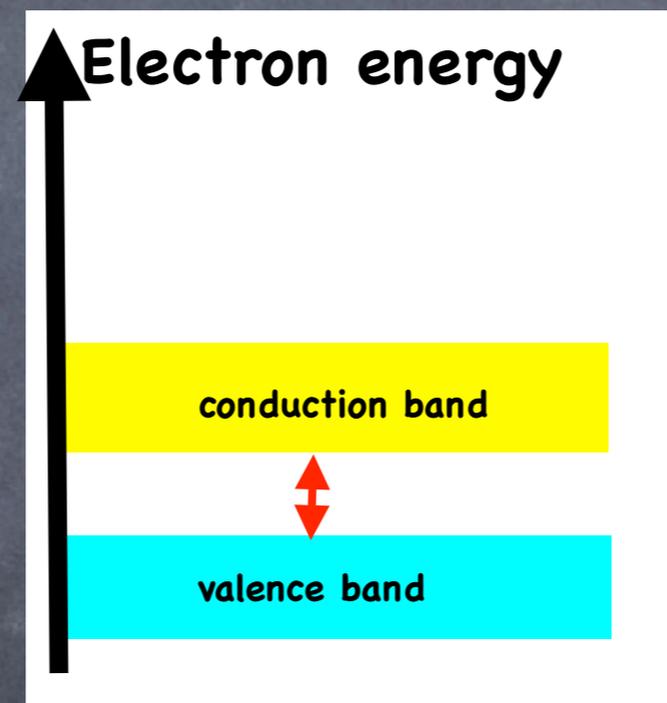


and it all comes down to the ...

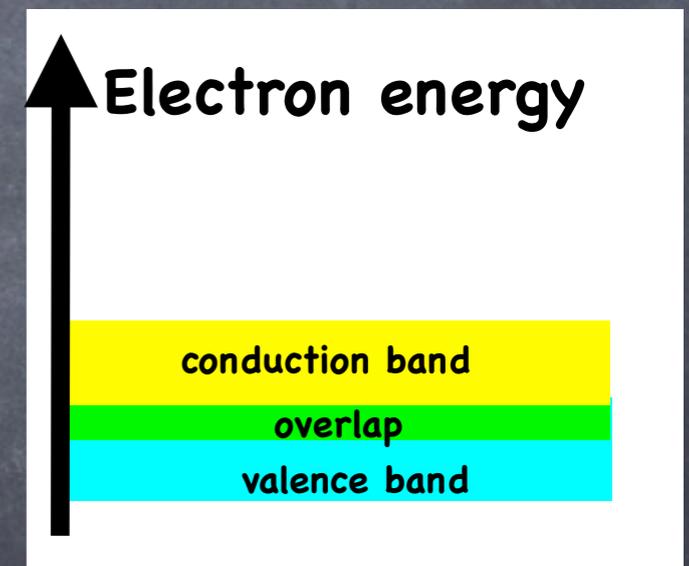
**energy gap** (forbidden zone) !!!



insulator

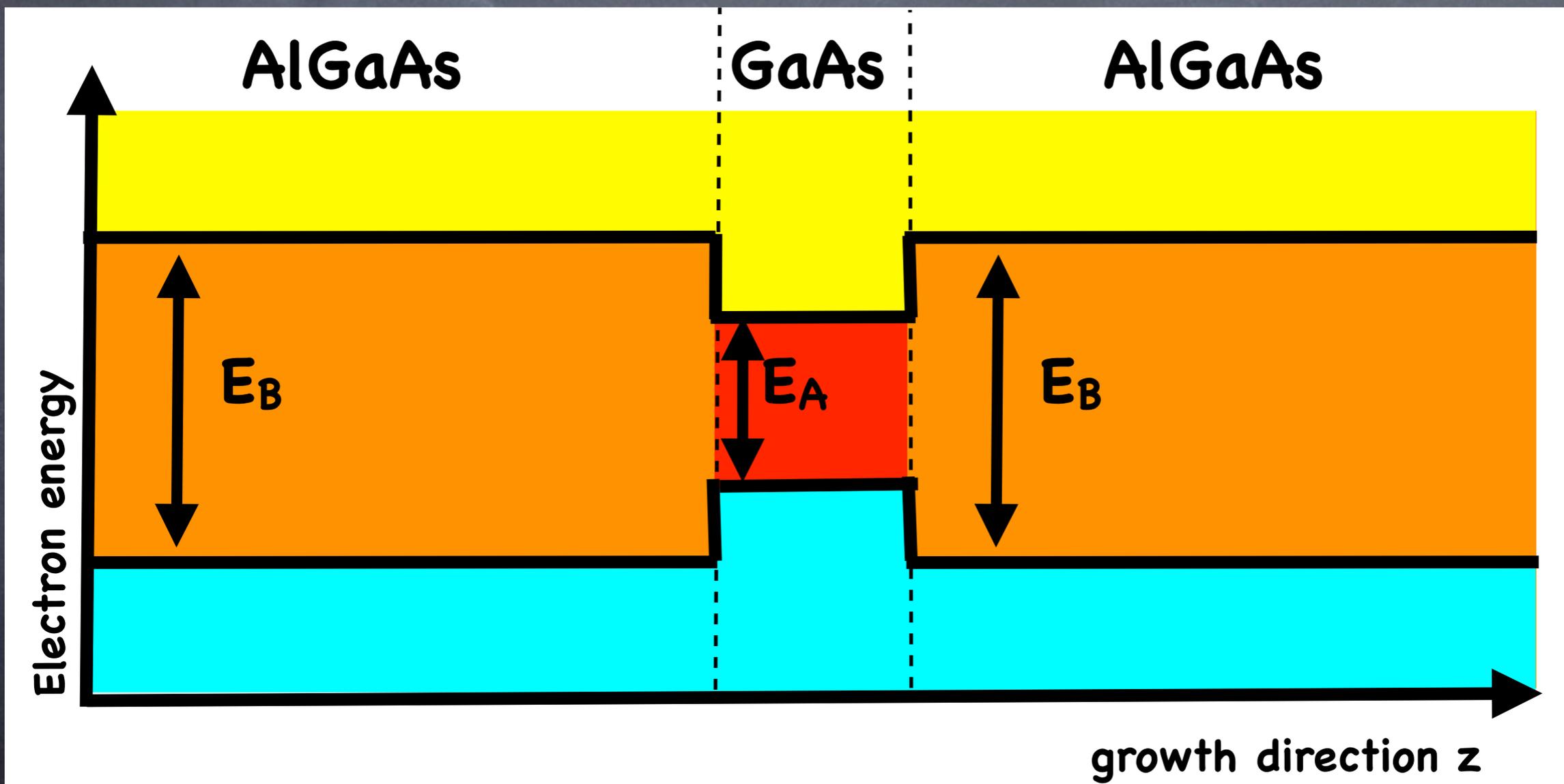


semiconductor

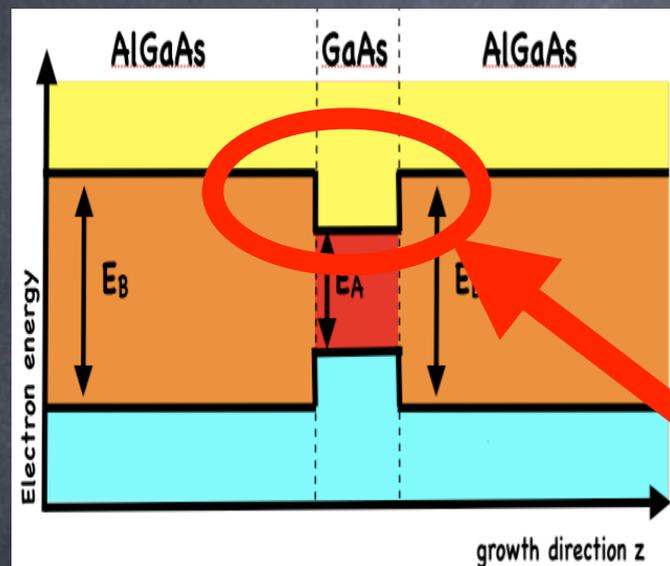


conductor

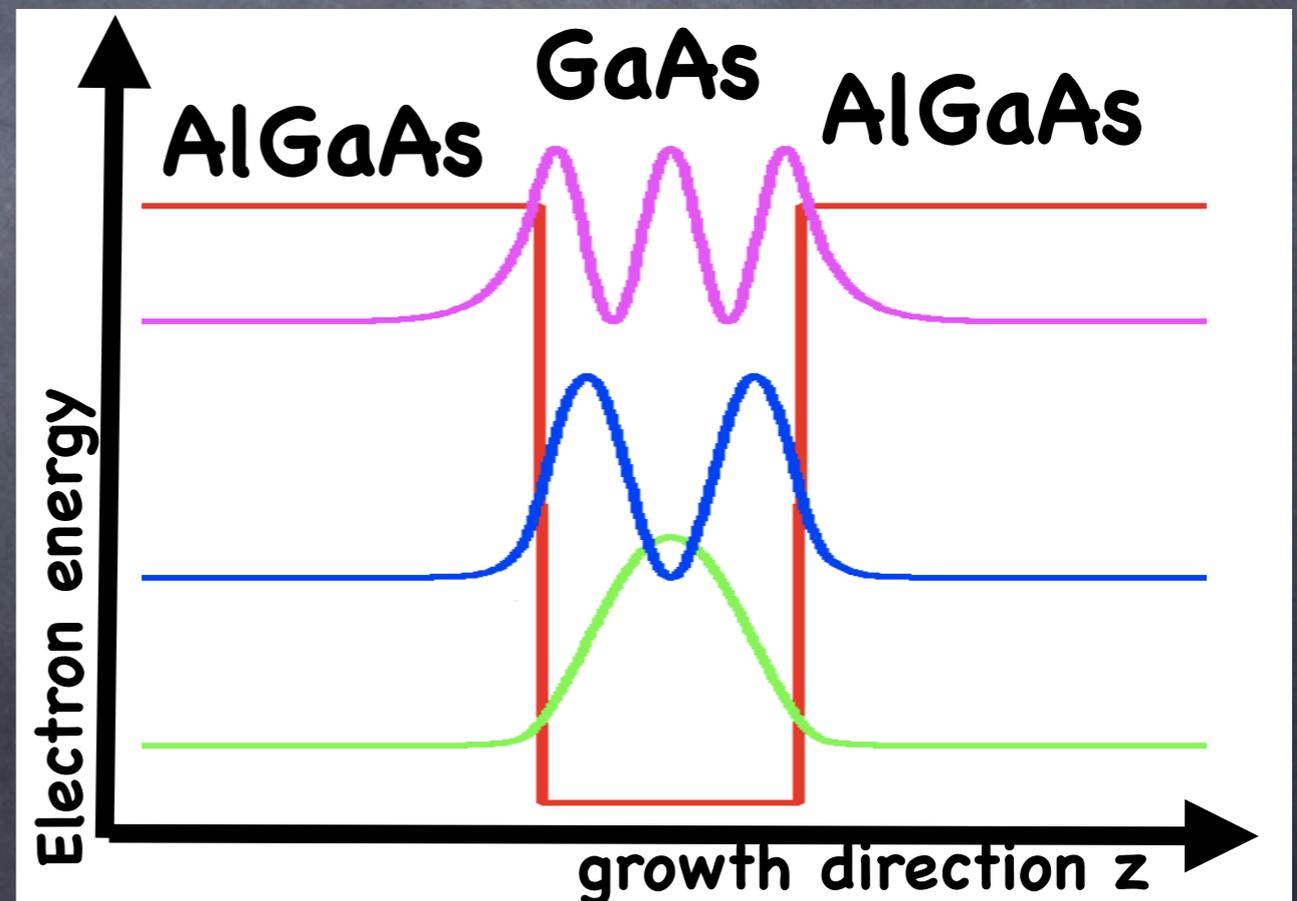
grow a layer of one semiconductor, e.g. GaAs ...  
... between two layers  
of another semiconductor, e.g. AlGaAs



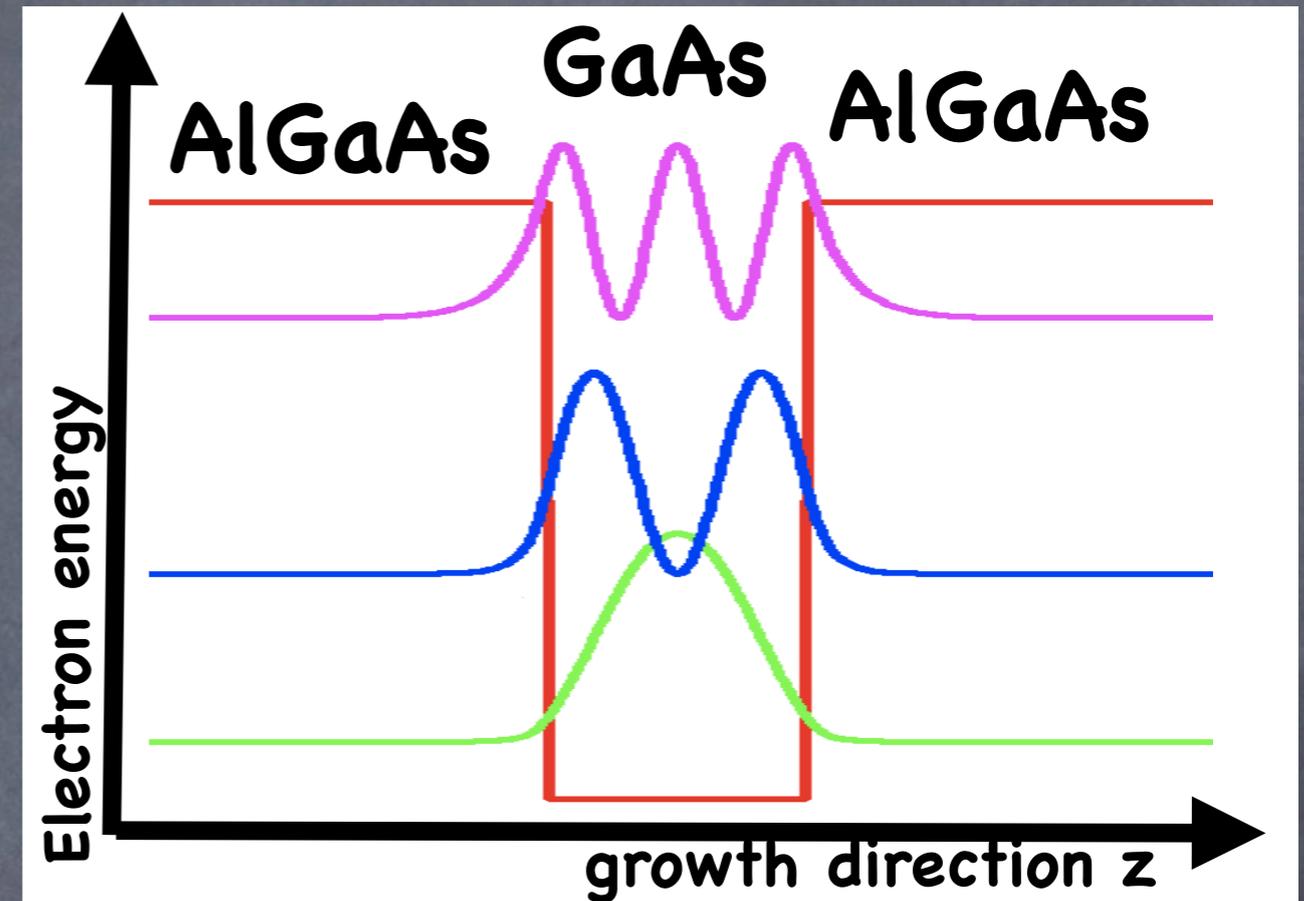
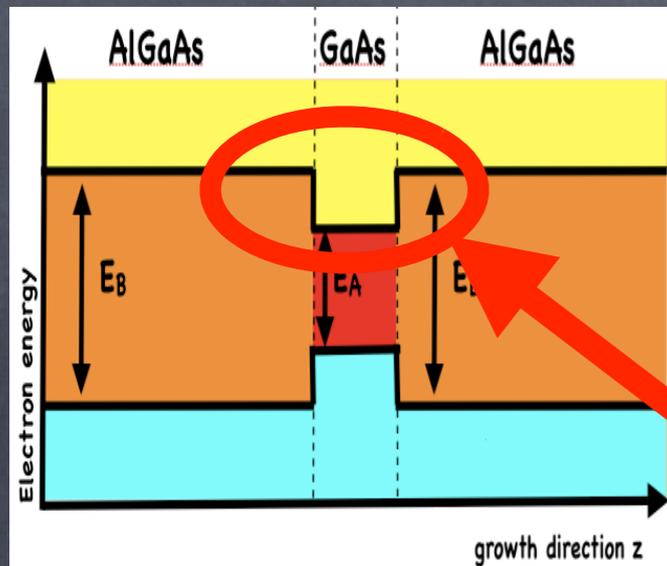
grow a layer of one semiconductor, e.g. GaAs ...  
... between two layers  
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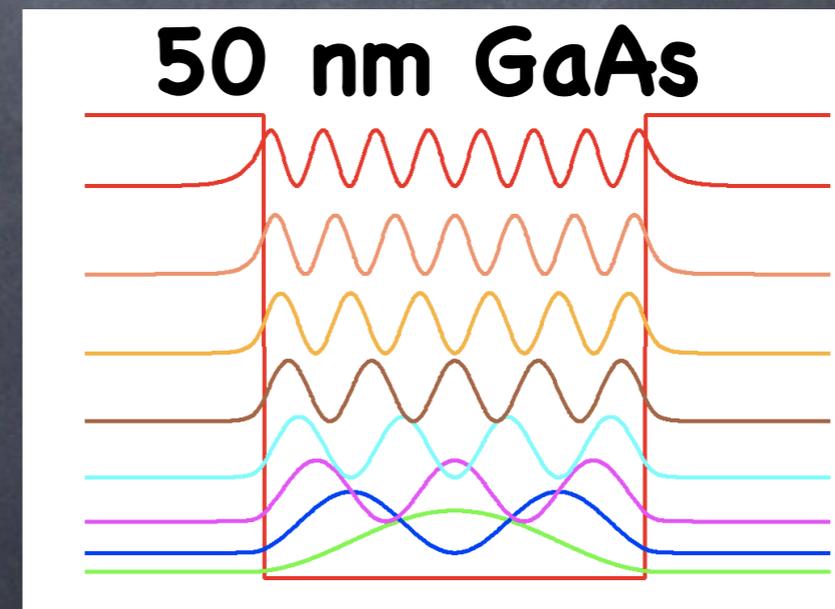
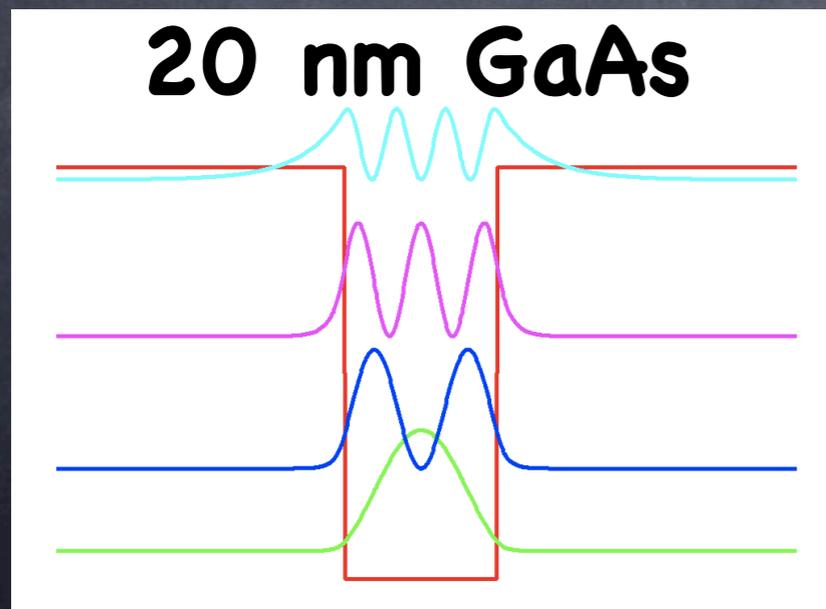
and we get a quantum well  
with discrete eigenstates !!!

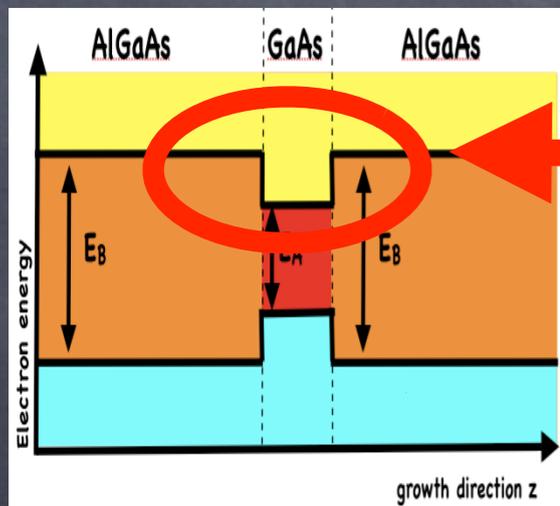


and we get a quantum well with discrete eigenstates !!!



