Understanding the high temperature limits of THz QCLs

SAND2012-1027P

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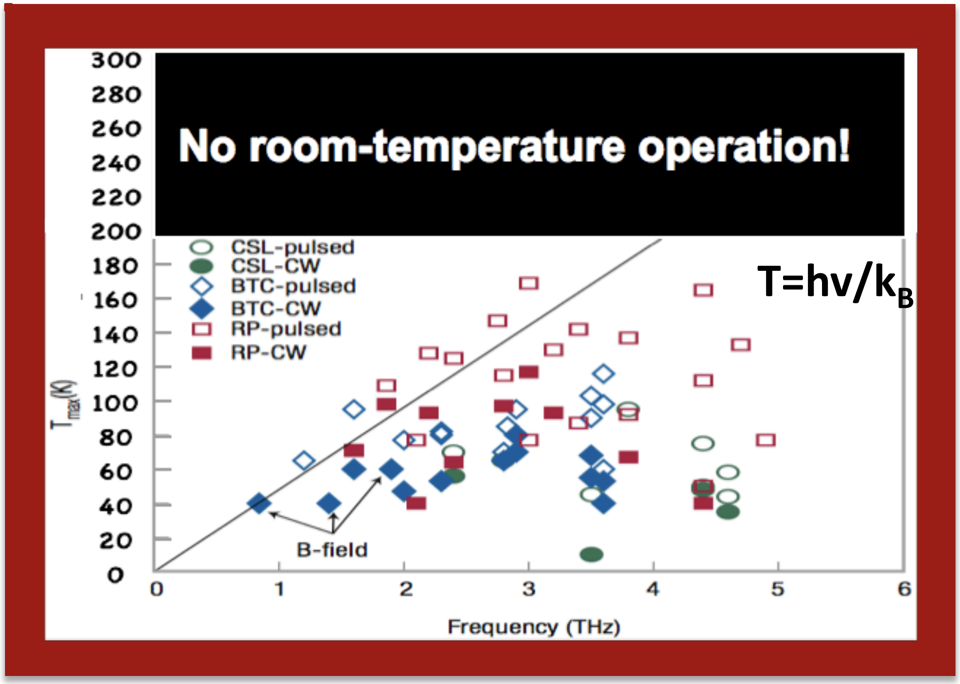
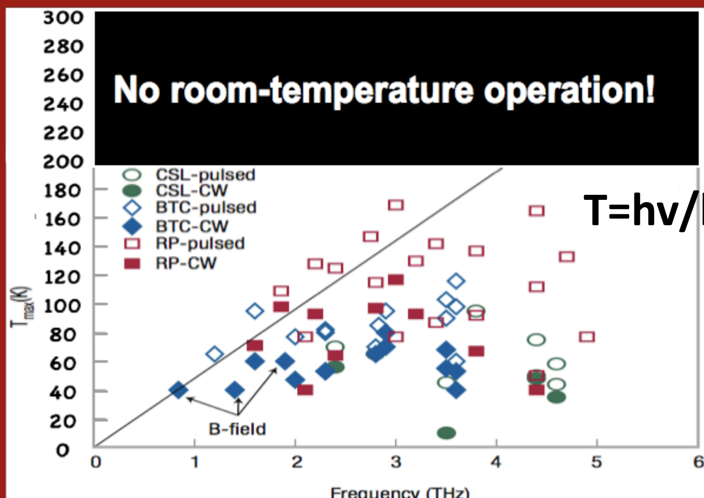
Key Team Members:
M.C. Wanke, M.J. Cich, A.D. Grine, C.T. Fuller, J.L. Reno



Understanding the high temperature limits of THz QCLs

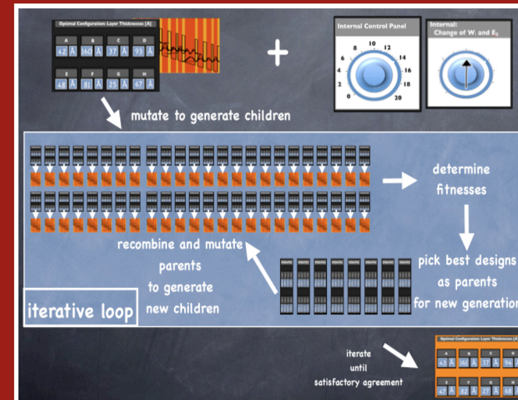
I.



$T=h\nu/k_B$

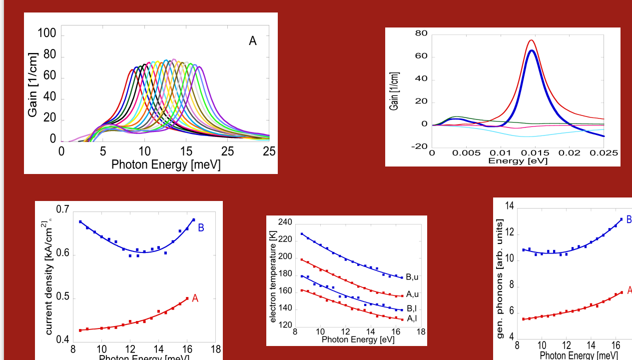
II.

IQE Design Tool

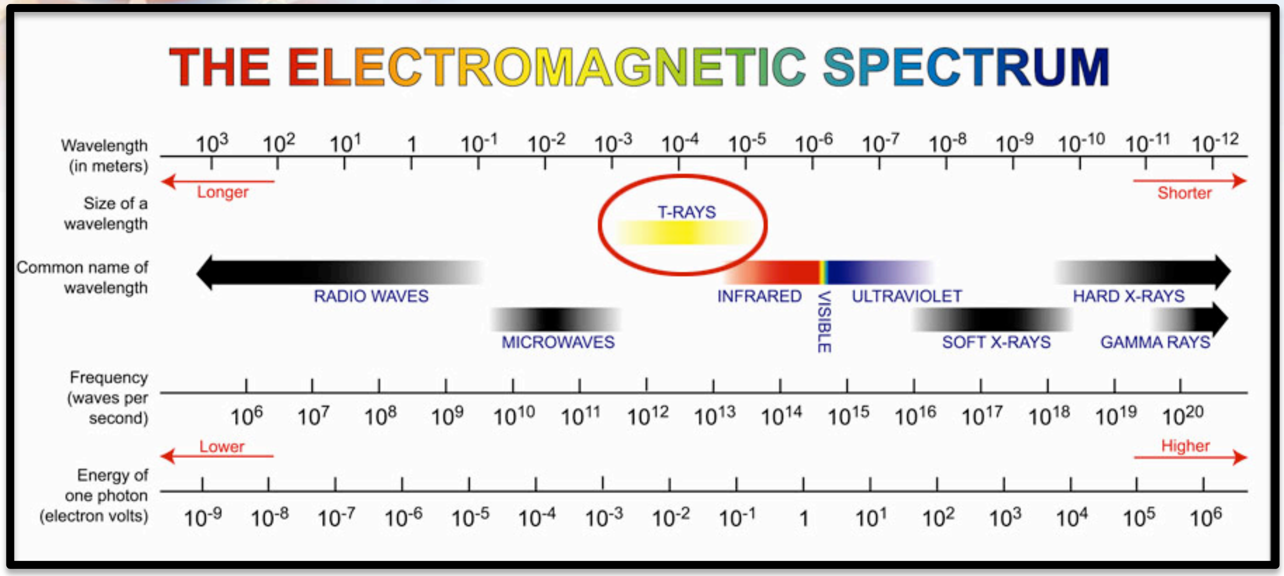


III.