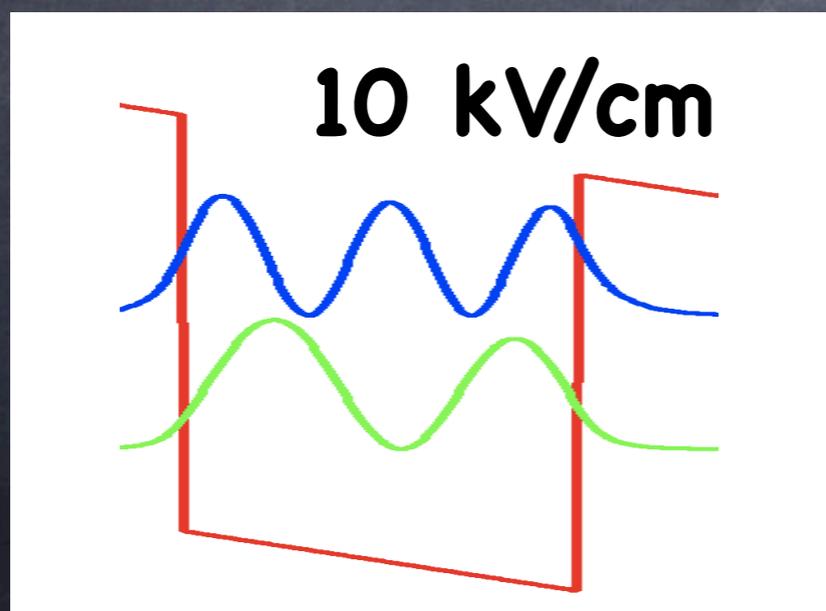
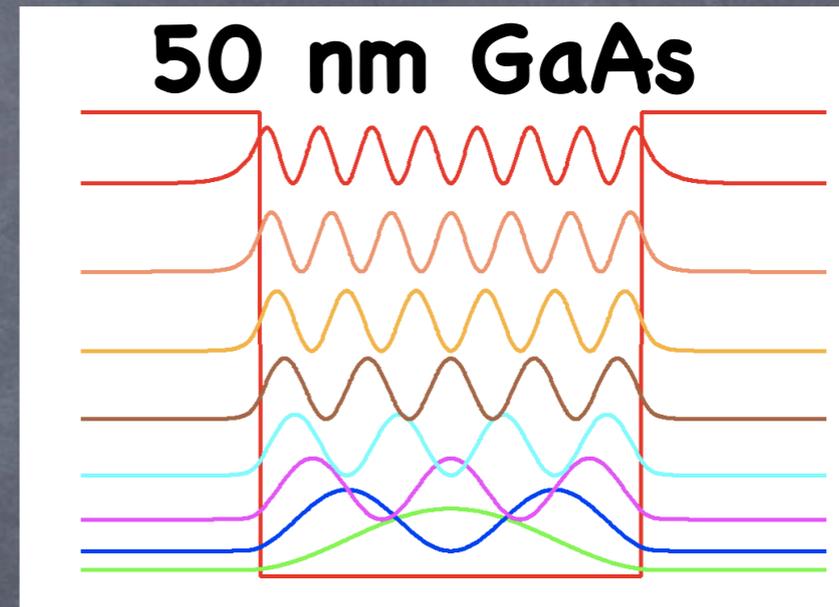
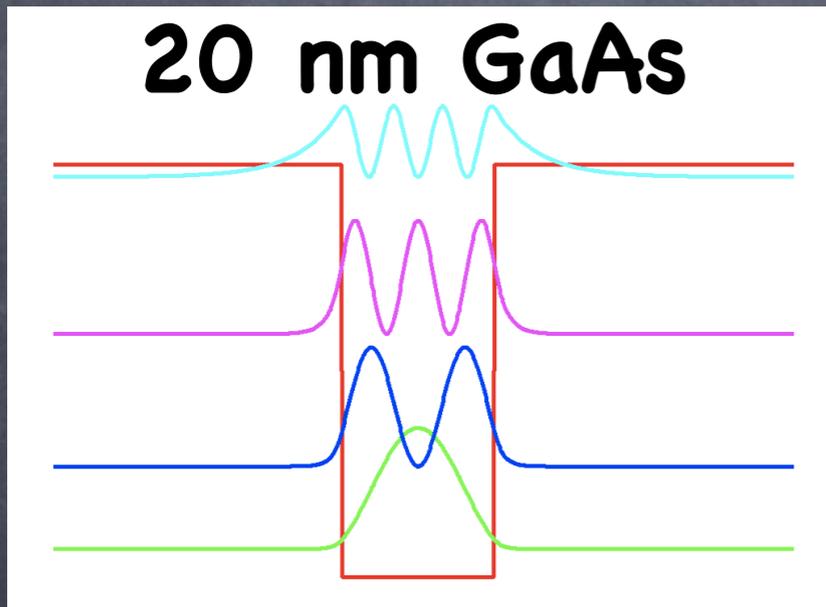
eigenstates can be changed over a) layer thickness:





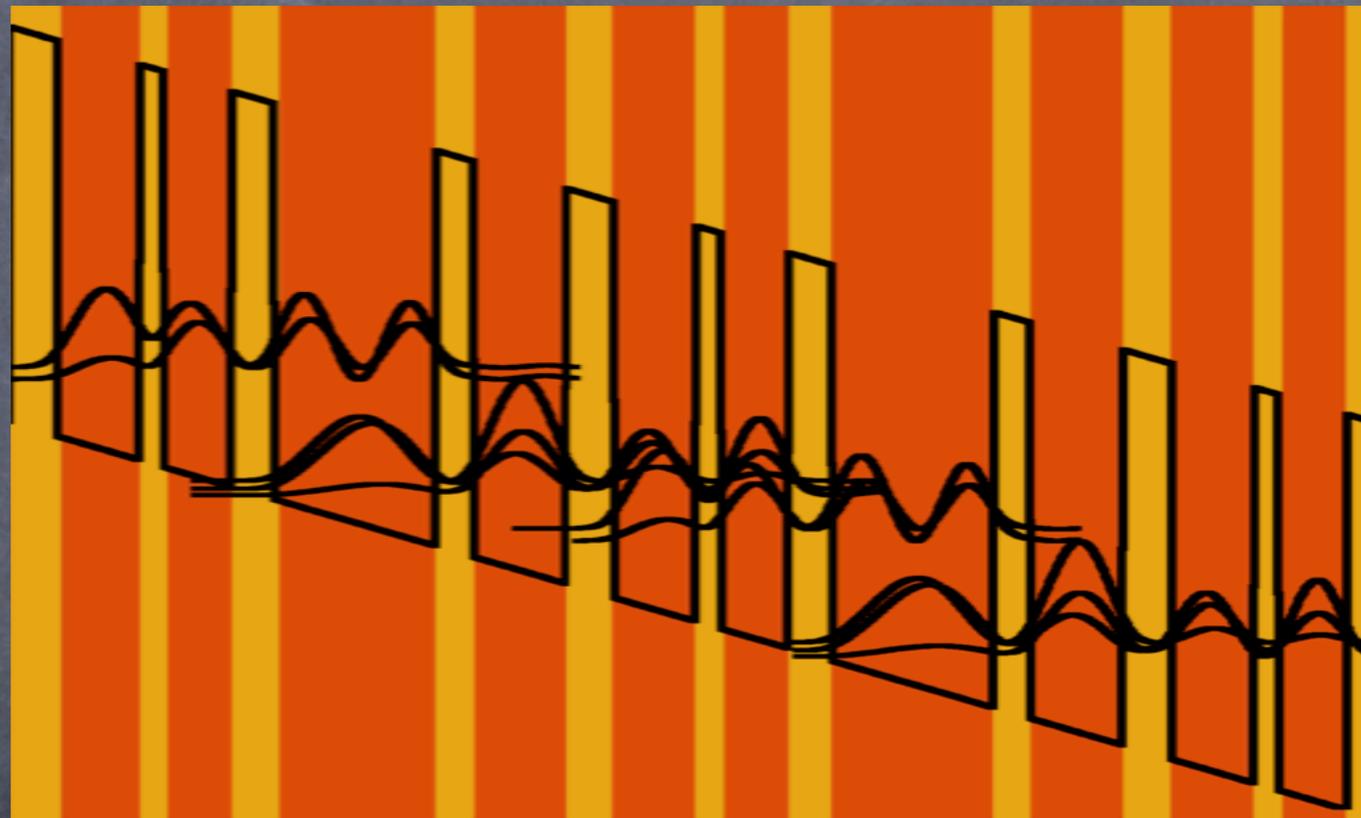
and we get a quantum well with discrete eigenstates !!!

eigenstates can be changed over a) layer thickness:



and also by b) applying an external electric field

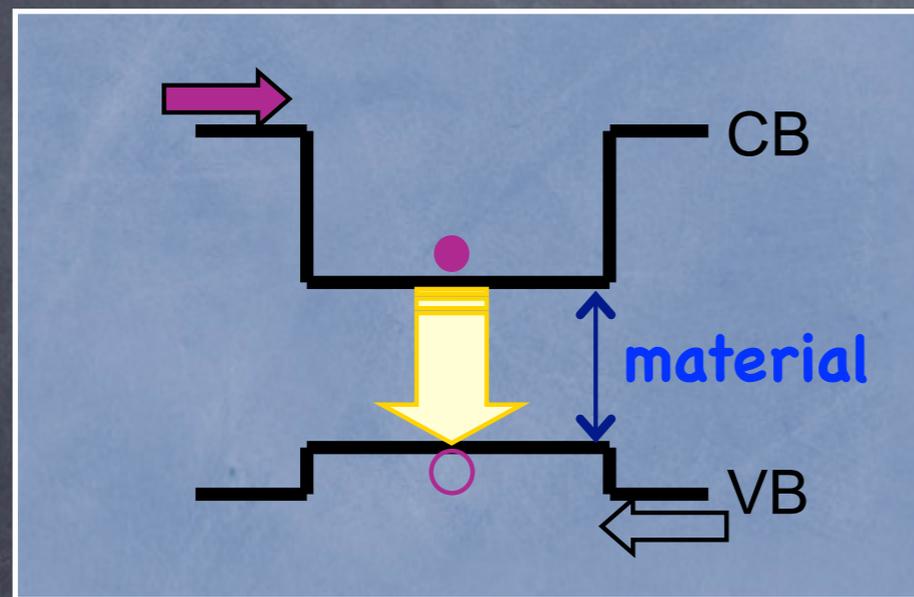
and if we add lots of those quantum wells...



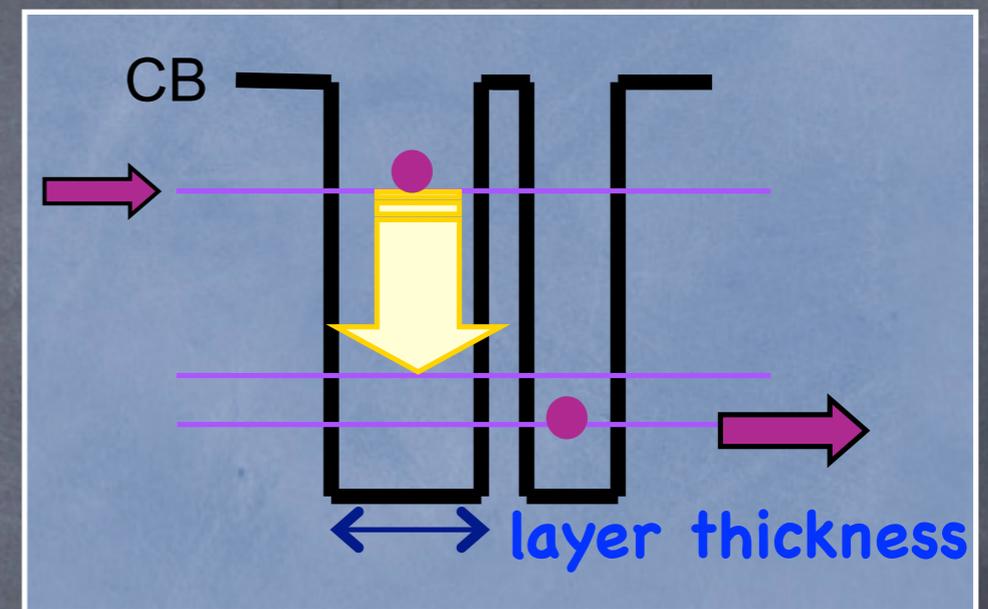
Quantum Cascade Laser: "Engineered collection of quantum wells with discrete eigenstates"

# What exactly are Quantum Cascade Lasers?

They are NOT  
Interband Lasers



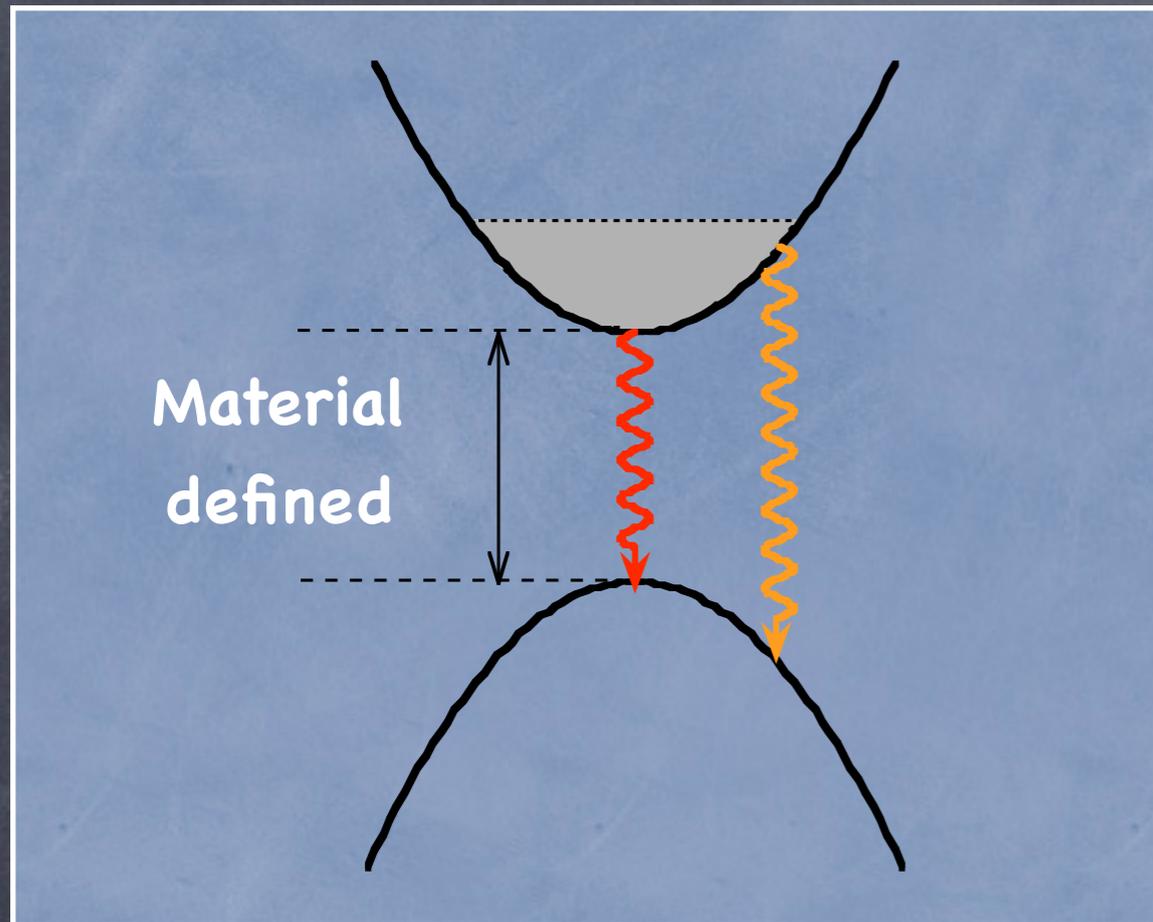
They are  
Inter**SUB**band Lasers



- Diode laser:
- interband transitions
  - $\lambda$  defined by material
  - immature materials at long  $\lambda$
  - bi-polar (interband)

- QCL:
- intersubband transitions
  - $\lambda$  defined by layer thickness
  - mature materials at long  $\lambda$
  - unipolar (intraband)

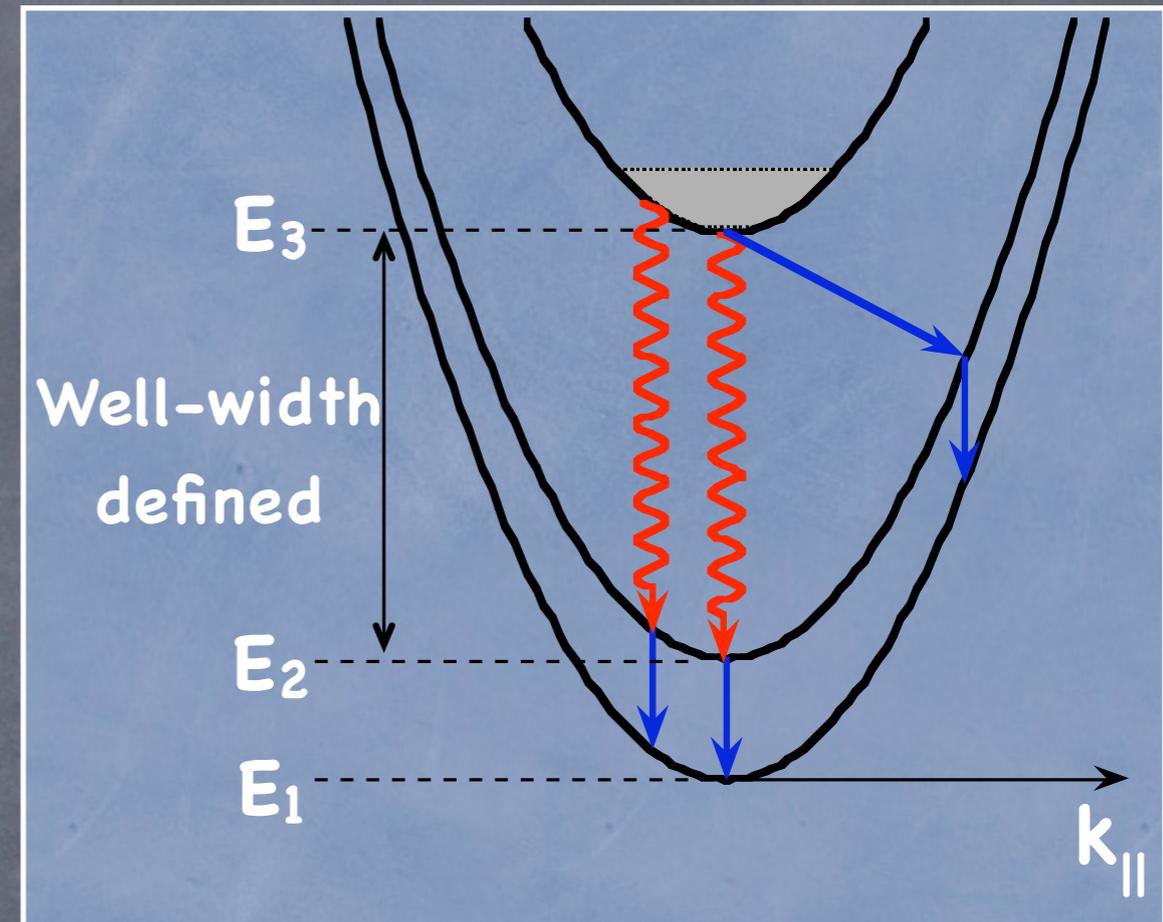
# Interband Transition



You would like a  
different photon energy ?

Sorry, but you will have to  
switch to a different material.

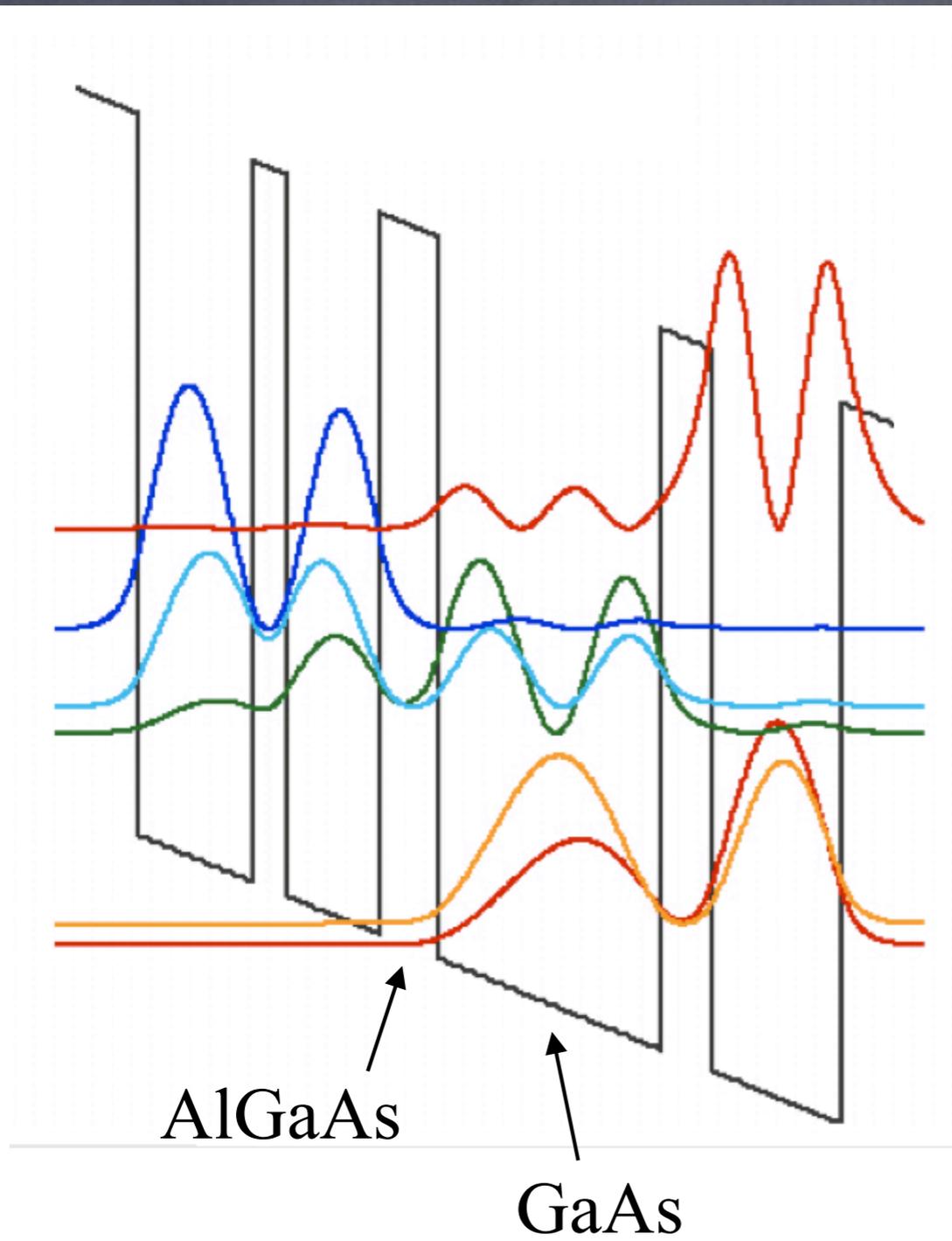
# InterSUBband Transition



You would like a  
different photon energy ?

Just change  
the width of the well.

# Engineered collection of quantum wells with discrete eigenstates



**Kazarinov/Suris (1971)**

(proposed amplification of light through intersubband transitions)



**Capasso et al. (1983)**

(showed sequential resonant tunneling through many quantum wells)



**Faist et al. (1994)**

(first QCL demonstration, 4  $\mu$ )

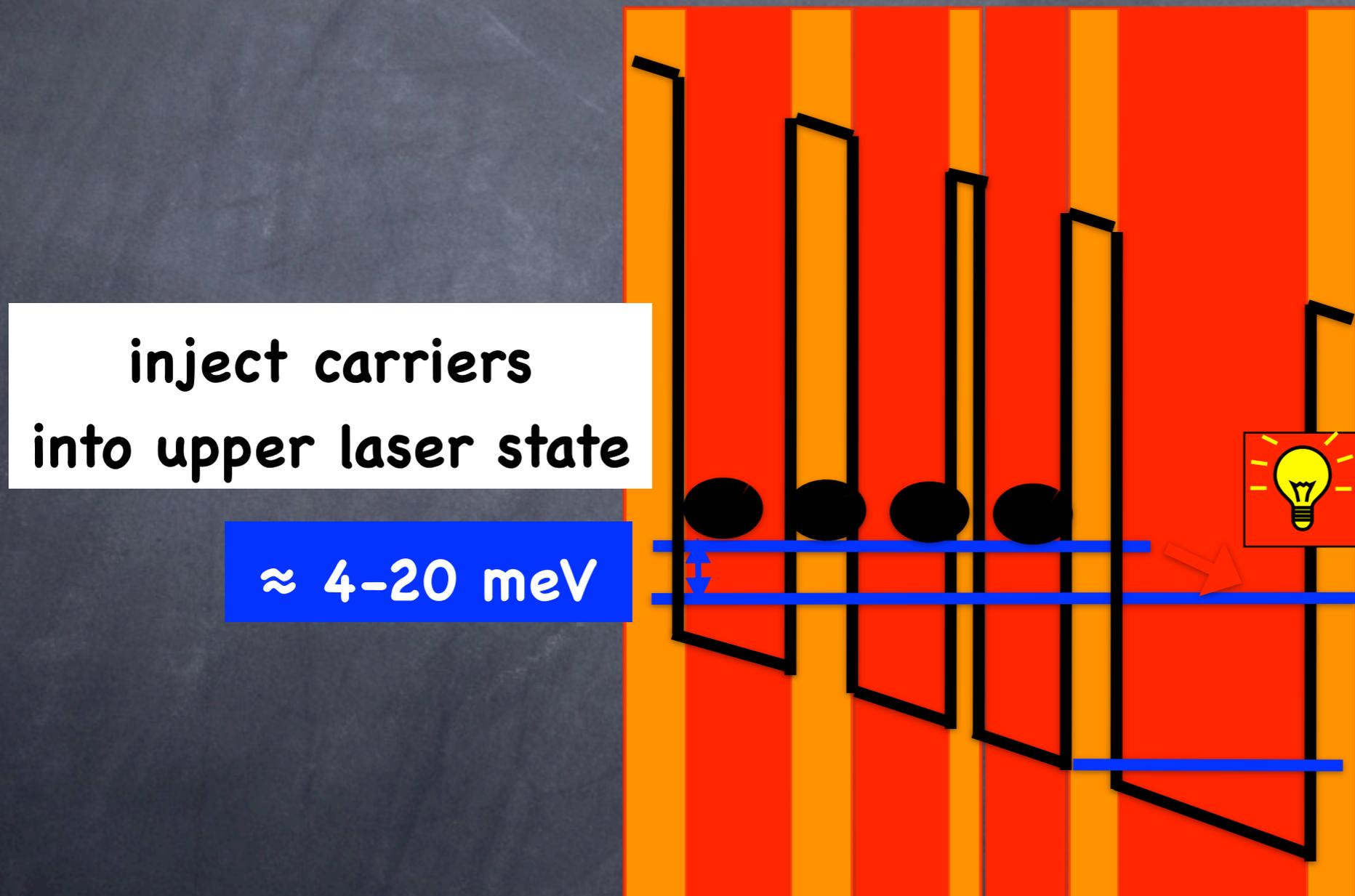


**Koehler et al. (2002)**

(first THz-QCL demonstration, 4.4 THz)