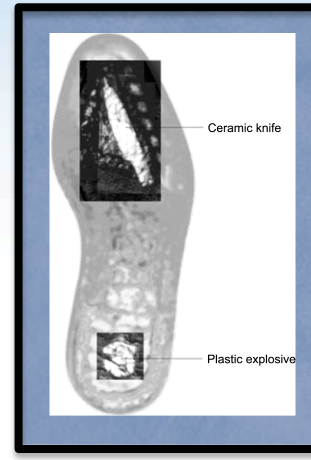
No-Fit Performance Simulator



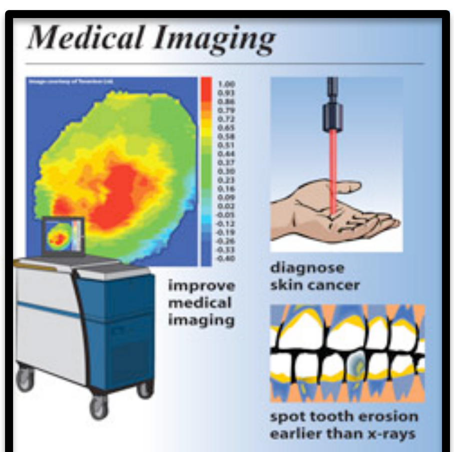
THz !!!

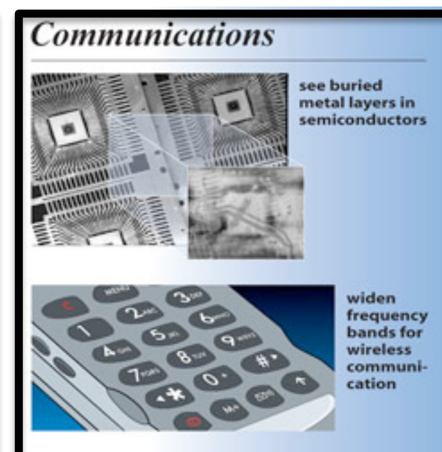


1 THz
1 ps
33 cm^{-1}
300 μm
48 K
4.1 meV



- **many materials (clothes, packaging materials) are transparent**
- **chemical signatures (THz-fingerprints)**
- **non-invasive, do not damage biological tissue**





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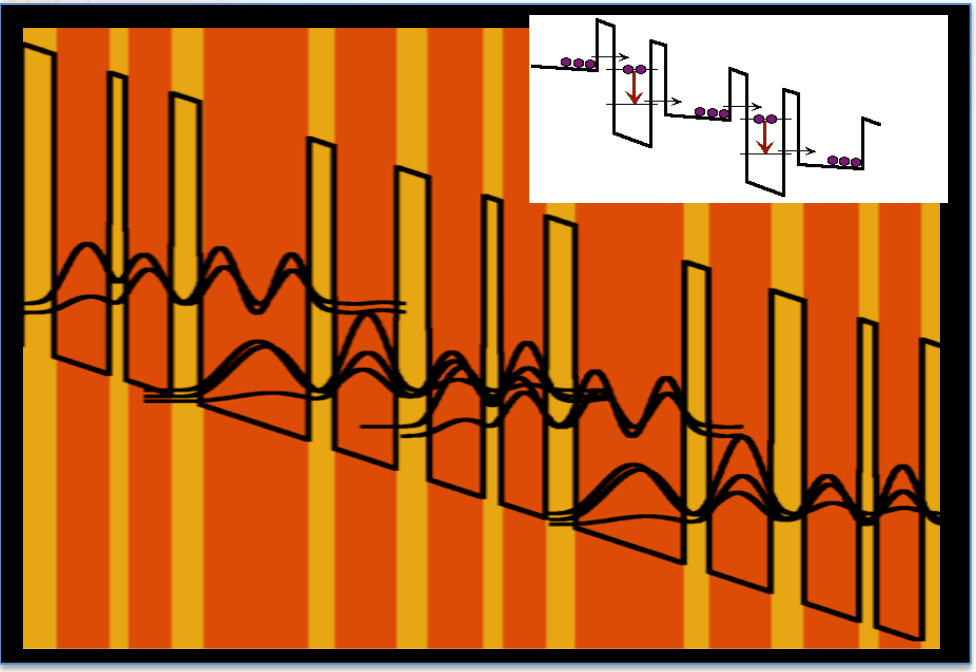
Quantum Cascade Laser: "Engineered collection of quantum wells with discrete eigenstates"