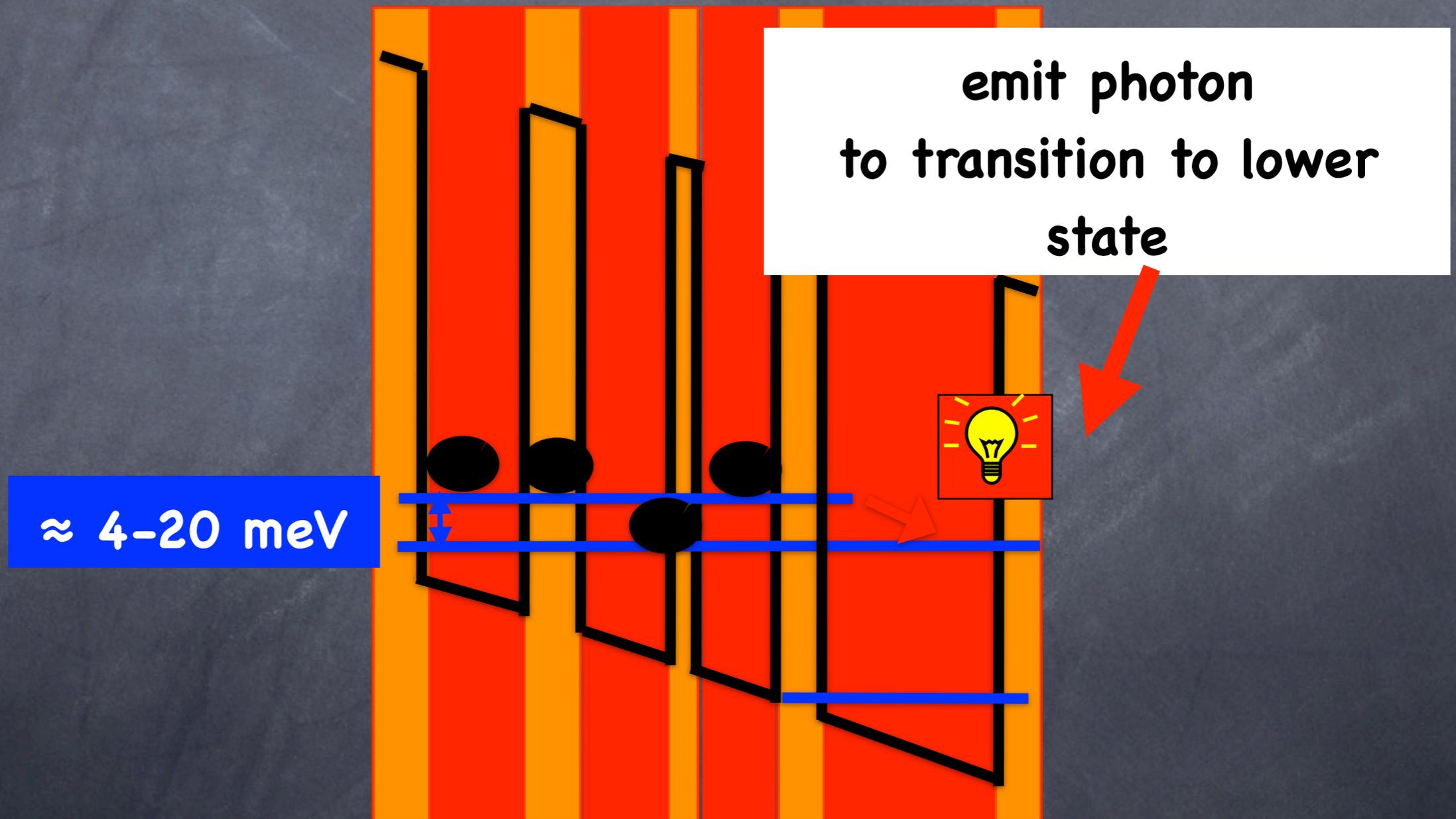
# 'Basic THz-QCL' in 4 steps.

## Step 1: inject carriers



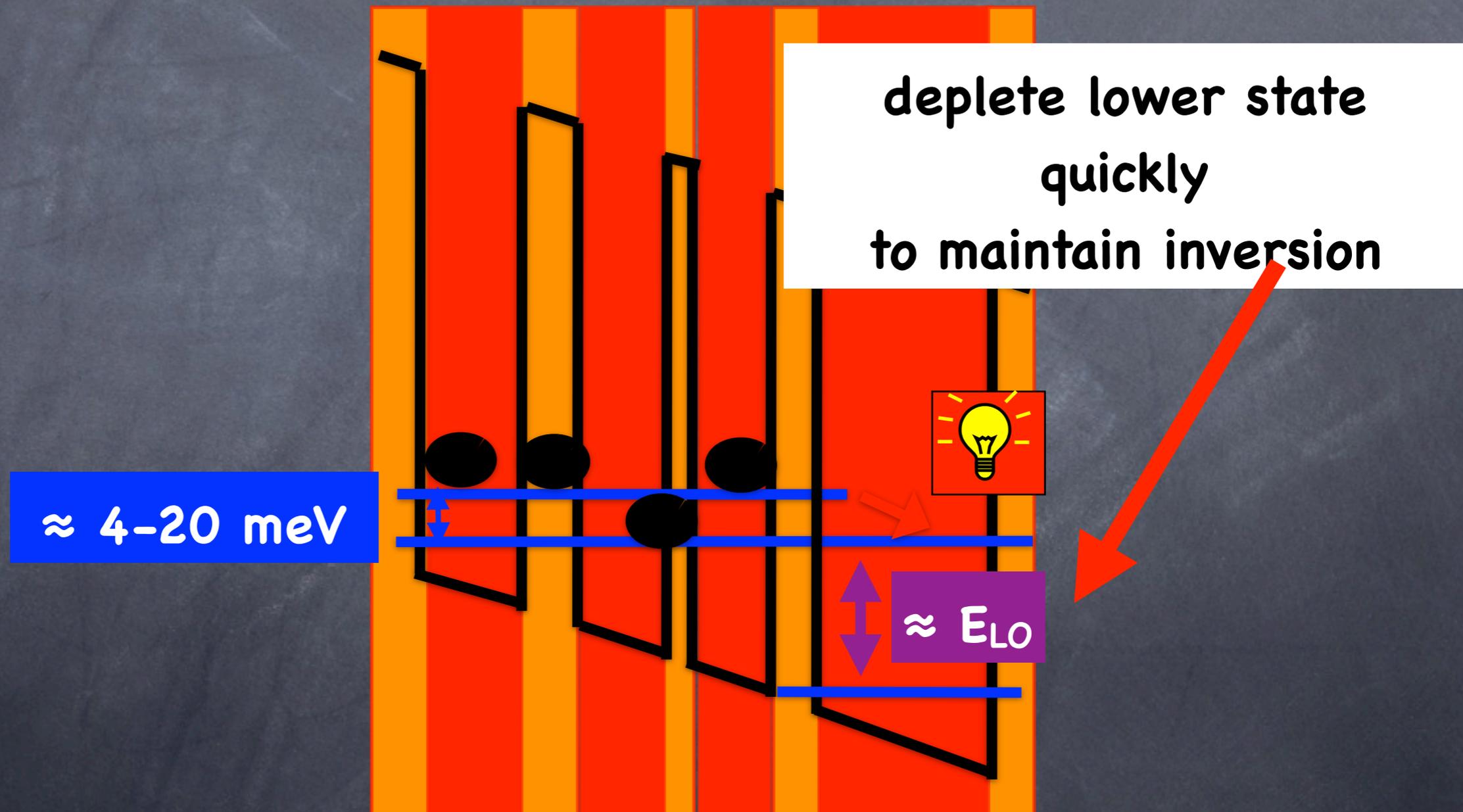
# 'Basic THz-QCL' in 4 steps.

## Step 2: emit photon



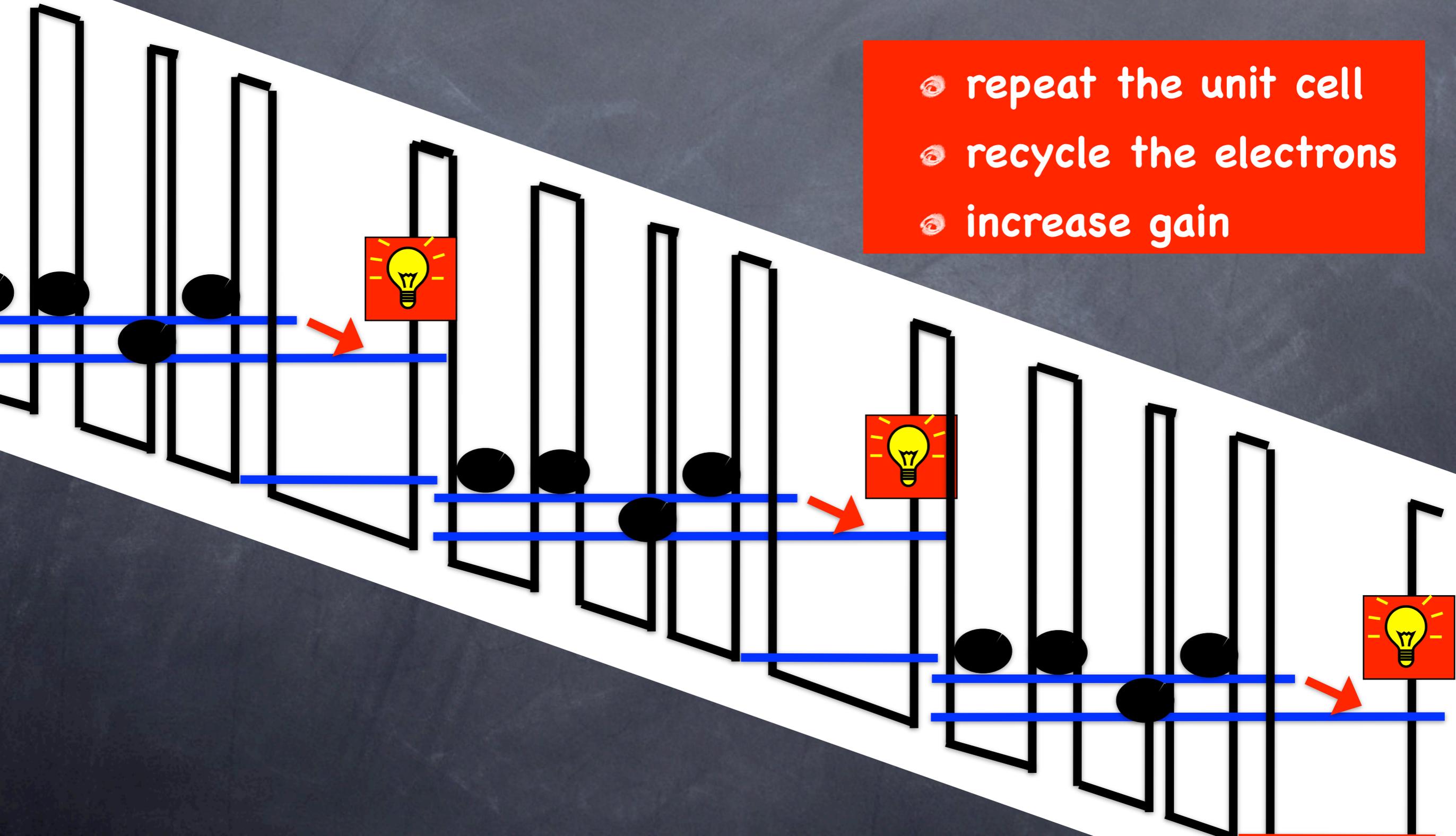
# 'Basic THz-QCL' in 4 steps.

## Step 3: deplete carriers



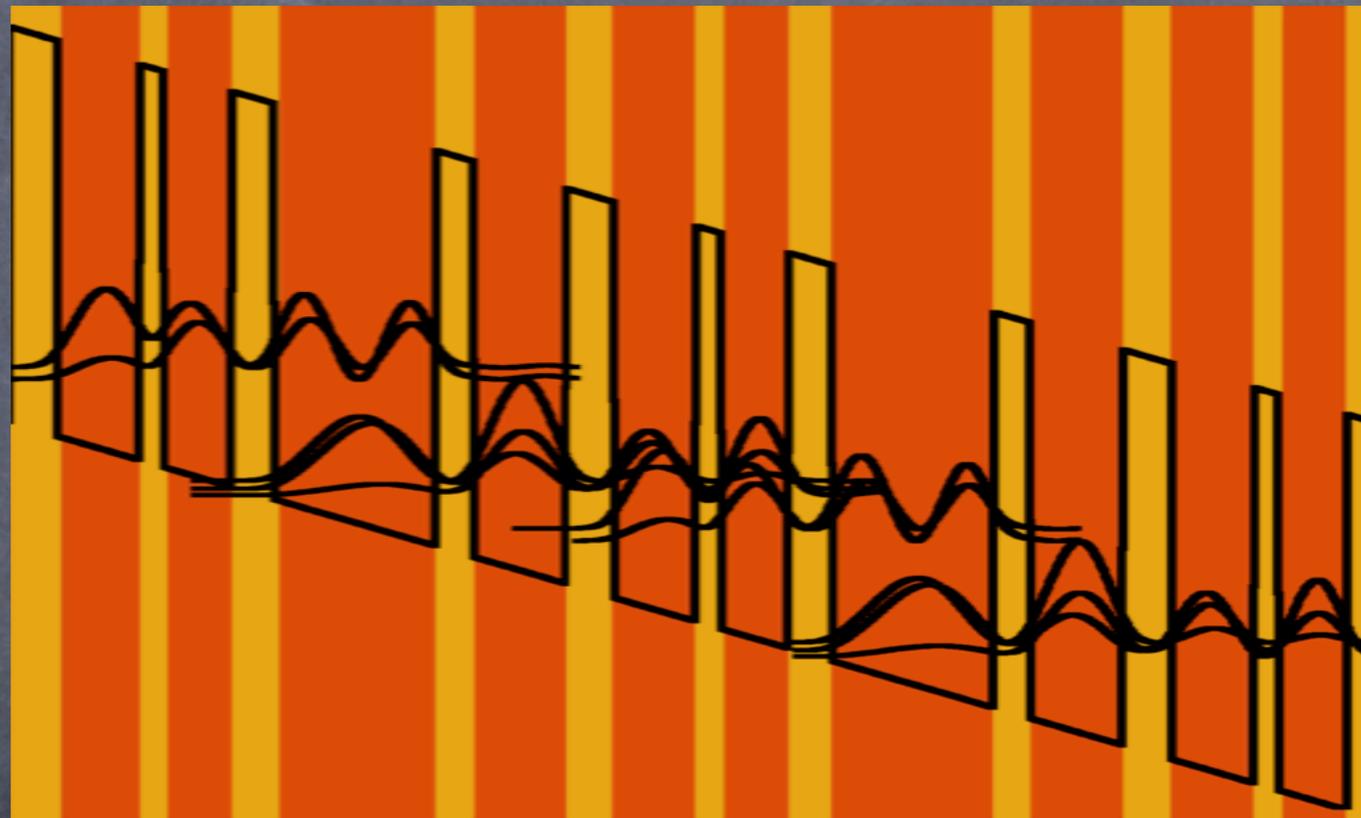
# 'Basic THz-QCL' in 4 steps.

Step 4: repeat, repeat, repeat



- repeat the unit cell
- recycle the electrons
- increase gain

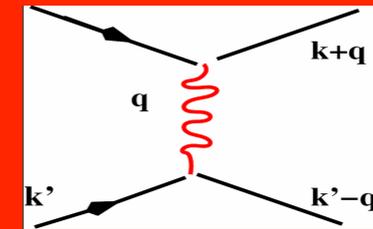
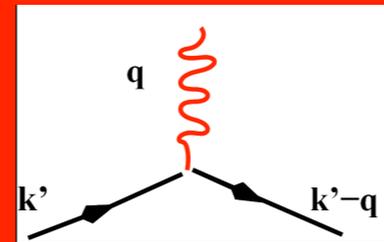
and there you have...



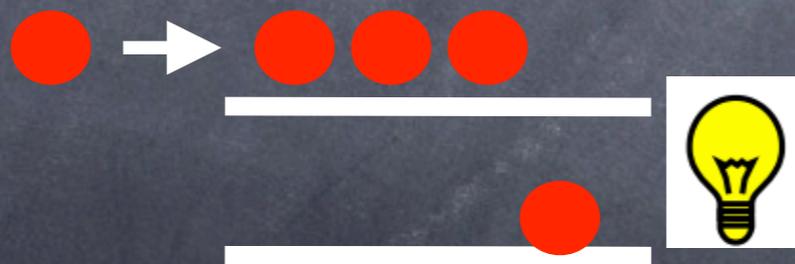
the Quantum Cascade Laser: "Engineered collection of quantum wells with discrete eigenstates"

The 'tricky' part:

Minimizing negative  
and  
maximizing positive  
effects of electron scattering

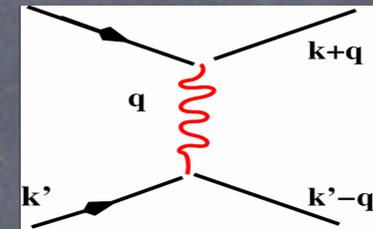
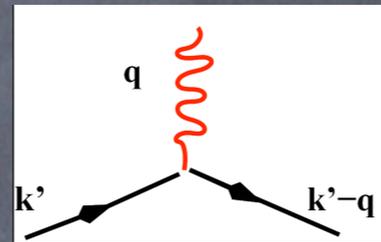


Scattering !!!

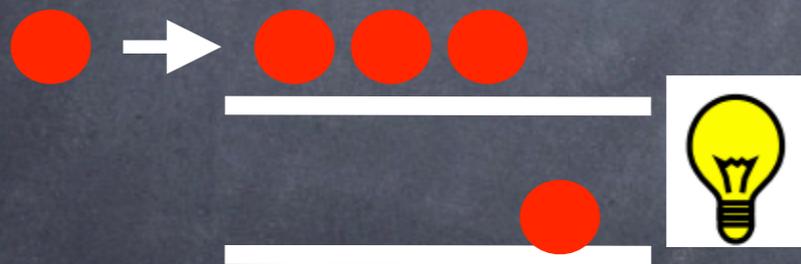


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Minimizing negative  
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maximizing positive  
effects of electron scattering



Scattering !!!

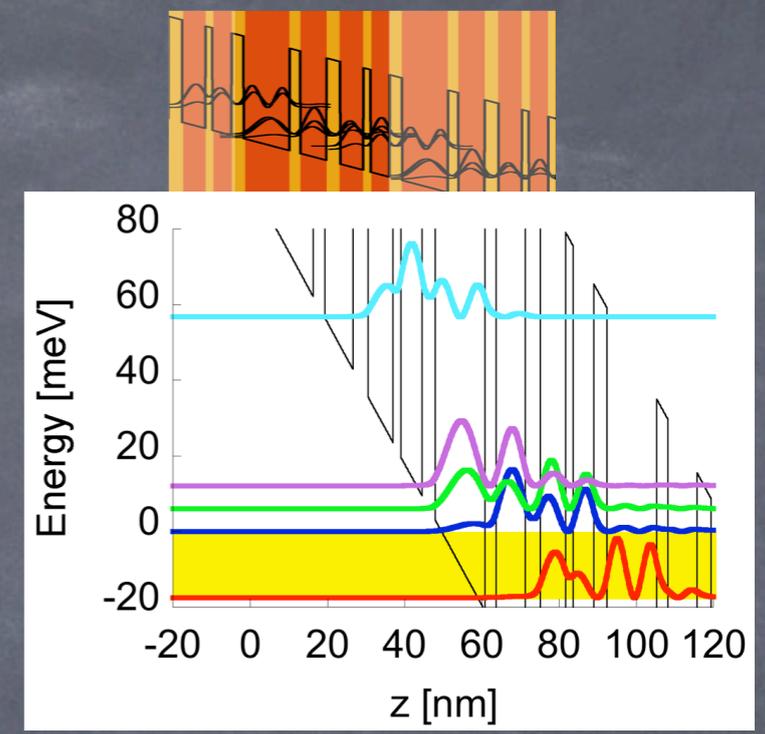
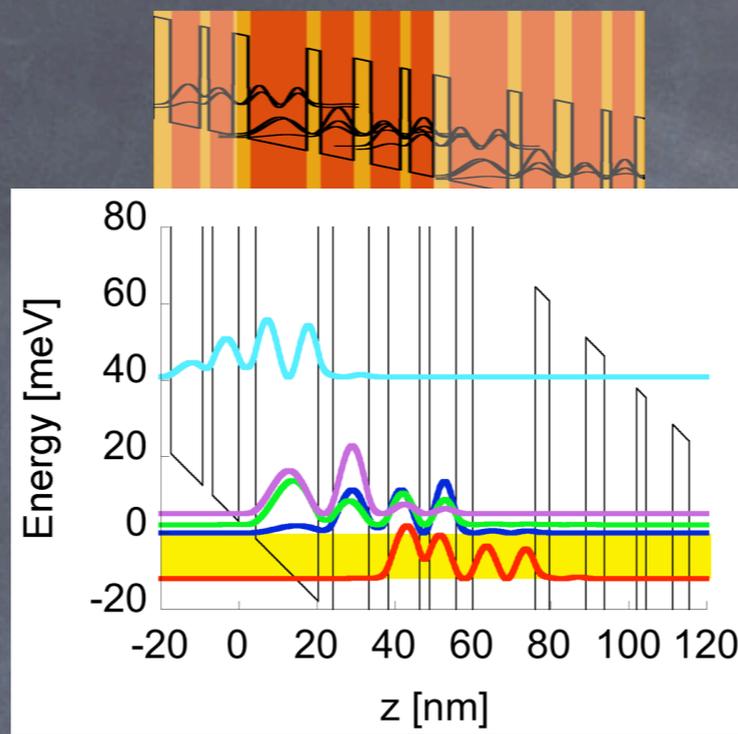
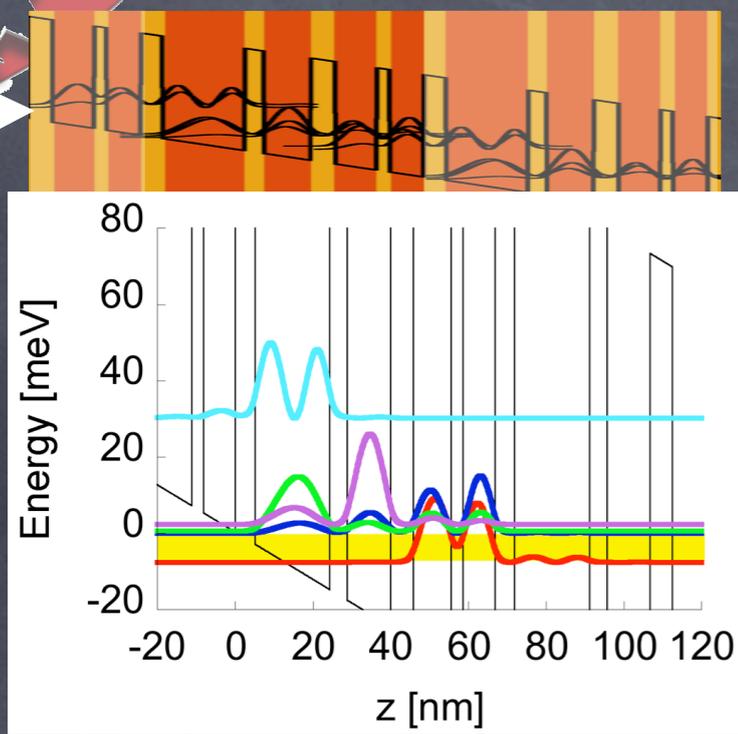


Scattering !!!