Kazarinov/Suris (1971)
(proposed amplification of light through intersubband transitions)

⬇

Capasso et al. (1983)
(showed sequential resonant tunneling through many quantum wells)

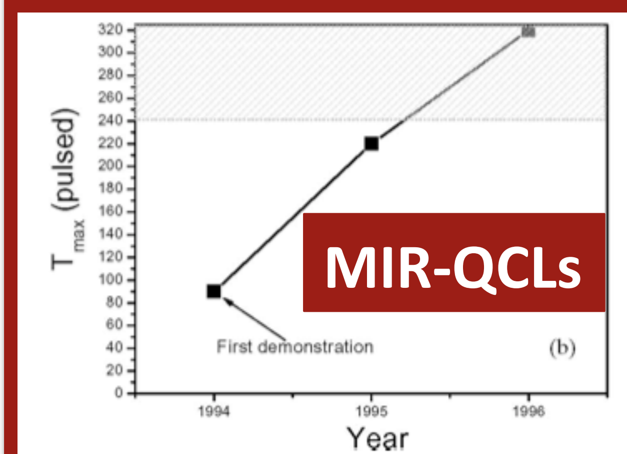
⬇

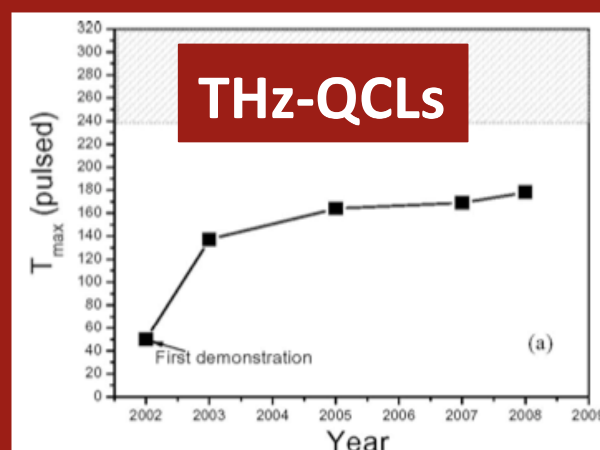
Faist et al. (1994)
(first QCL demonstration, 4 μ)

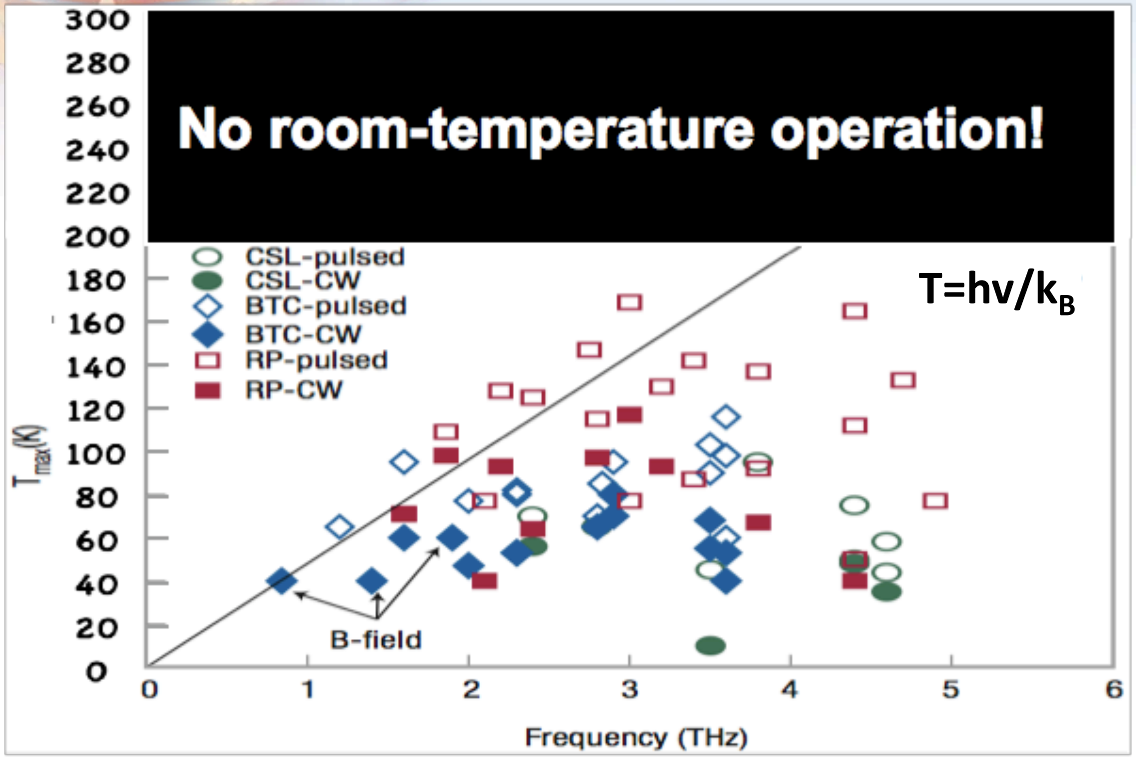
⬇

Koehler et al. (2002)
(first THz-QCL demonstration, 4.4 THz)

The path to room temperature….







But why?
Is there a fundamental limit?
$T_{MAX} \leq h\nu/k_B$?

Question from all potential sponsors:

"Can I get a room temperature THz QCL?"

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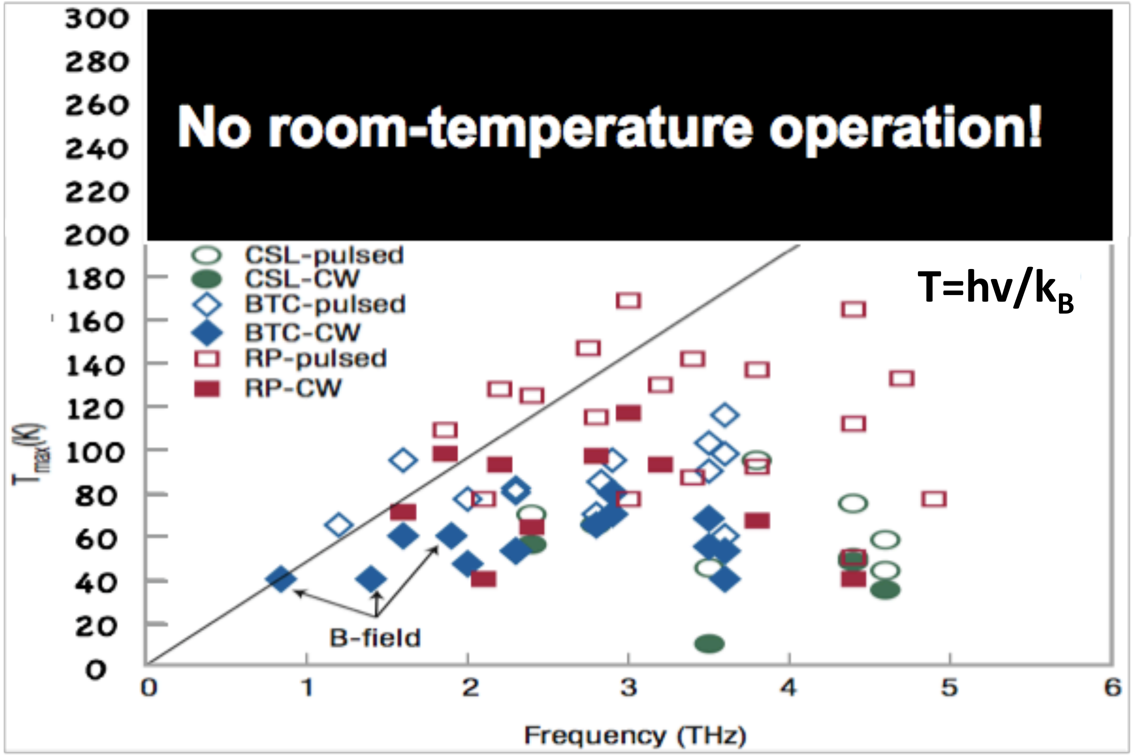
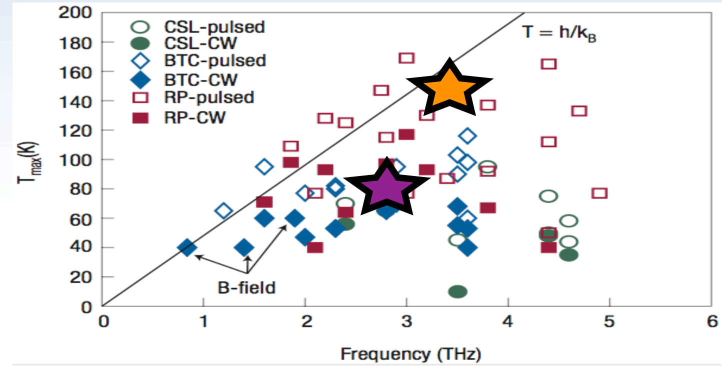
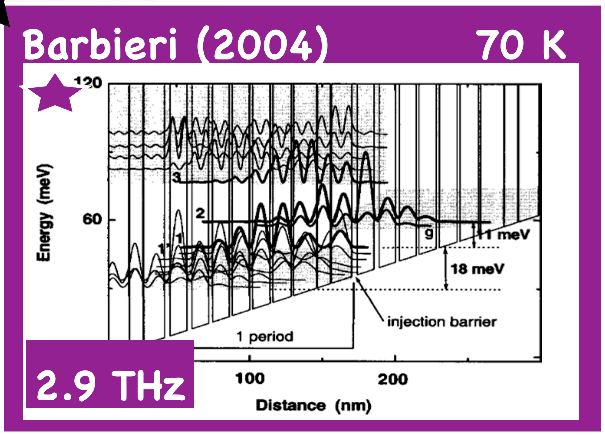
How do you 'improve understanding'? (and preferably in an efficient way)