Scattering !!!

Wavefunctions/  
Separation Energies



## Wavefunction shapes:

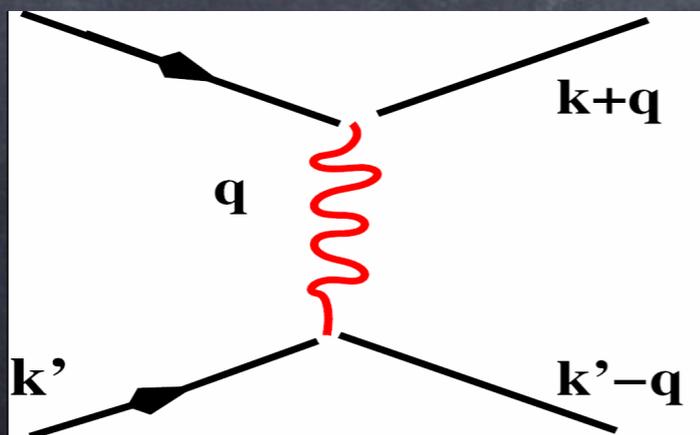
• Coulomb matrix elements:

$$V_{\mathbf{k}_{||}}^{abcd} \propto \frac{1}{|\mathbf{k}_{||}|} \int dz \int dz' \phi_a(z) \phi_b(z') \phi_c(z) \phi_d(z') e^{-i\mathbf{k}_{||}|z-z'|}$$

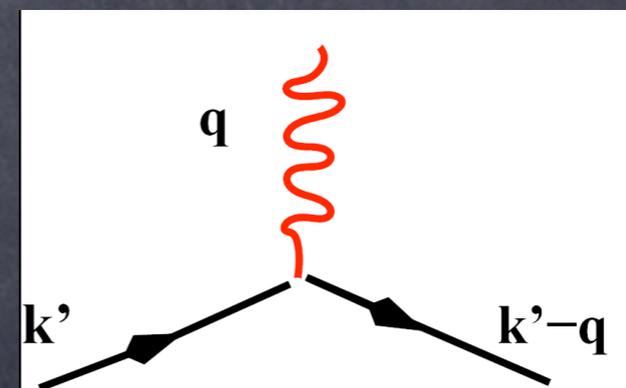
• Froehlich matrix elements:

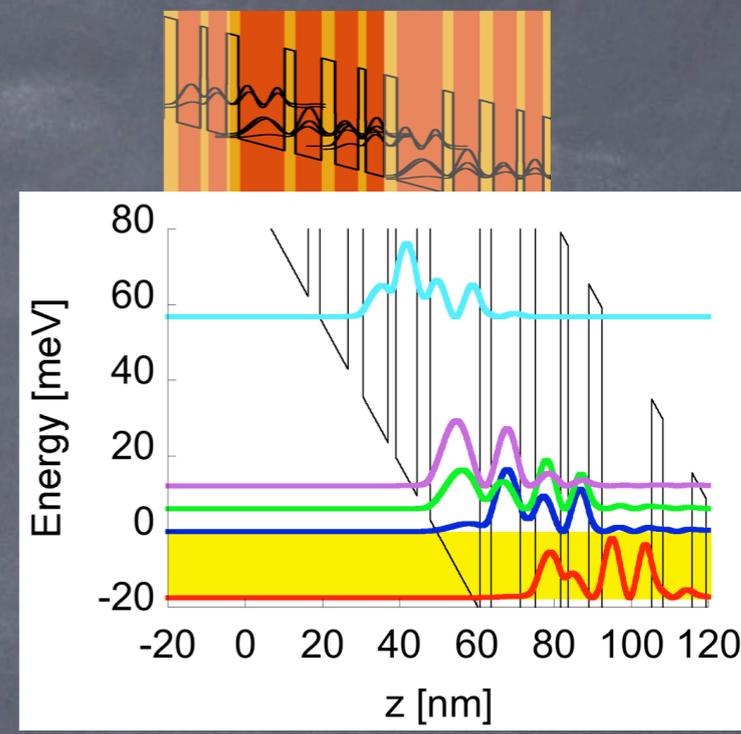
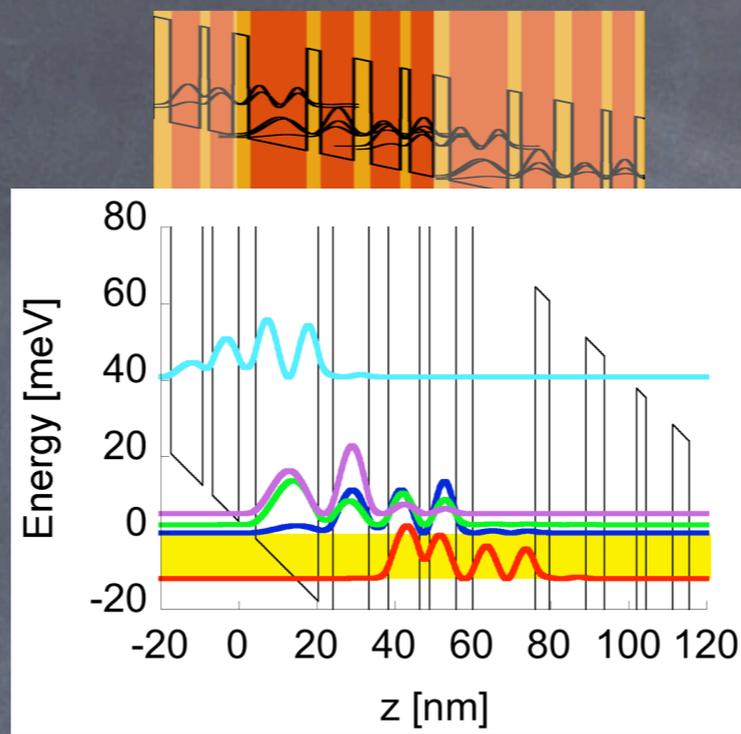
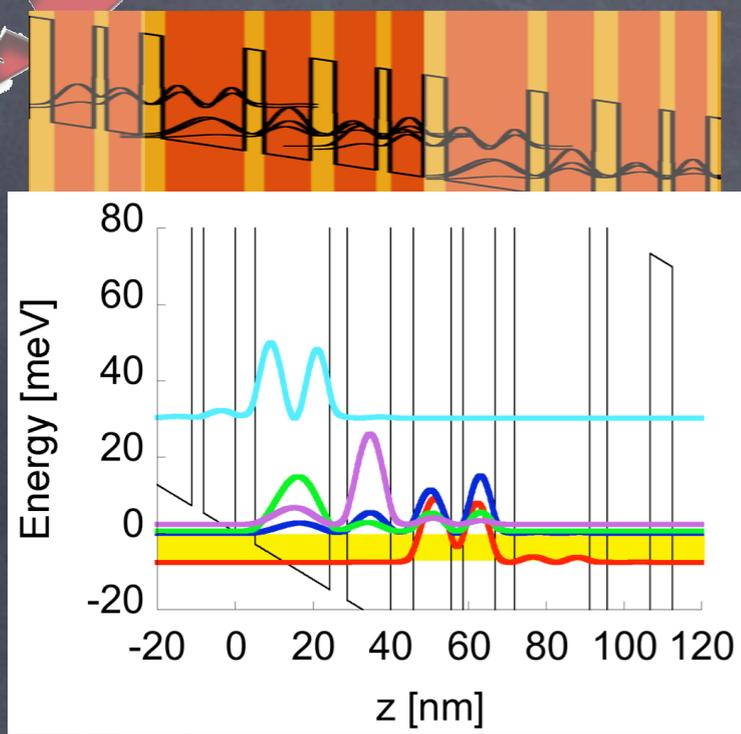
$$g_q^{ab} \propto \frac{1}{\sqrt{q_{||}^2 + q_{\perp}^2}} \int dz \phi_a(z) \phi_b(z) e^{iq_{\perp}z}$$

carrier-carrier scattering



carrier-phonon scattering





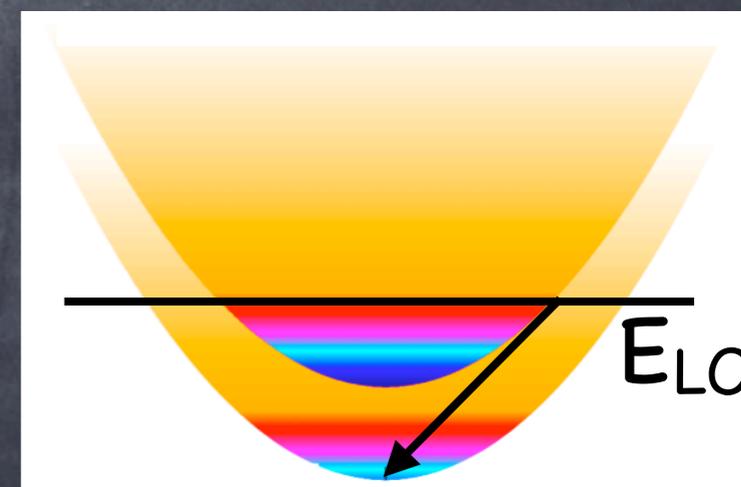
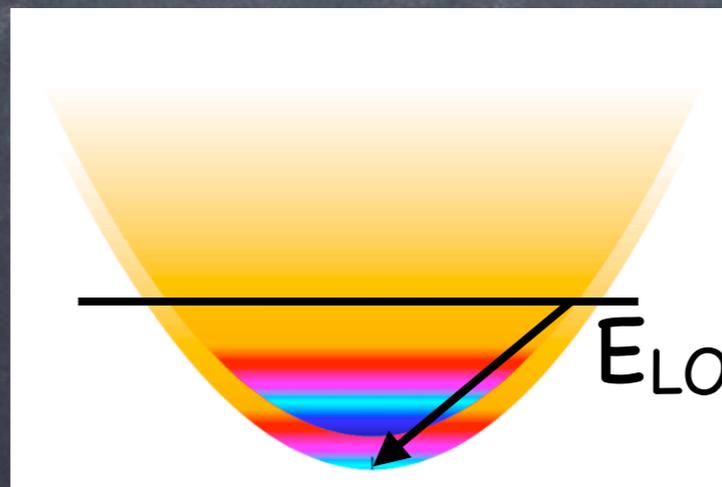
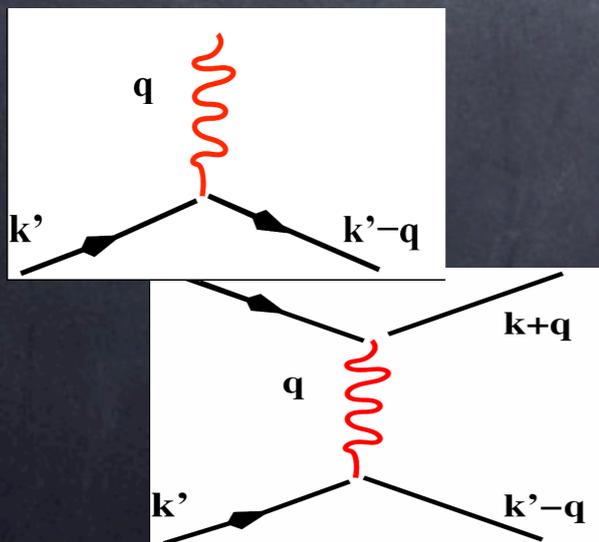
## Separation energies:

allowed transitions for cc-scattering:

$$\delta(\epsilon_{a,k} + \epsilon_{b,k'} - \epsilon_{c,k+q} + \epsilon_{d,k'-q})$$

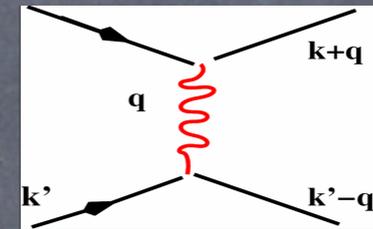
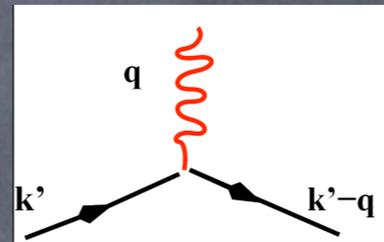
allowed transitions for cp-scattering:

$$\delta(\epsilon_{a,k} - \epsilon_{b,k+q} \pm \hbar\omega_{LO})$$

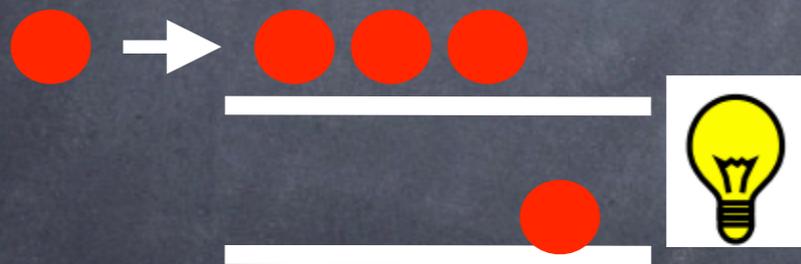


The 'tricky' part:

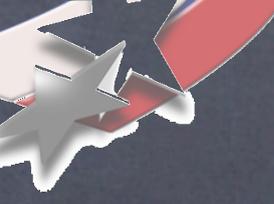
Minimizing negative  
and  
maximizing positive  
effects of electron scattering



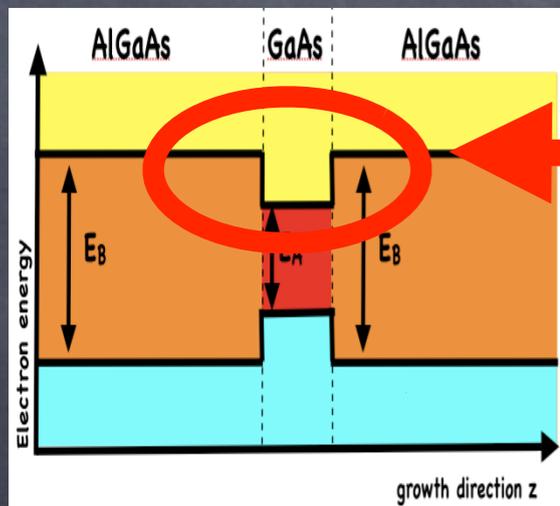
Scattering !!!



Design Question!!!

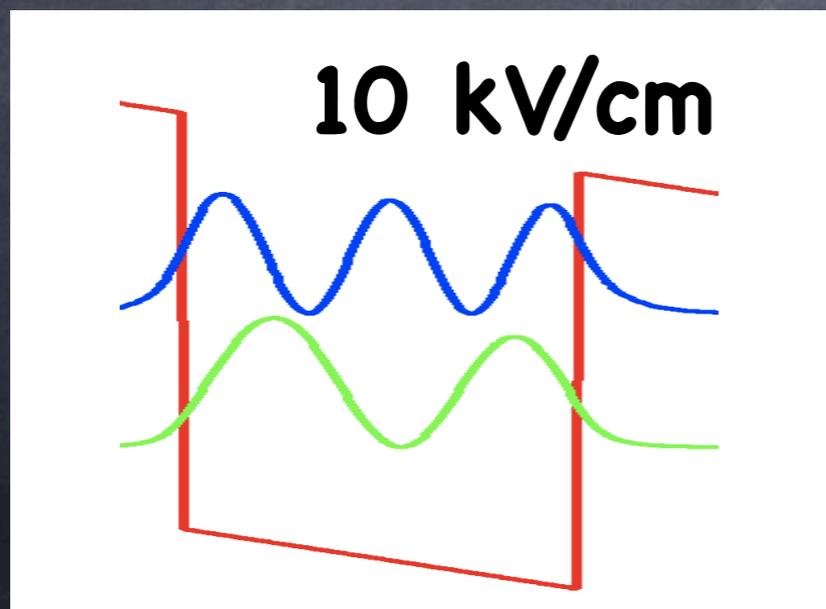
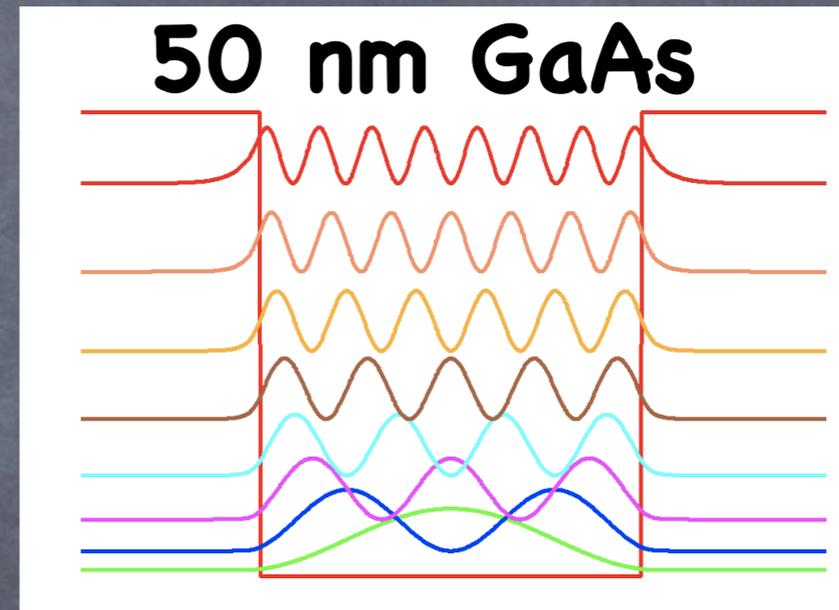
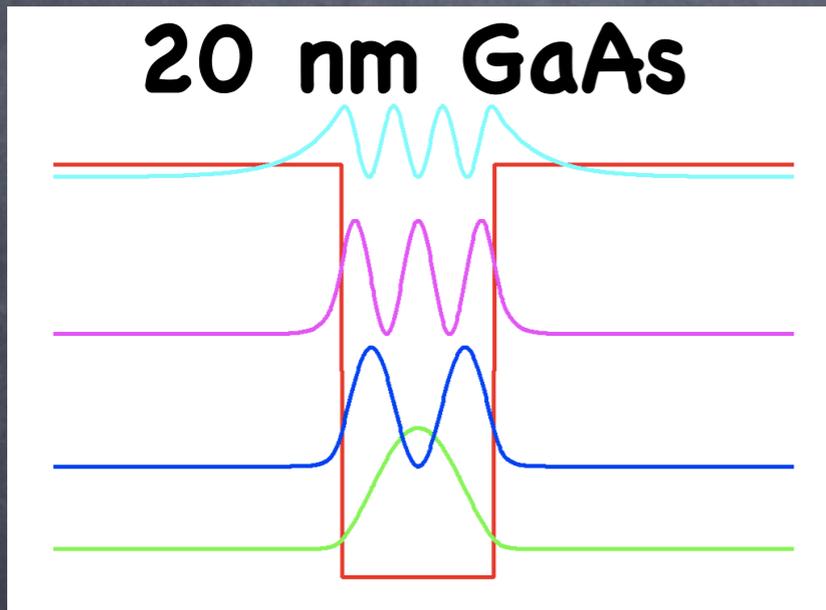


# Designing a QCL



and we get a quantum well with discrete eigenstates !!!

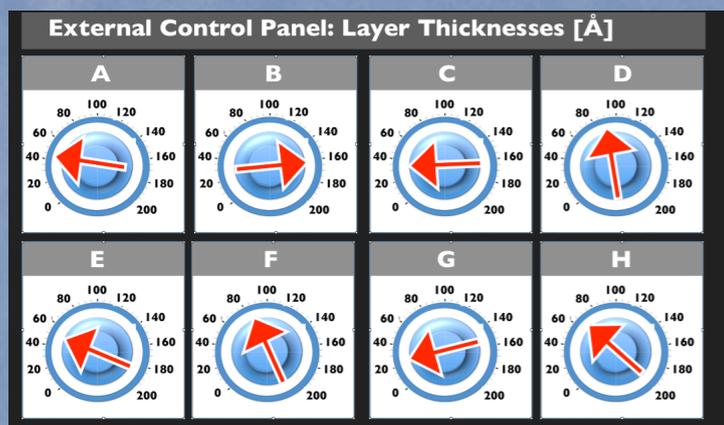
eigenstates can be changed over a) layer thickness:



and also by b) applying an external electric field



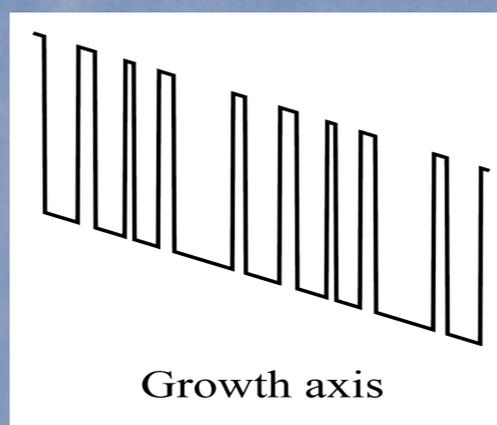
# 1. 'Educated' guess



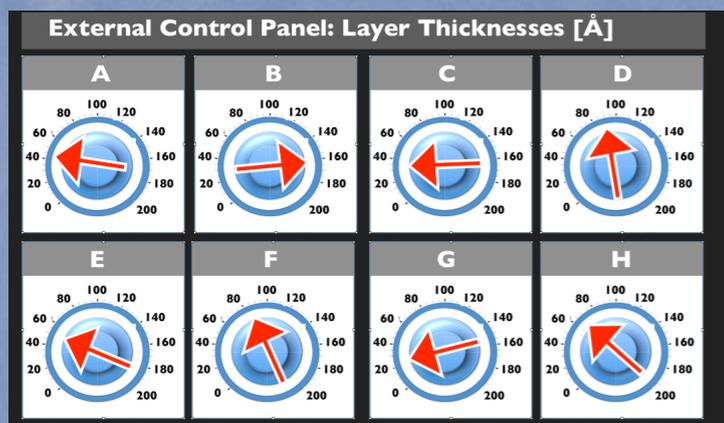
material



# 2. Potential



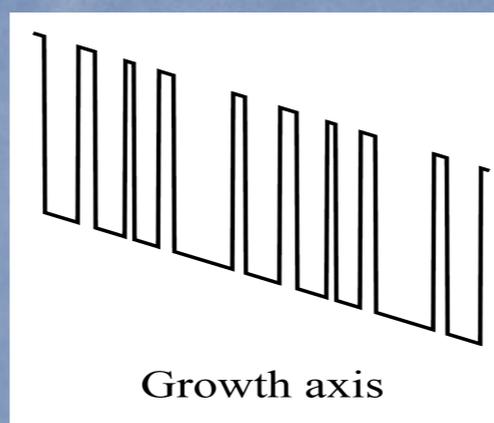
# 1. 'Educated' guess



material



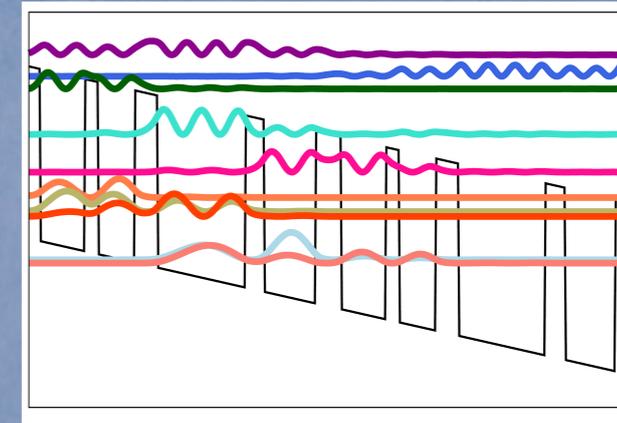
# 2. Potential



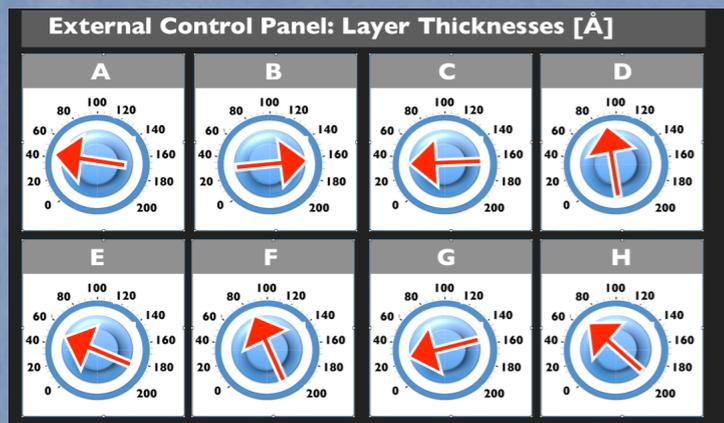
k.p.



# 3. Bandstructure



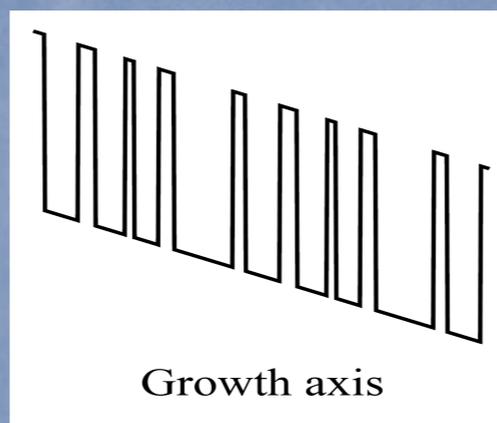
# 1. 'Educated' guess



material



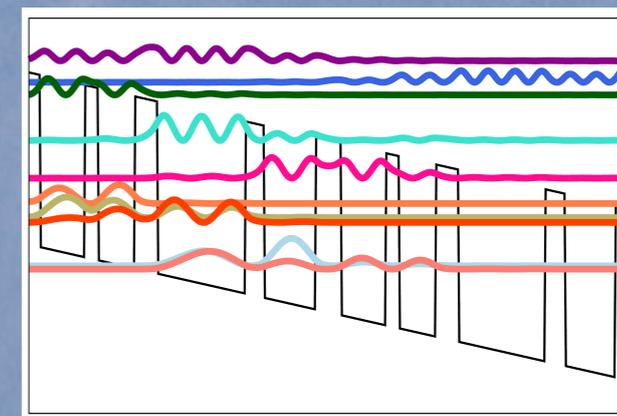
# 2. Potential



k.p.



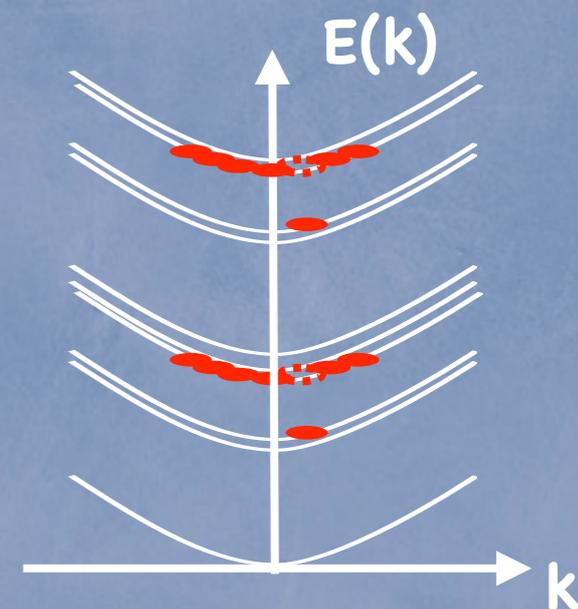
# 3. Bandstructure



QKC



# 4. Carrier distribution

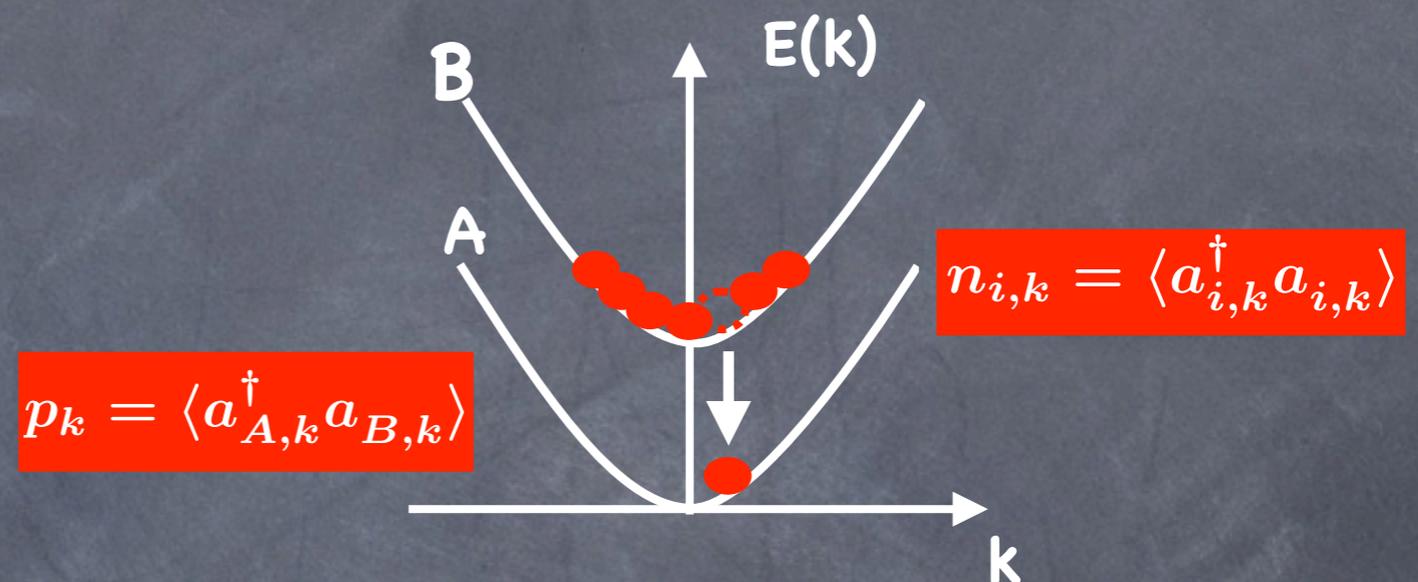


# How do we calculate those carrier distributions...

## QKC

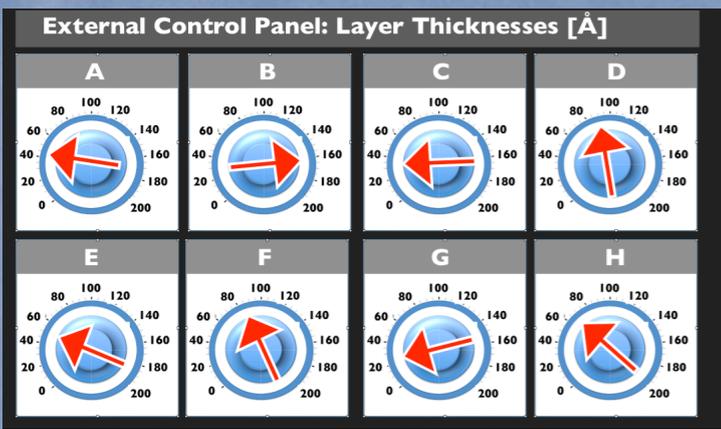
### Quantum Kinetic Calculation

- treat carriers in second quantization
- solve Heisenberg Equation time-resolved for carrier distributions and microscopic polarizations
- microscopic scattering in 2. Born approximation (pauli blocking, non-diagonal scattering contributions)



$$-i\hbar \frac{d}{dt} \langle a_{A,k}^\dagger a_{B,k} \rangle = \langle [(H_0 + H_{cf} + H_{cc} + H_{cp}), a_{A,k}^\dagger a_{B,k}] \rangle$$

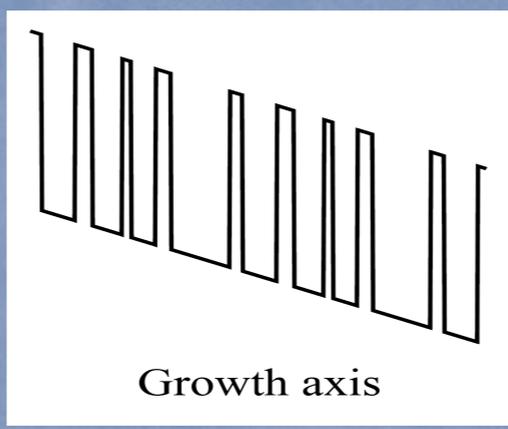
# 1. 'Educated' guess



material



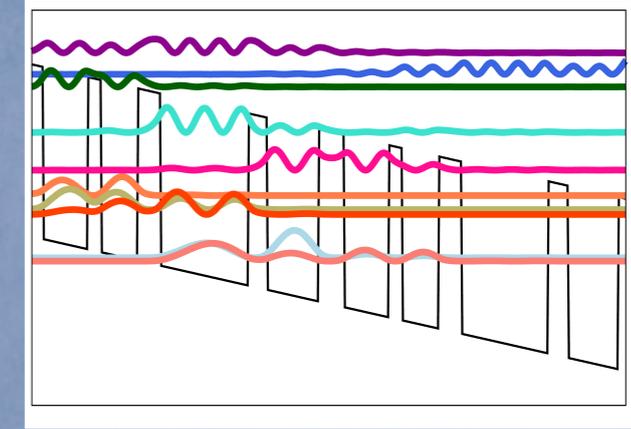
# 2. Potential



k.p.



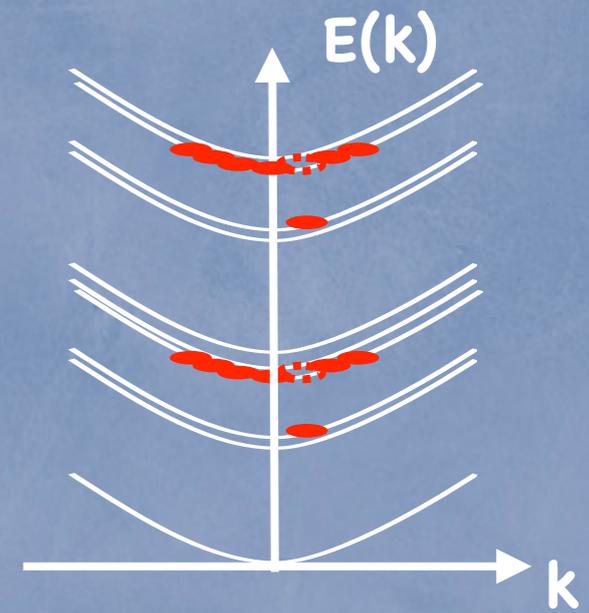
# 3. Bandstructure



QKC



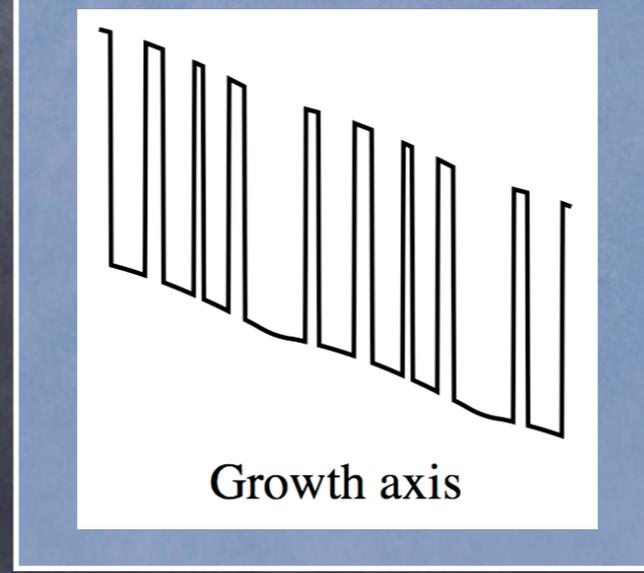
# 4. Carrier distribution



back to k.p.



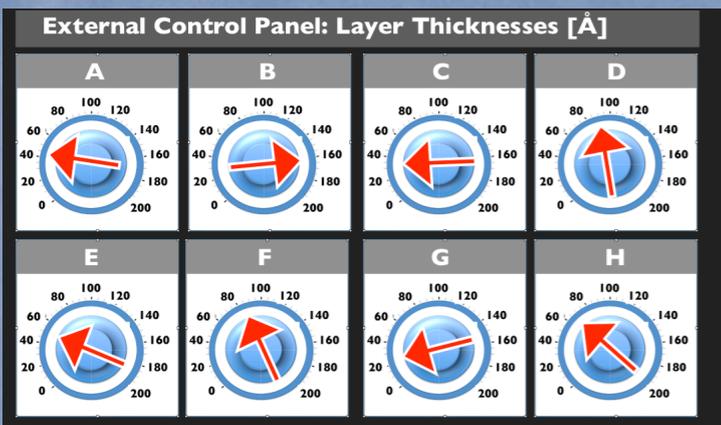
# 5. Updated potential



Poisson

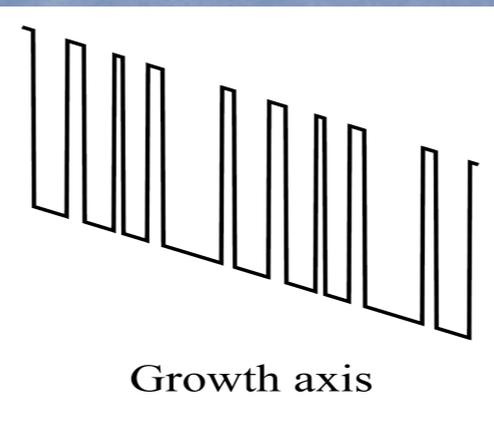


# 1. 'Educated' guess



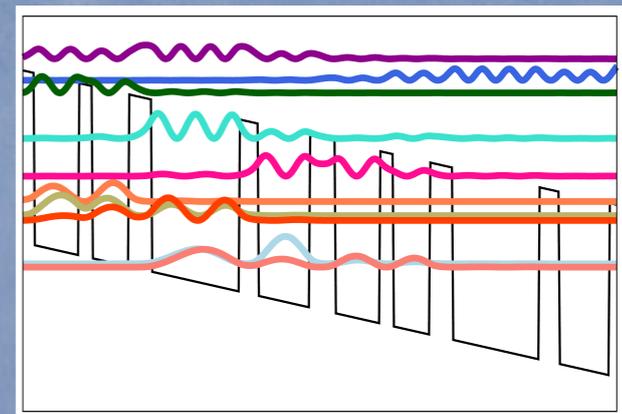
material

# 2. Potential



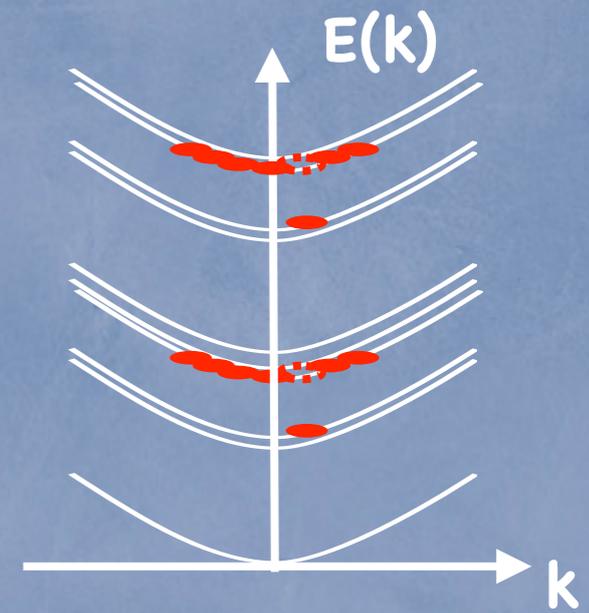
k.p.

# 3. Bandstructure



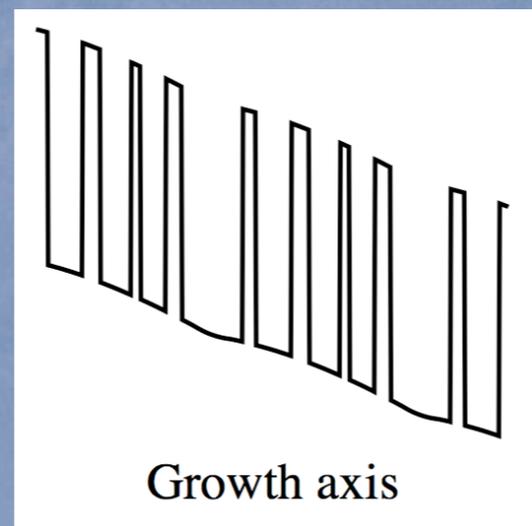
QKC

# 4. Carrier distribution

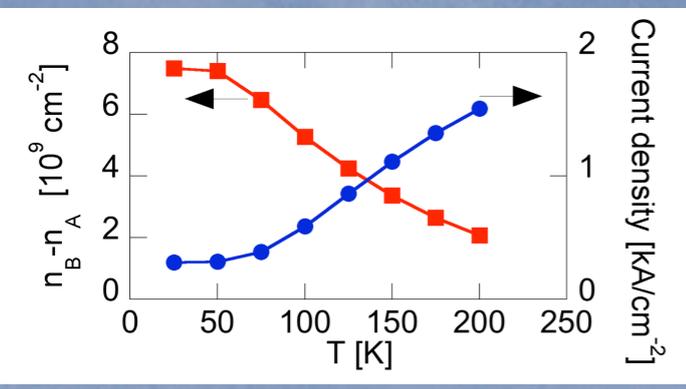


Poisson

# 5. Updated potential

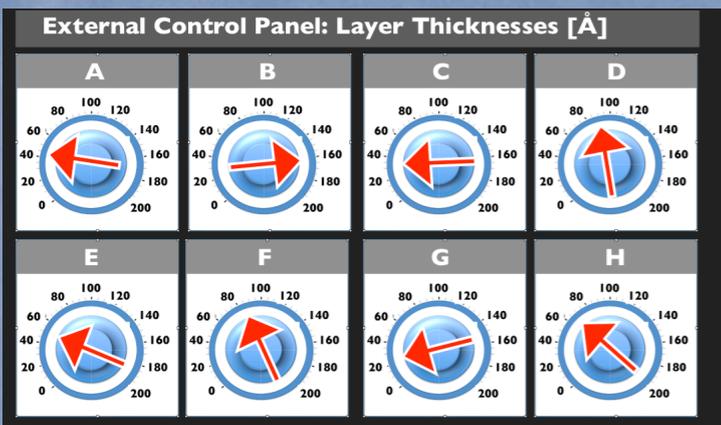


# 5. Laser Characteristics



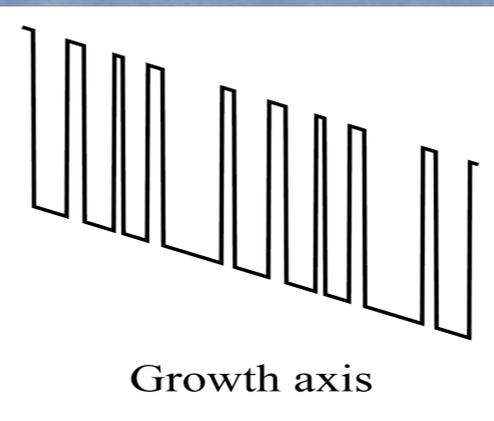
back to k.p.

# 1. 'Educated' guess



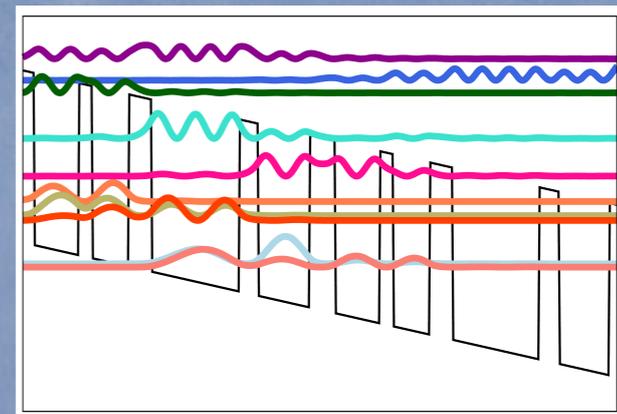
material

# 2. Potential



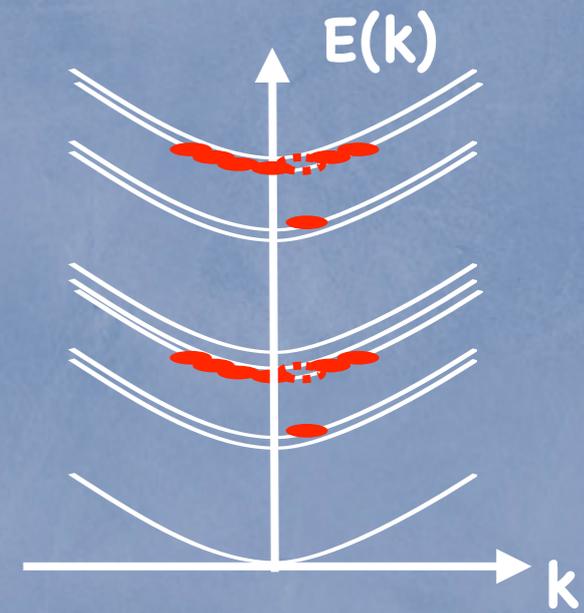
k.p.

# 3. Bandstructure



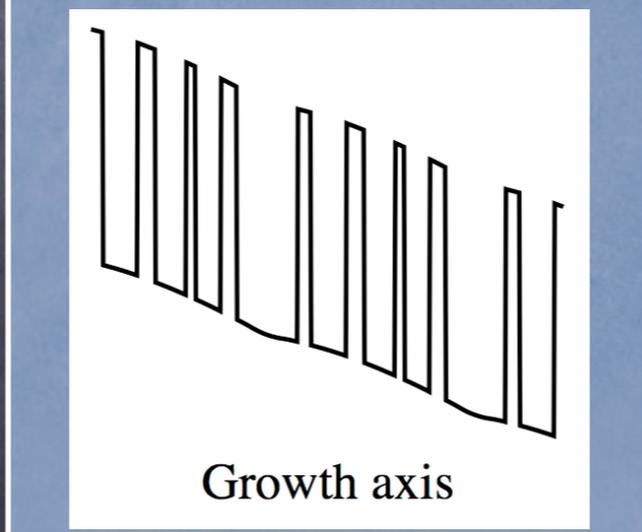
QKC

# 4. Carrier distribution



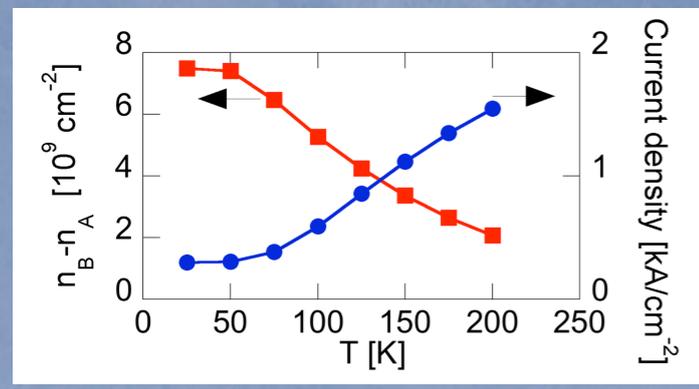
Poisson

# 5. Updated potential



# 5. Laser Characteristics

Design Emission Frequency  
2.9 THz



Done! Yeah!

sorry, try again

back to k.p.

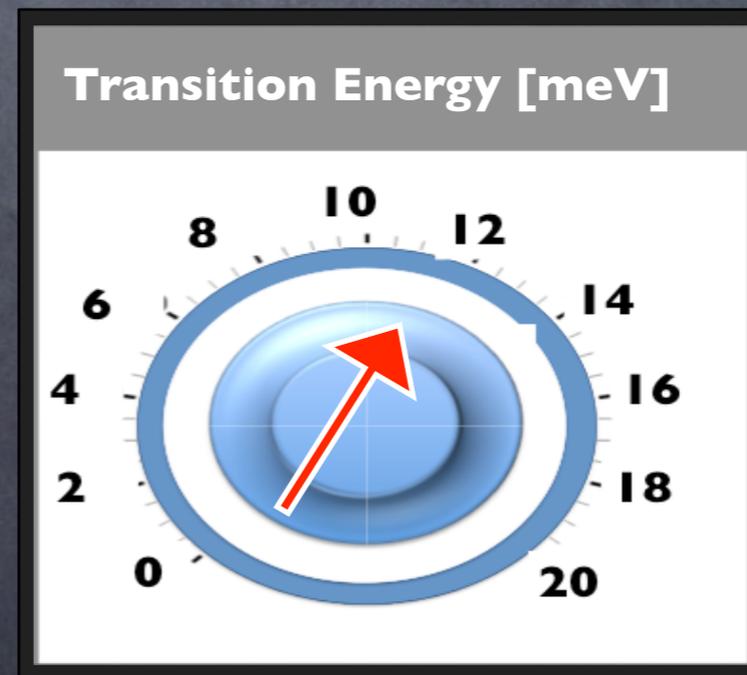


Replace  
EXTERNAL with INTERNAL  
Control Panel



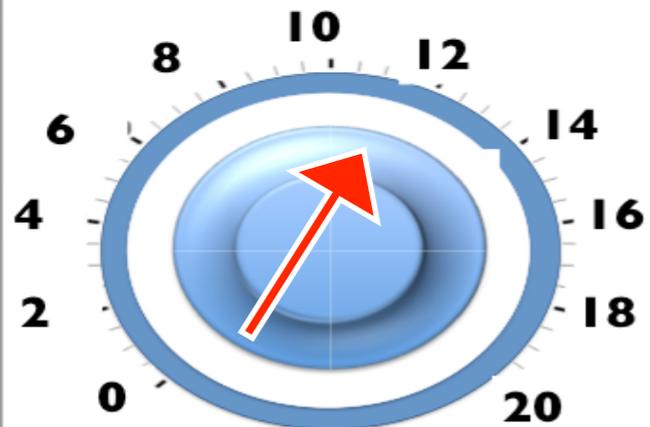
Inverse

Quantum Engineering



# Inverse Quantum Engineering (IQE)

Internal Control Panel



evolutionary algorithm  
coupled with  
Schroedinger-Poisson-Solver:  
find optimal configuration  
for specific system  
under specific constraints



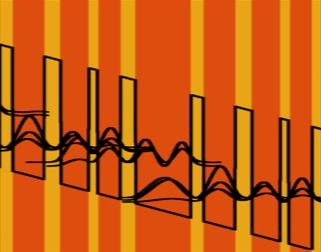
Optimal Configuration: Layer Thicknesses [ $\text{\AA}$ ]

A	B	C	D
42 $\text{\AA}$	160 $\text{\AA}$	37 $\text{\AA}$	93 $\text{\AA}$
E	F	G	H
48 $\text{\AA}$	81 $\text{\AA}$	25 $\text{\AA}$	67 $\text{\AA}$

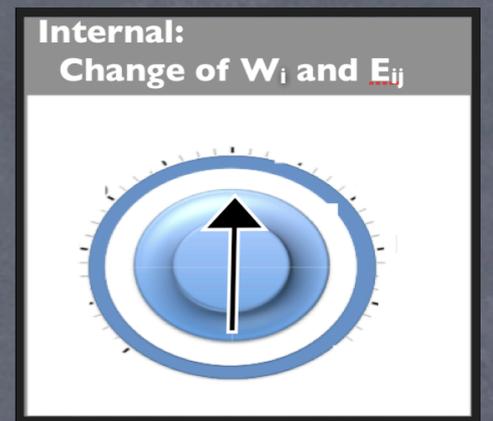
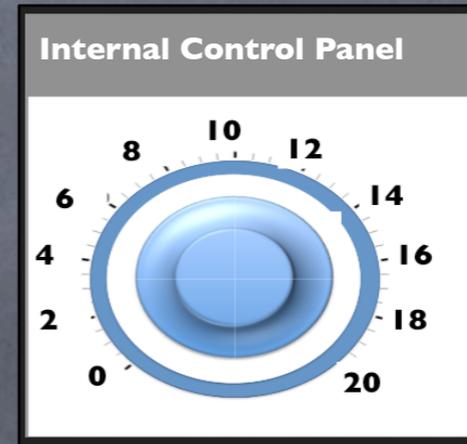
# Inverse Quantum Engineering (IQE)

Optimal Configuration: Layer Thicknesses [Å]

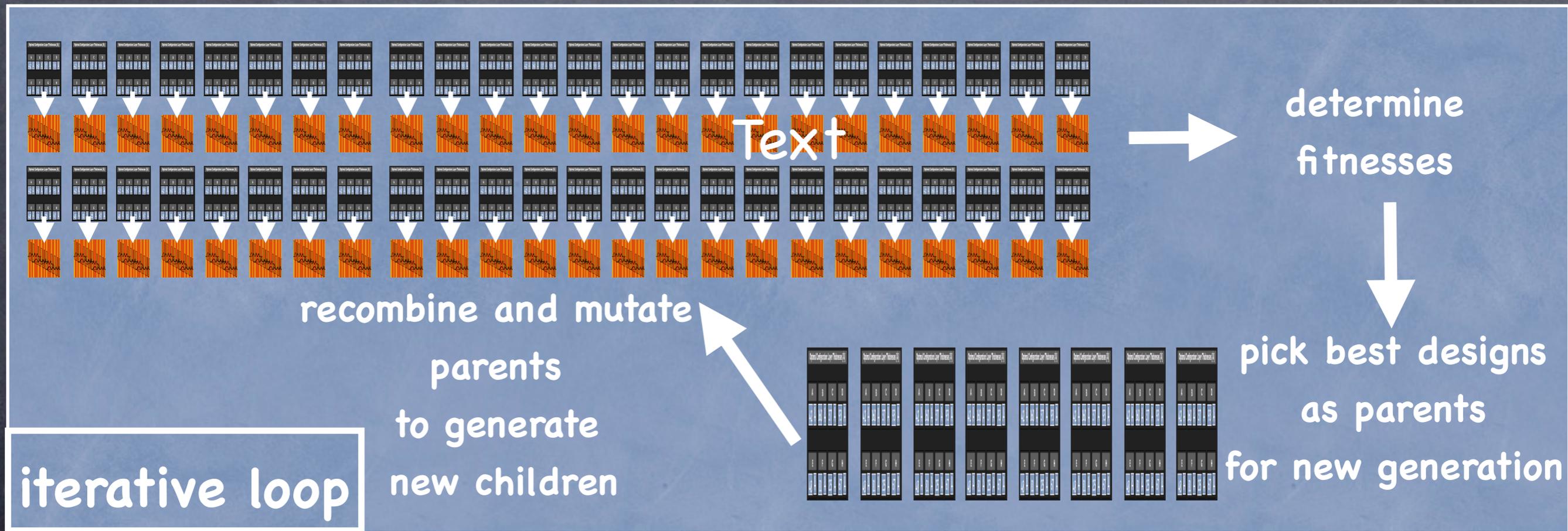
A	B	C	D
42 Å	160 Å	37 Å	93 Å
E	F	G	H
48 Å	81 Å	25 Å	67 Å



+



mutate to generate children

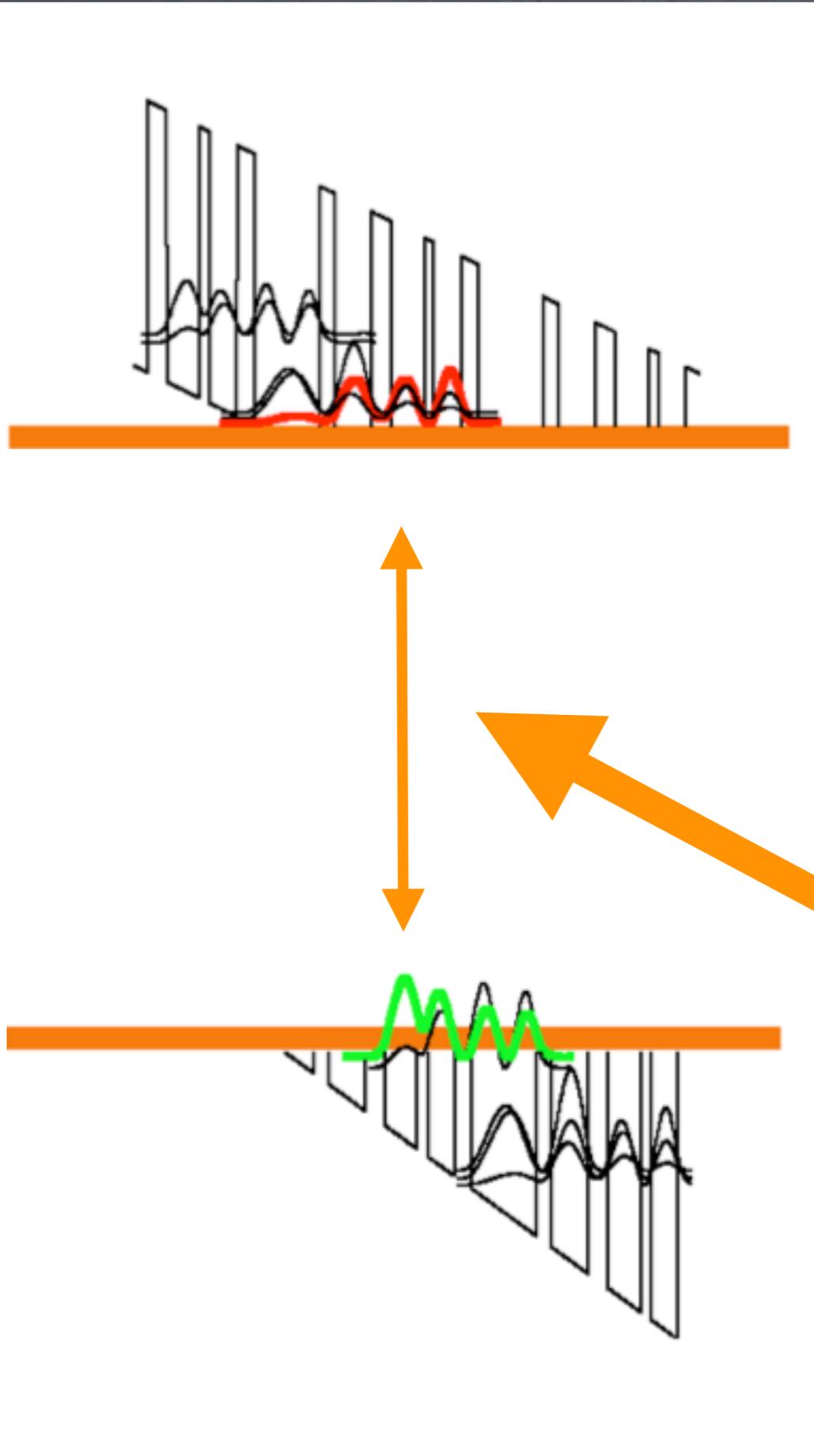


iterate until satisfactory agreement

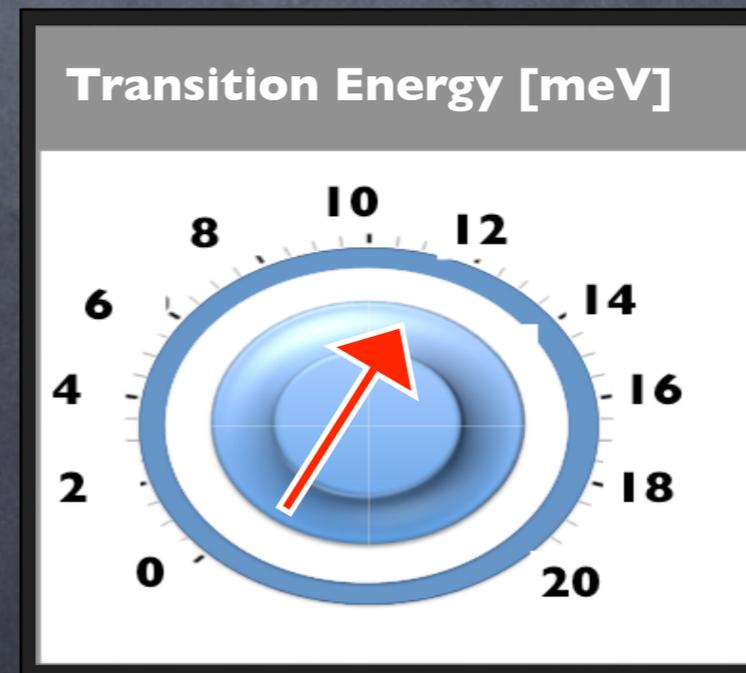
Optimal Configuration: Layer Thicknesses [Å]

A	B	C	D
43 Å	161 Å	37 Å	94 Å
E	F	G	H
47 Å	82 Å	27 Å	68 Å

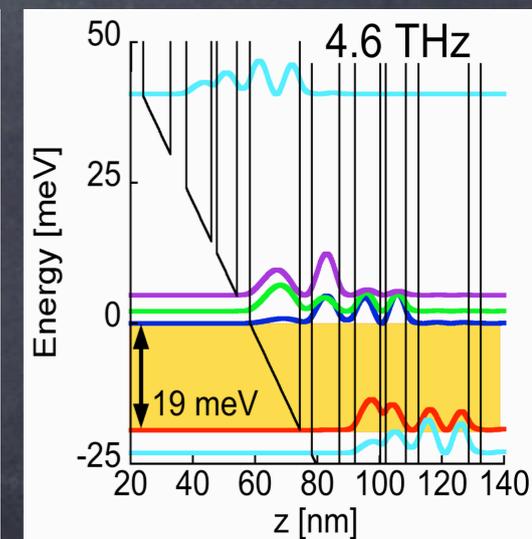
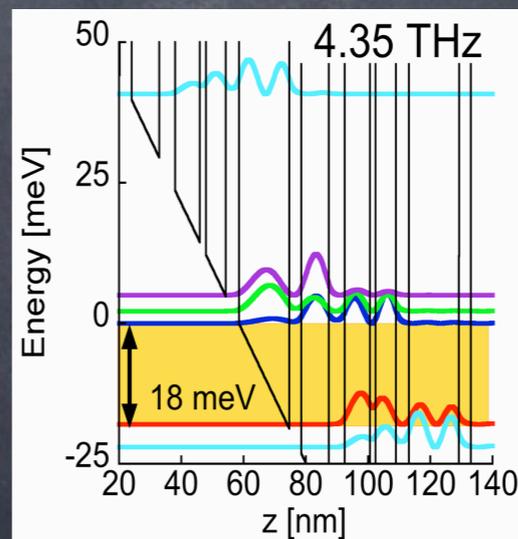
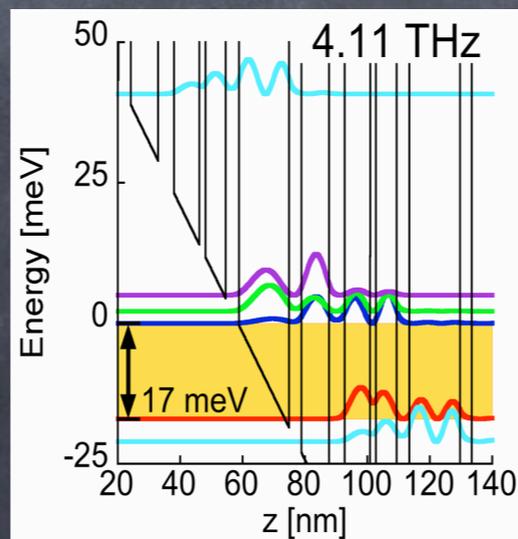
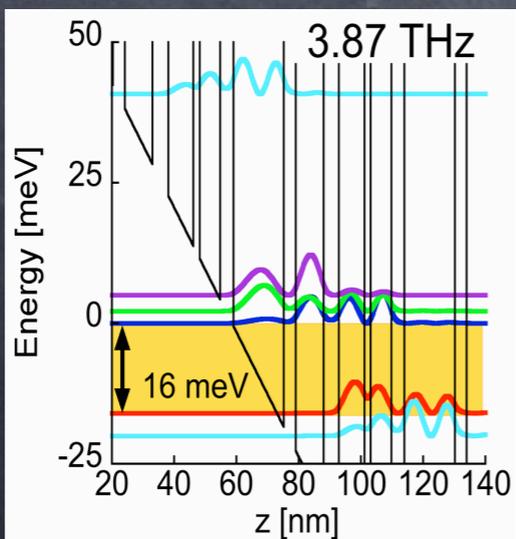
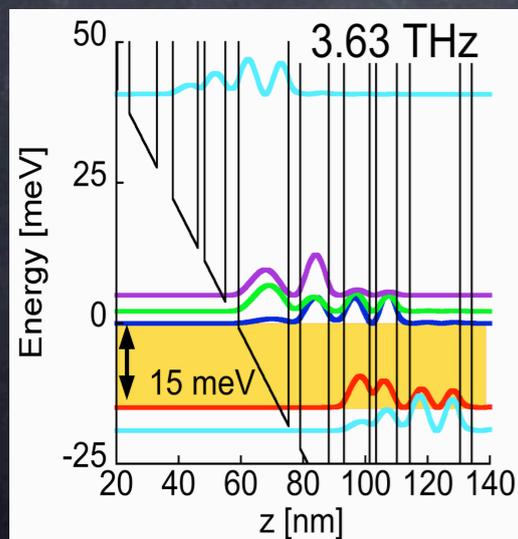
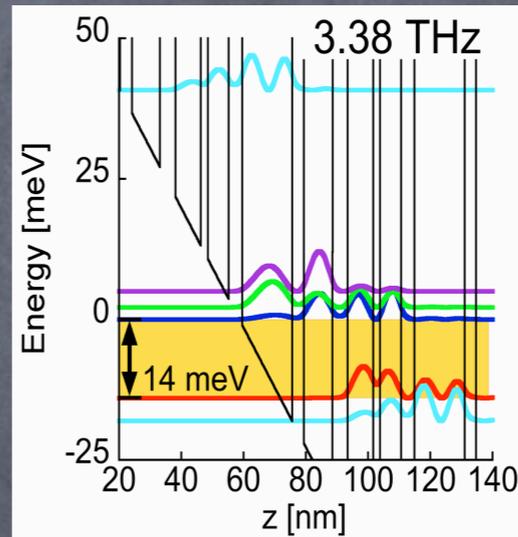
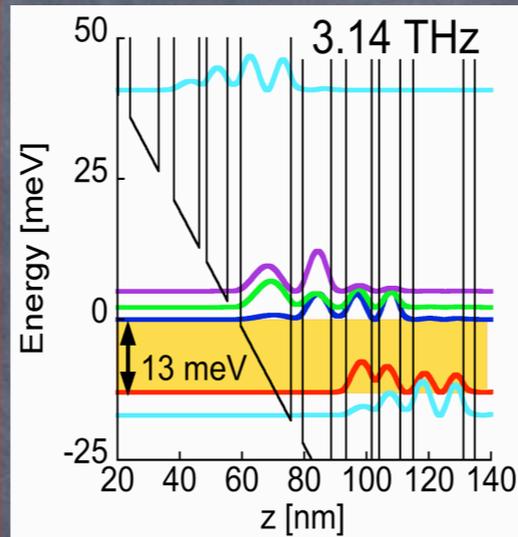
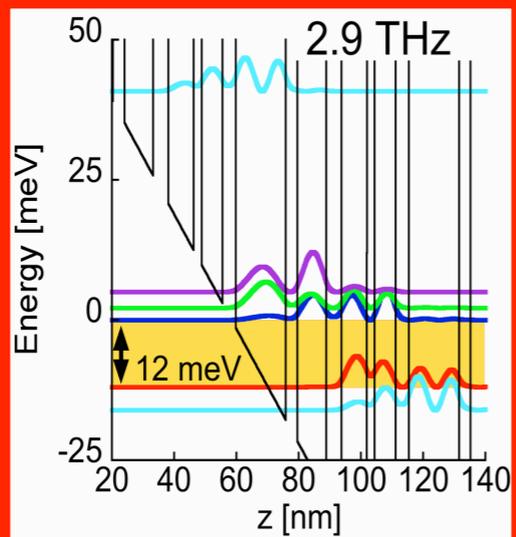
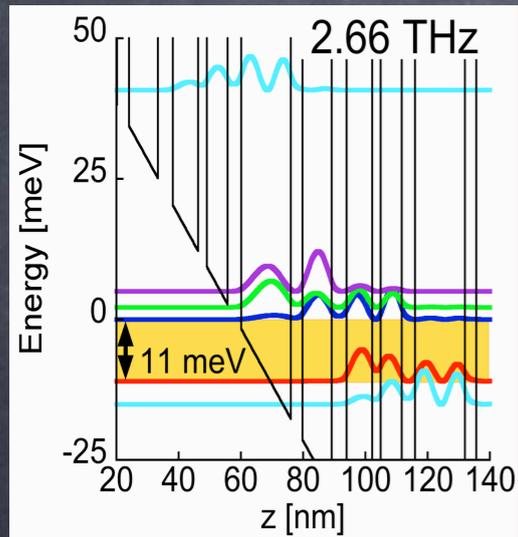
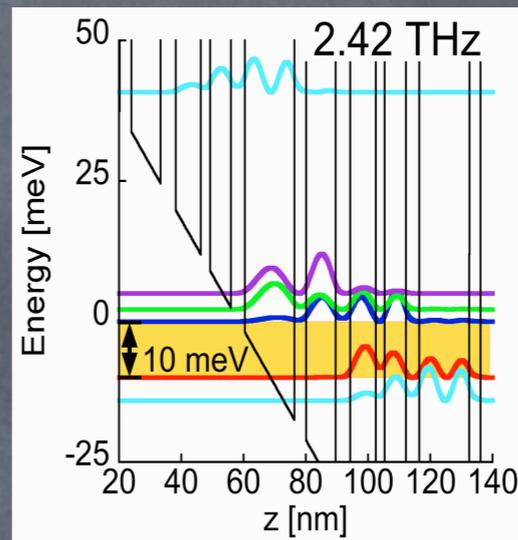
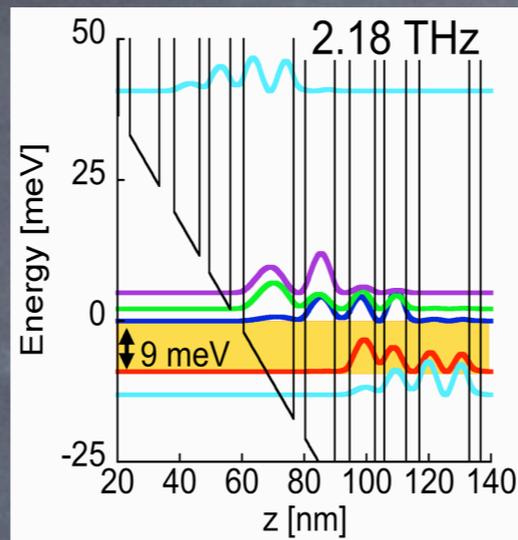
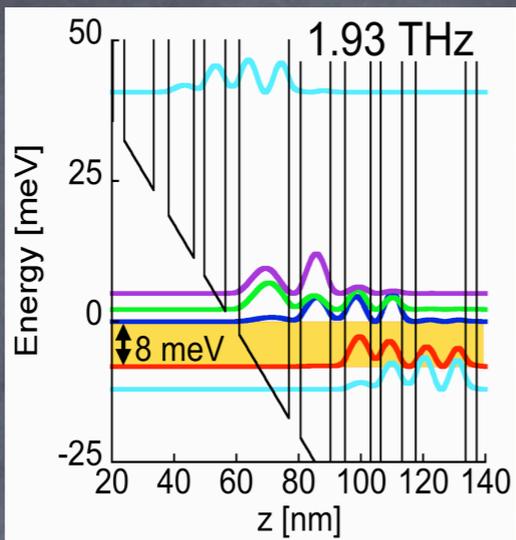
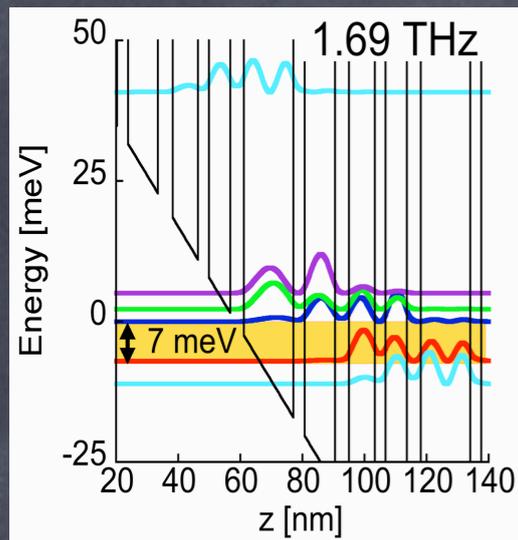
# First application: Frequency tuning!!!



Inverse  
Quantum Engineering



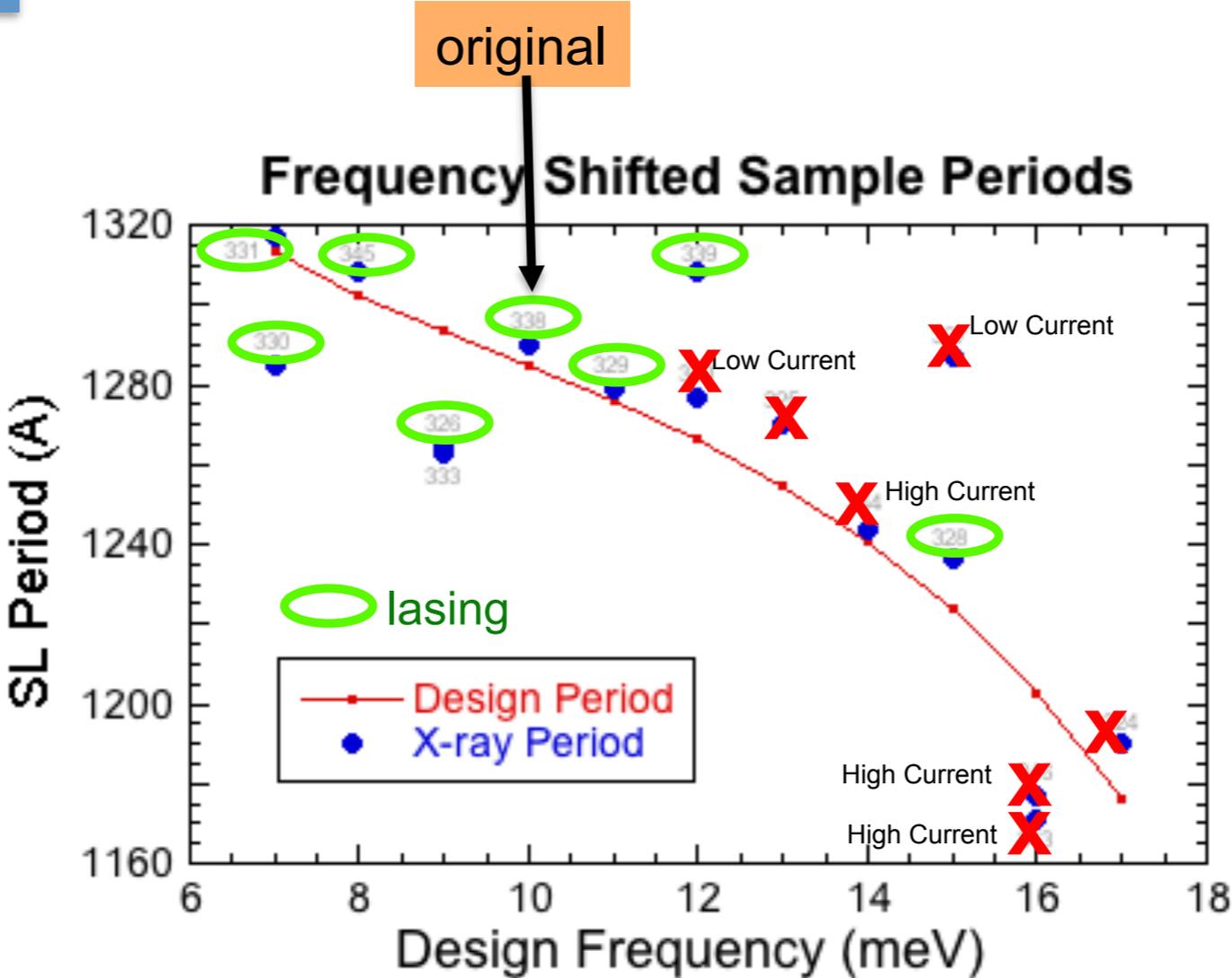
# Tuning the emission frequency of a THz QCL



1.69 THz  
to  
4.6 THz

- Growth
- Fabrication
- Experiment

# Series of IQE-designed lasers at 11 frequencies

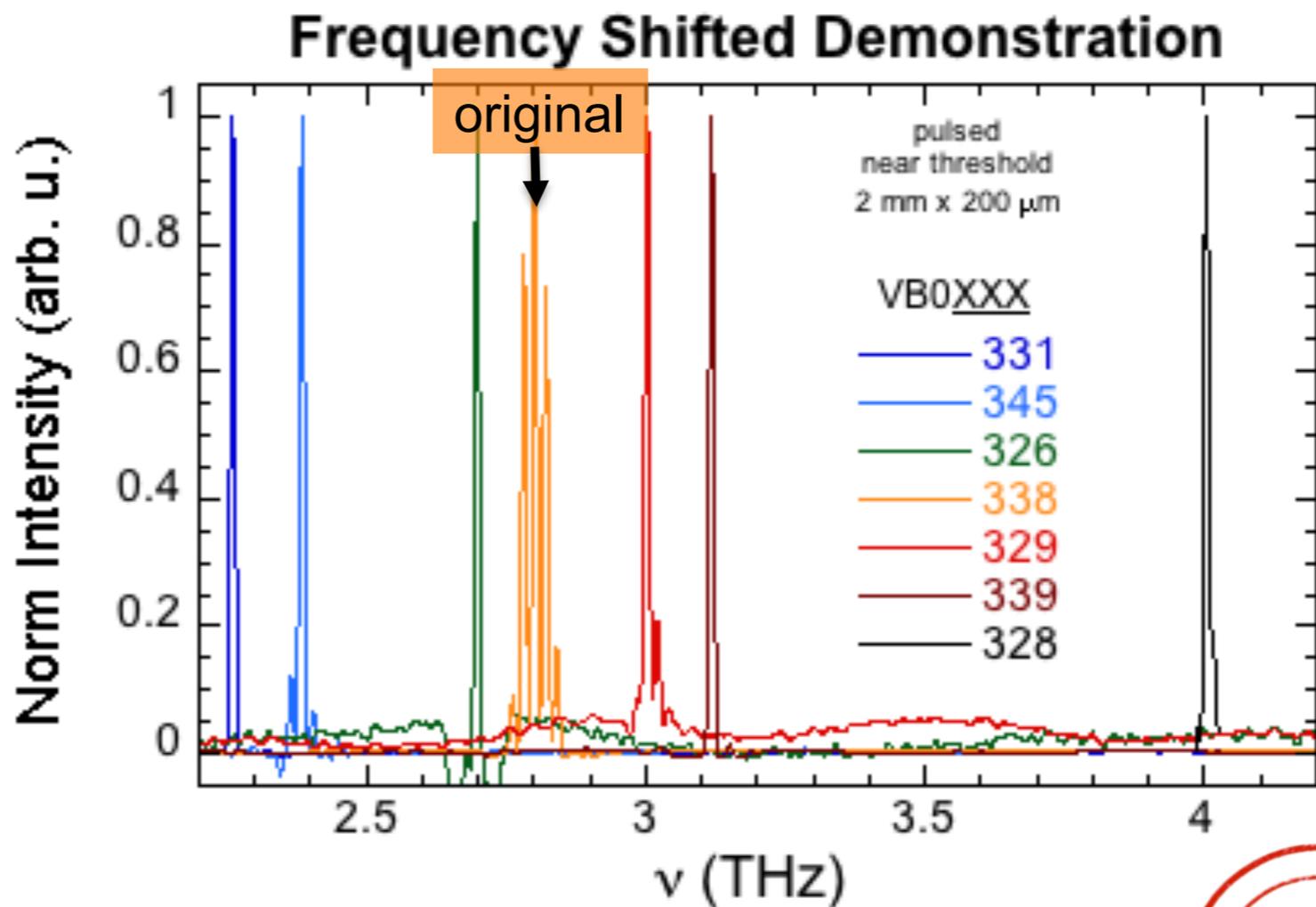


Growth

Fabrication

Experiment

## Observed lasing at 7 frequencies



# PROOF: IQE Design Tool WORKS !

VALIDATED!!



Growth

Fabrication

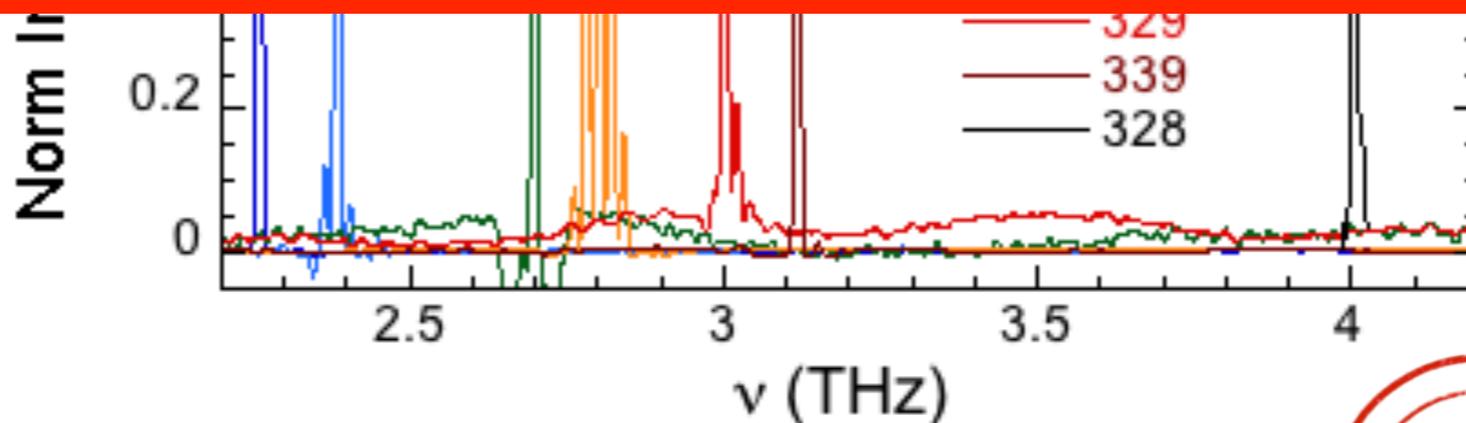
Experiment

## Observed lasing at 7 frequencies

### Frequency Shifted Demonstration

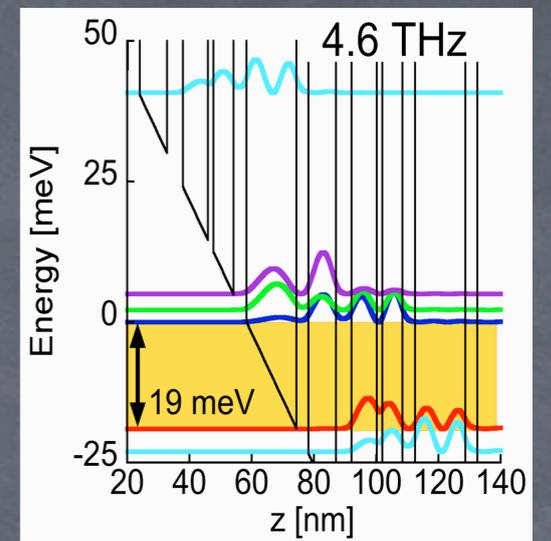
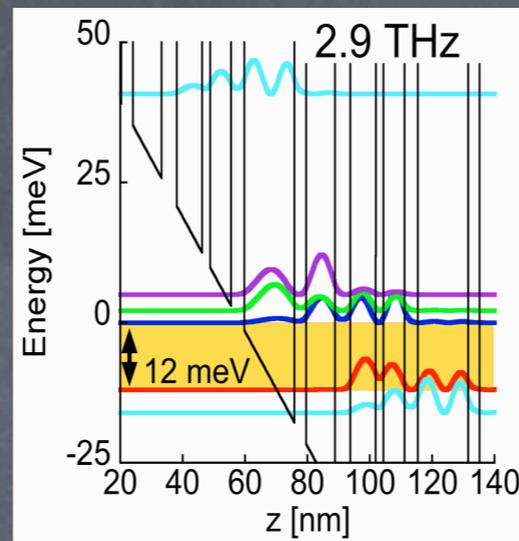
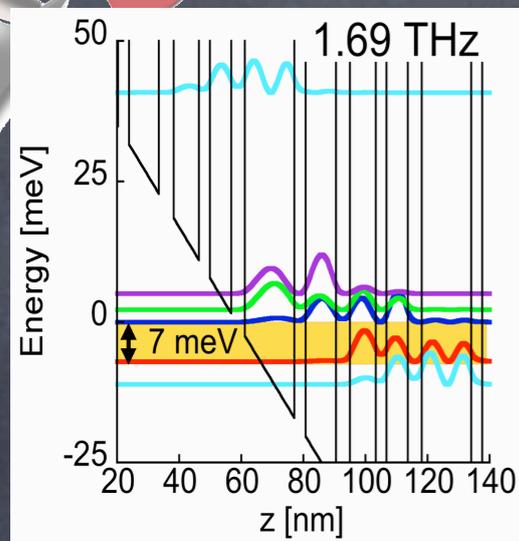


Works because we kept wavefunctions and transition energies the same!!!



**PROOF: IQE Design Tool WORKS !**





And same wavefunction shapes means:

- same Coulomb matrix elements:  $V_{\mathbf{k}_{||}}^{abcd} \propto \frac{1}{|\mathbf{k}_{||}|} \int dz \int dz' \phi_a(z) \phi_b(z') \phi_c(z) \phi_d(z') e^{-i\mathbf{k}_{||}|z-z'|}$

- same Froehlich matrix elements:  $g_{\mathbf{q}}^{ab} \propto \frac{1}{\sqrt{q_{||}^2 + q_{\perp}^2}} \int dz \phi_a(z) \phi_b(z) e^{i\mathbf{q}_{\perp}z}$

And same separation energies means:

- same allowed transitions for cc-scattering:  $\delta(\epsilon_{a,\mathbf{k}} + \epsilon_{b,\mathbf{k}'} - \epsilon_{c,\mathbf{k}+\mathbf{q}} - \epsilon_{d,\mathbf{k}'-\mathbf{q}})$

- same allowed transitions for cp-scattering:  $\delta(\epsilon_{a,\mathbf{k}} - \epsilon_{b,\mathbf{k}+\mathbf{q}} \pm \hbar\omega_{\text{LO}})$

**ONE difference: photon energy (laser frequency!)**

Simulation

Code

# Needed: Performance simulator without fit parameters !!!

Fully-microscopic, k-resolved,  
quantum kinetic simulator  
(for electrons and phonons):

$$\frac{d}{dt}\sigma_{\mathbf{k}}^{ij} = \frac{d}{dt}\langle a_{j,\mathbf{k}}^\dagger a_{j',\mathbf{k}} \rangle = \frac{i}{\hbar}\langle [H, a_{j,\mathbf{k}}^\dagger a_{j',\mathbf{k}}] \rangle$$

carrier-field

carrier-phonon

carrier-impurity

carrier-carrier

$$H_{cl} = \sum_{a,b,\mathbf{k}} \int dz \mathbf{d}_{ab}(z) \cdot \mathbf{E}(z,t) a_{a\mathbf{k}}^\dagger a_{b\mathbf{k}}$$

$$H_{cp} = \sum_{a,b,\mathbf{k}} \sum_{\mathbf{Q}} [g_{\mathbf{Q}}^{ab} a_{a\mathbf{k}}^\dagger b_{\mathbf{Q}} a_{b\mathbf{k}-\mathbf{Q}} + h.a.]$$

$$H_{ci} = \sum_{c,d} \sum_l \sum_{\mathbf{q},\mathbf{k}} V_{cd}^l(\mathbf{q}) a_{c,\mathbf{k}+\mathbf{q}}^\dagger a_{d,\mathbf{k}}$$

$$H_{cc} = \frac{1}{2} \sum_{abcd} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{q}}^{abcd} a_{a\mathbf{k}+\mathbf{q}}^\dagger a_{b\mathbf{k}'-\mathbf{q}}^\dagger a_{d\mathbf{k}} a_{c\mathbf{k}}$$

$$\frac{d}{dt}\sigma_{\mathbf{k}}^{ii} = \frac{2}{\hbar} \sum_{a \neq j} \Im[d_{a,i} \sigma_{\mathbf{k}}^{aj} E(t)]$$

$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ii}|_{cp} = & \mp \frac{2\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{a,b,c} \text{Re}[g_{\hat{\mathbf{q}}||}^{bc,ia} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{ac} \sigma_{\mathbf{k}}^{bi}] \delta(\epsilon_{\mathbf{k}}^b - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^c \pm \hbar\omega_{LO}) \\ & - \frac{2\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{a,b} \text{Re}[g_{\hat{\mathbf{q}}||}^{ba,ia} \sigma_{\mathbf{k}}^{bi}] \delta(\epsilon_{\mathbf{k}}^b - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^a \pm \hbar\omega_{LO}) (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \mp \frac{1}{2}) \\ & + \frac{2\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{a,b} \text{Re}[g_{\hat{\mathbf{q}}||}^{ib,ia} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{ab}] \delta(\epsilon_{\mathbf{k}}^i - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^b \pm \hbar\omega_{LO}) (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \pm \frac{1}{2}) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ii} = & -\frac{2\pi}{\hbar} \sum_{c,c'} \sum_{\mathbf{q}} \text{Re}[V_{\mathbf{q}}^{ci,c'} \sigma_{\mathbf{k}}^{c'ij}] \delta(\epsilon_{c,\mathbf{k}} - \epsilon_{c,\mathbf{k}+\mathbf{q}}) \\ & + \frac{2\pi}{\hbar} \sum_{c,c'} \sum_{\mathbf{q}} \text{Re}[V_{\mathbf{q}}^{ci,c'} \sigma_{\mathbf{k}+\mathbf{q}}^{cc'}] \delta(\epsilon_{i,\mathbf{k}} - \epsilon_{c',\mathbf{k}+\mathbf{q}}) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ii}|_{scatt(cc)} = & \frac{4\pi}{\hbar} \sum_{\mathbf{k}',\mathbf{q}} \sum_{w,x,y,z,g} \Re[V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}+\mathbf{q}}^{wx} \sigma_{\mathbf{k}'-\mathbf{q}}^{zg} (V_{\mathbf{q}}^{iyzg} - \sum_0 \sigma_{\mathbf{k}'}^{oy} V_{\mathbf{q}}^{iozg}) \\ & \times \delta(\epsilon_{i,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\ & + \sum_0 V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}}^{xi} (-\sigma_{\mathbf{k}'-\mathbf{q}}^{gz} \sigma_{\mathbf{k}+\mathbf{q}}^{ow} V_{\mathbf{q}}^{iyog} + \sigma_{\mathbf{k}'}^{yo} (\sigma_{\mathbf{k}+\mathbf{q}}^{gw} V_{\mathbf{q}}^{iogz} + \sigma_{\mathbf{k}'-\mathbf{q}}^{gz} V_{\mathbf{q}}^{iowg} \\ & - V_{\mathbf{q}}^{io wz})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ij} = & -\frac{i}{\hbar} \sum_a [d_{j,i} \sigma_{\mathbf{k}}^{jj} - d_{j,i} \sigma_{\mathbf{k}}^{ii}] E(t) \\ & - \frac{i}{\hbar} \sum_{a \neq j} d_{a,i} \sigma_{\mathbf{k}}^{aj} E(t) + \frac{i}{\hbar} \sum_{a \neq i} d_{j,a} \sigma_{\mathbf{k}}^{ia} E(t) \end{aligned}$$

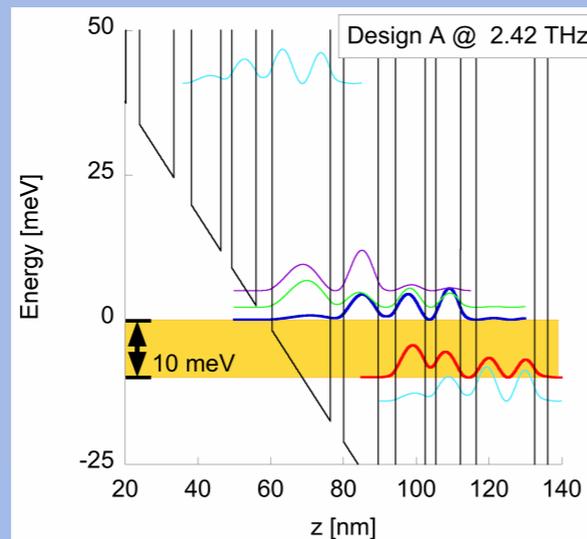
$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ij}|_{cp} = & \frac{\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{b,c} [\mp \sum_a g_{\hat{\mathbf{q}}||}^{bc,ia} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{ac} \sigma_{\mathbf{k}}^{bj} - g_{\hat{\mathbf{q}}||}^{bc,ic} (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \mp \frac{1}{2}) \sigma_{\mathbf{k}}^{bj} \\ & \mp \sum_a g_{\hat{\mathbf{q}}||}^{ja,bc} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{ca} \sigma_{\mathbf{k}}^{ib} - g_{\hat{\mathbf{q}}||}^{jc,bc} (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \mp \frac{1}{2}) \sigma_{\mathbf{k}}^{ib}] \delta(\epsilon_{\mathbf{k}}^b - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^c \pm \hbar\omega_{LO}) \\ & + \frac{\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{c,b} g_{\hat{\mathbf{q}}||}^{jb,ic} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{cb} \delta(\epsilon_{\mathbf{k}}^j - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^b \pm \hbar\omega_{LO}) (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \pm \frac{1}{2}) \\ & + \frac{\pi}{\hbar} \sum_{\hat{\mathbf{q}}} \sum_{c,b} g_{\hat{\mathbf{q}}||}^{jc,ib} \sigma_{\mathbf{k}+\hat{\mathbf{q}}}^{bc} \delta(\epsilon_{\mathbf{k}}^i - \epsilon_{\mathbf{k}+\hat{\mathbf{q}}}^b \pm \hbar\omega_{LO}) (n_{\hat{\mathbf{q}}||} + \frac{1}{2} \pm \frac{1}{2}) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ij} = & -\frac{\pi}{\hbar} \sum_{c,c'} \sum_{\mathbf{q}} [V_{\mathbf{q}}^{ci,c'} \sigma_{\mathbf{k}}^{c'ij} + V_{\mathbf{q}}^{c'c,ic'} \sigma_{\mathbf{k}}^{ic'}] \delta(\epsilon_{c,\mathbf{k}} - \epsilon_{c,\mathbf{k}+\mathbf{q}}) \\ & + \frac{\pi}{\hbar} \sum_{c,c'} \sum_{\mathbf{q}} \sigma_{\mathbf{k}+\mathbf{q}}^{cc'} [V_{\mathbf{q}}^{ci,c'} \delta(\epsilon_{j,\mathbf{k}} - \epsilon_{c,\mathbf{k}+\mathbf{q}}) + \delta(\epsilon_{i,\mathbf{k}} - \epsilon_{c,\mathbf{k}+\mathbf{q}})] \end{aligned}$$

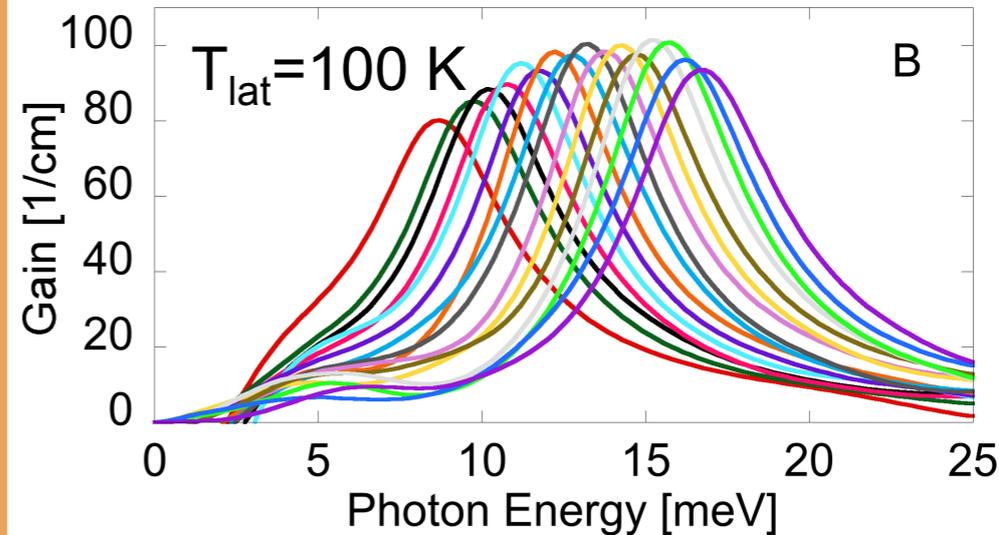
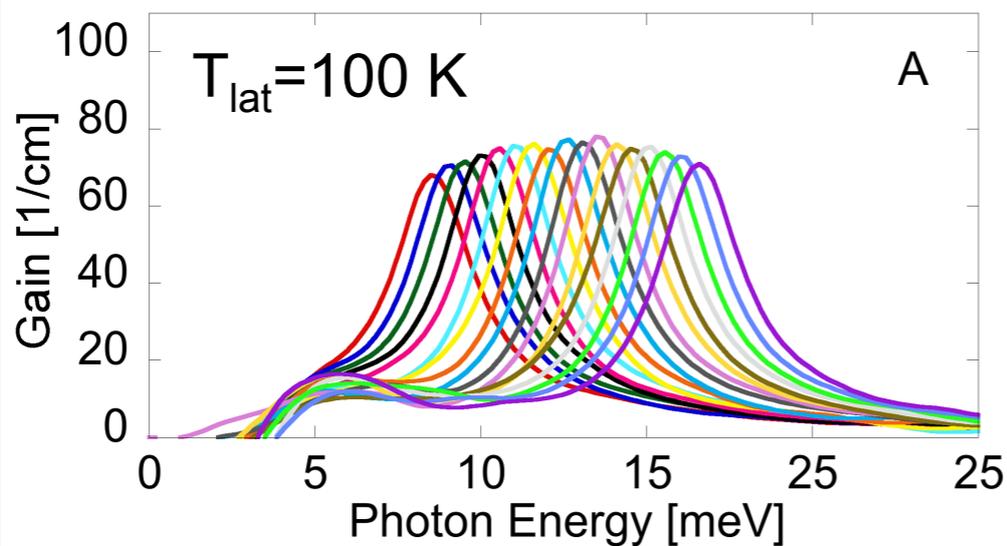
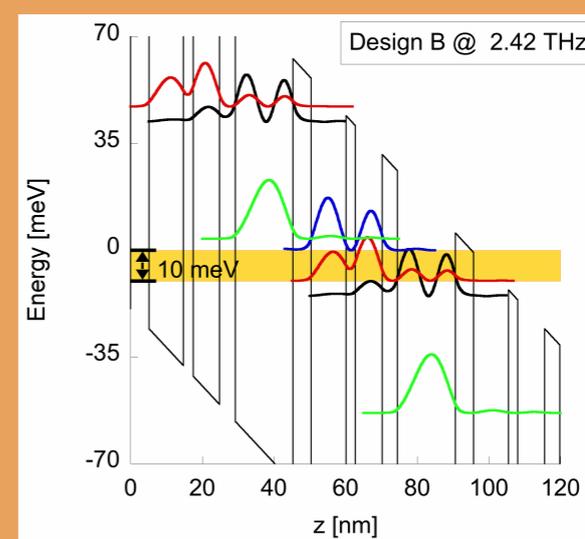
$$\begin{aligned} \frac{d}{dt}\sigma_{\mathbf{k}}^{ij}|_{scatt(cc)} = & \frac{2\pi}{\hbar} \sum_{\mathbf{k}',\mathbf{q}} \sum_{w,x,y,z,g} [V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}+\mathbf{q}}^{wx} \sigma_{\mathbf{k}'-\mathbf{q}}^{zg} (V_{\mathbf{q}}^{iyzg} - \sum_0 \sigma_{\mathbf{k}'}^{oy} V_{\mathbf{q}}^{iozg}) \\ & \times \delta(\epsilon_{i,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\ & + V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}+\mathbf{q}}^{xw} \sigma_{\mathbf{k}'-\mathbf{q}}^{gz} (V_{\mathbf{q}}^{iyzq} - \sum_0 \sigma_{\mathbf{k}'}^{yo} V_{\mathbf{q}}^{iozg}) \\ & \times \delta(\epsilon_{j,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\ & + \sum_0 V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}}^{xj} (-\sigma_{\mathbf{k}'-\mathbf{q}}^{gz} \sigma_{\mathbf{k}+\mathbf{q}}^{ow} V_{\mathbf{q}}^{iyog} + \sigma_{\mathbf{k}'}^{yo} (\sigma_{\mathbf{k}+\mathbf{q}}^{gw} V_{\mathbf{q}}^{iogz} + \sigma_{\mathbf{k}'-\mathbf{q}}^{gz} V_{\mathbf{q}}^{iowg} \\ & - V_{\mathbf{q}}^{io wz})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\ & + \sum_0 V_{\mathbf{q}}^{xywz} \sigma_{\mathbf{k}}^{ix} (-\sigma_{\mathbf{k}'-\mathbf{q}}^{zg} \sigma_{\mathbf{k}+\mathbf{q}}^{wo} V_{\mathbf{q}}^{jyog} + \sigma_{\mathbf{k}'}^{yo} (\sigma_{\mathbf{k}+\mathbf{q}}^{wg} V_{\mathbf{q}}^{jogz} + \sigma_{\mathbf{k}'-\mathbf{q}}^{gz} V_{\mathbf{q}}^{jowg} \\ & - V_{\mathbf{q}}^{jowz})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \end{aligned}$$

# Use quantum kinetic performance simulator to investigate $1/kt$

## Frequency-shift design A

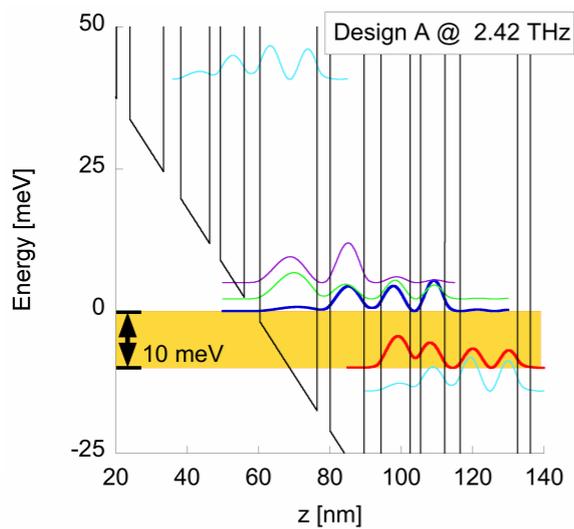
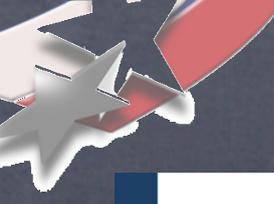


## Frequency-shift design B



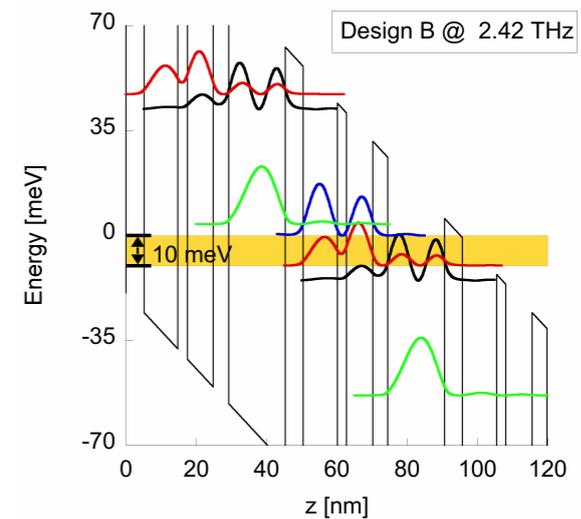
**Max. gain depends on design not frequency**



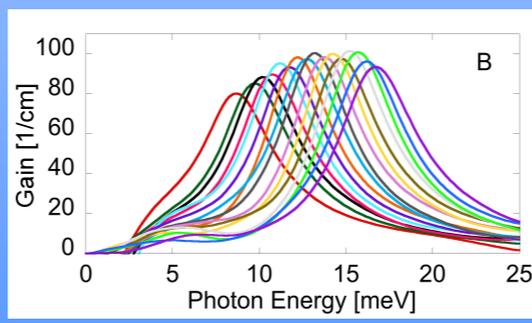
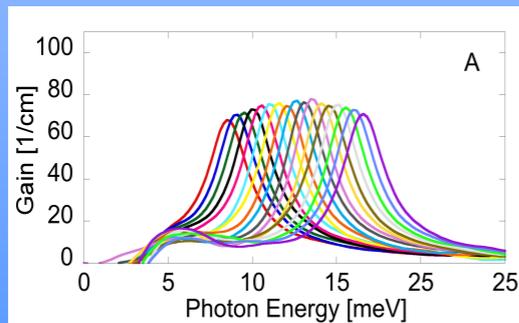


Which design is better???

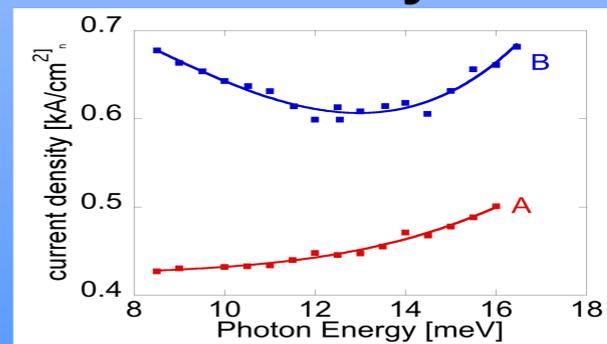
And WHY ???



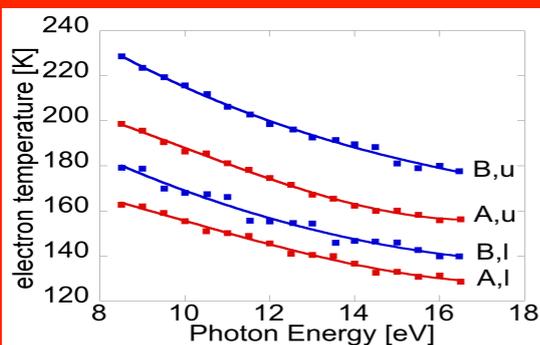
gain...



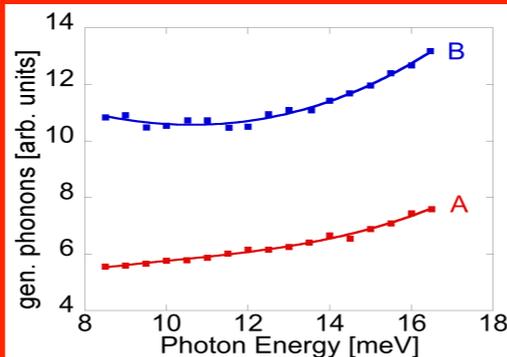
current density...



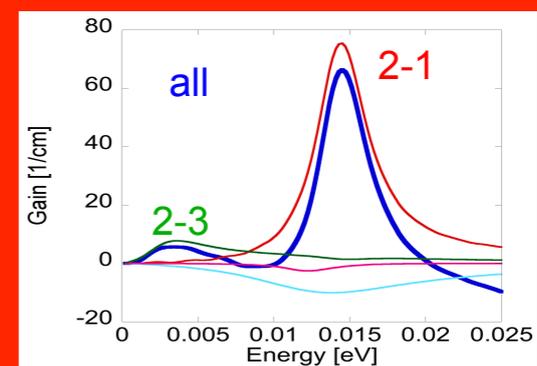
electrons...



phonons...

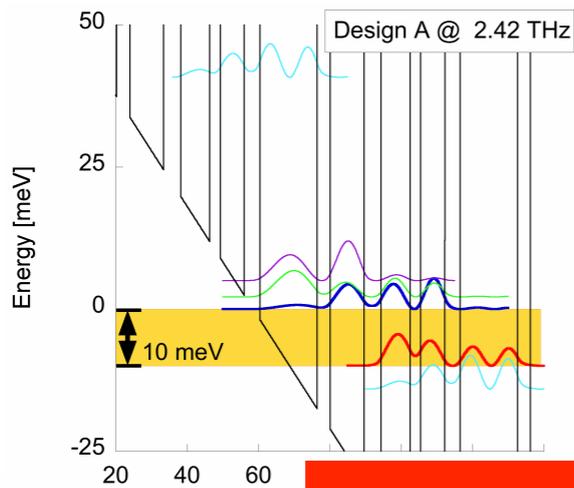
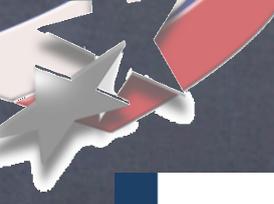


diff. gain contrib....



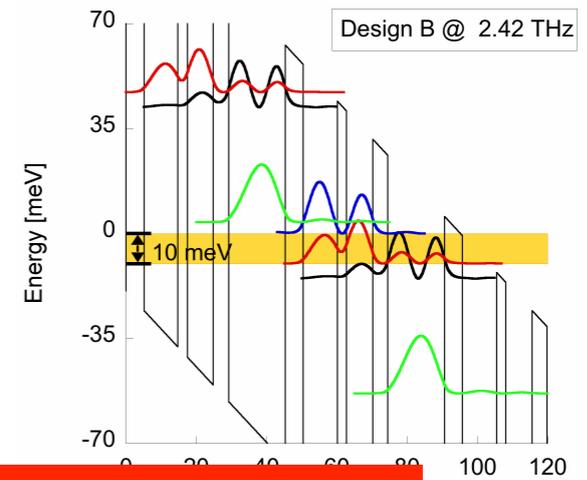
Discovery at the Interface  
of Science and Engineering:  
**Science Matters!**

Cannot "simply" simulate... can actually start understanding.

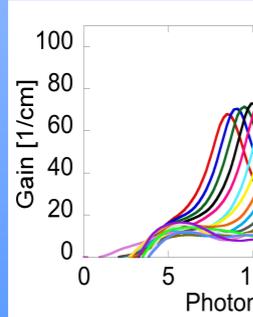


Which design is better???

And WHY ???

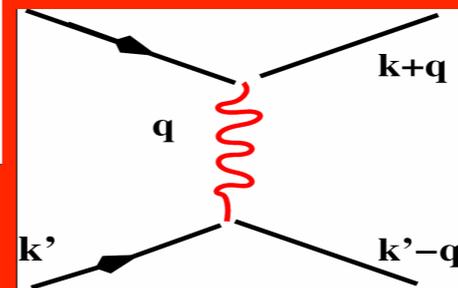
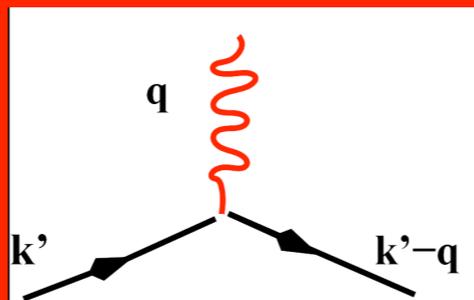
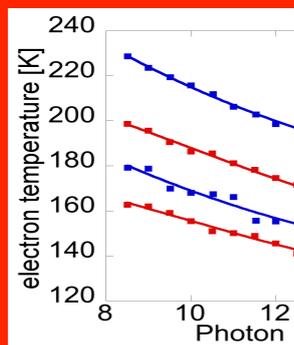


gain...



Minimizing negative  
and  
maximizing positive  
effects of electron scattering

electrons

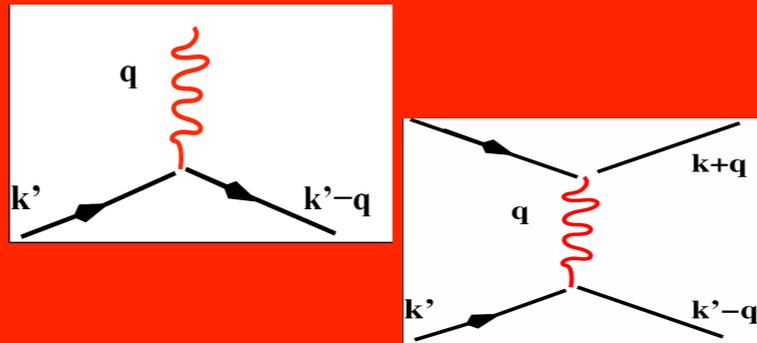


Discovery at the Interface  
of Science and Engineering:

Science Matters!

Cannot "simply" simulate... can actually start understanding.

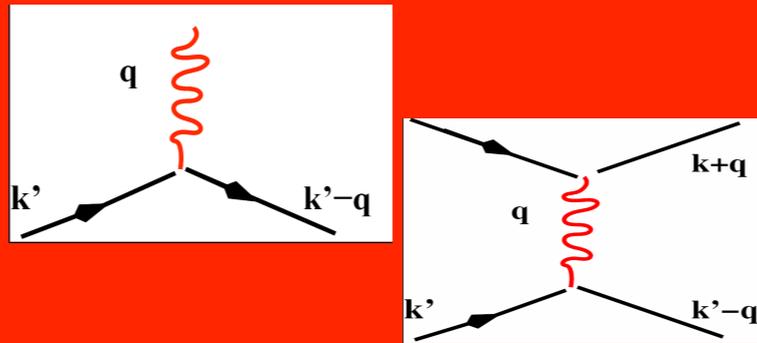
Minimizing negative  
and  
maximizing positive  
effects of electron scattering



Quantum Cascade Lasers !!!

300–500 nm Photocathodes (???)

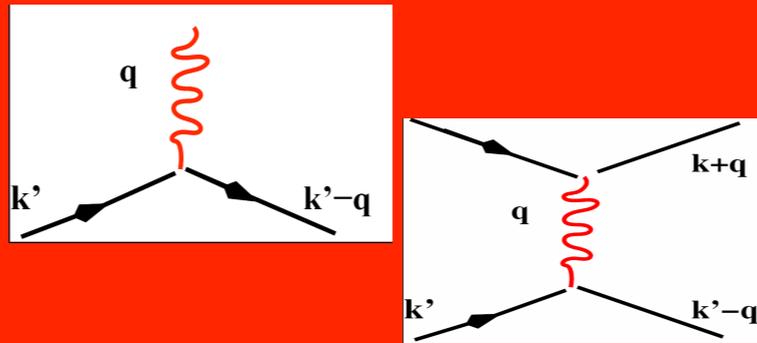
Minimizing negative  
and  
maximizing positive  
effects of electron scattering



300–500 nm Photocathodes

Spicer's 3-step model:  
Absorption, Transport, Emission

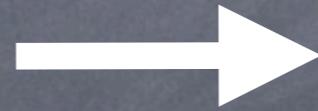
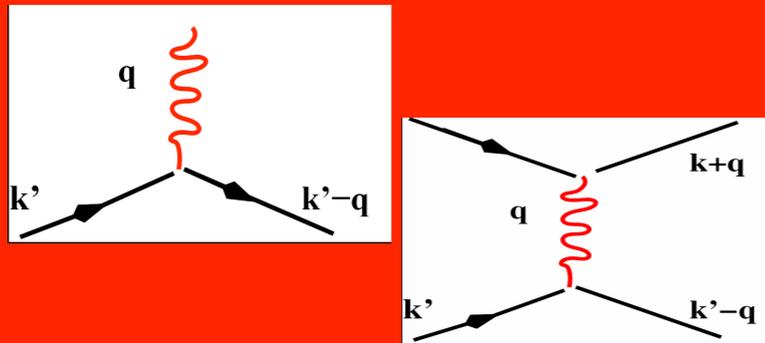
Minimizing negative  
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300–500 nm Photocathodes

Spicer's 3-step model:  
Absorption, **Transport**, Emission

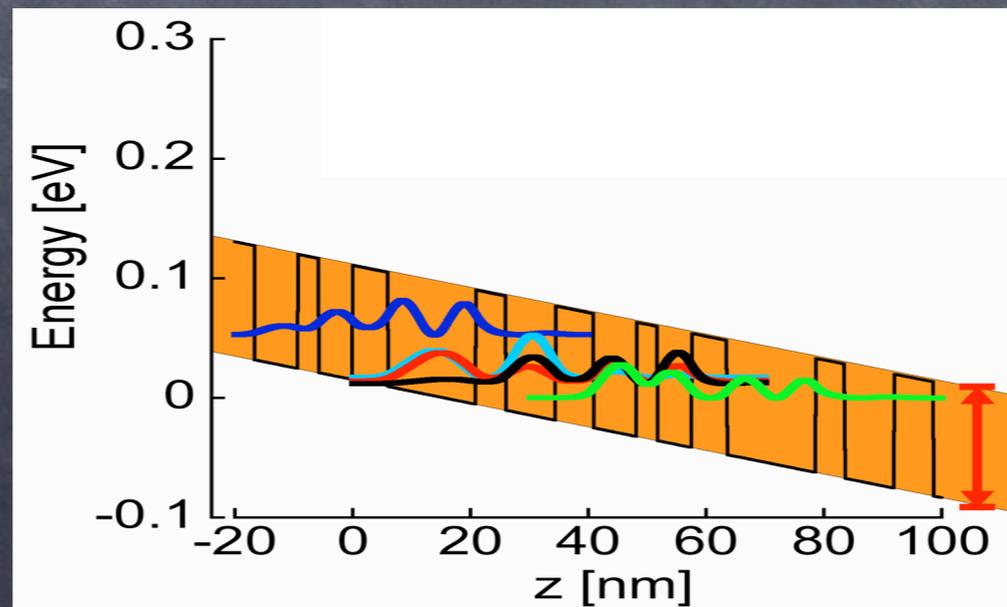
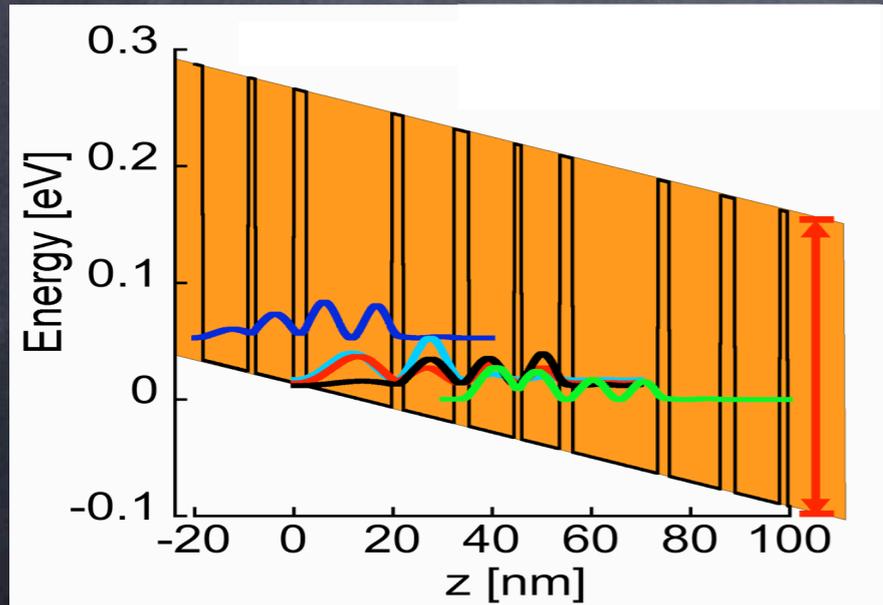
Minimizing negative  
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effects of electron scattering



300-500 nm  
Photocathodes



Spicer's 3-step model:  
Absorption, **Transport**, Emission



e.g. GaN ?