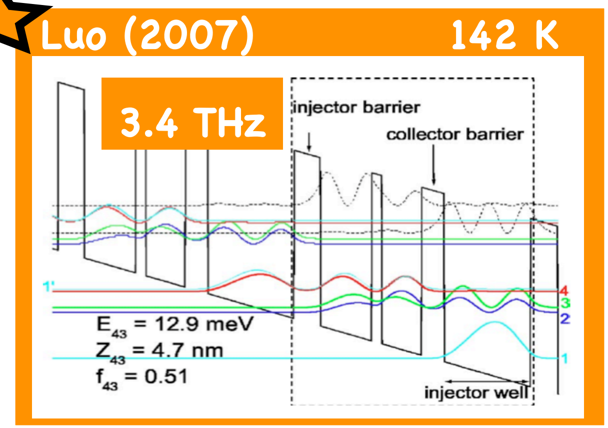


Maybe by comparing the different QCLs?

Comparing QCLs:







and have:

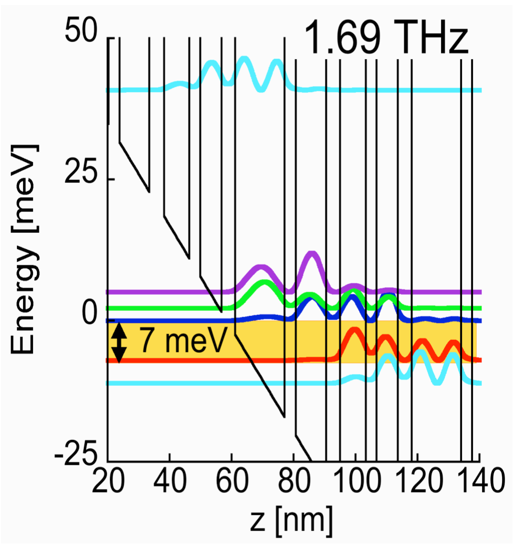
- different depletion (BTC vs RP)
- different number of quantum wells (9 vs 3)
- different photon energy (12 vs 13 meV)
- different wavefunctions..

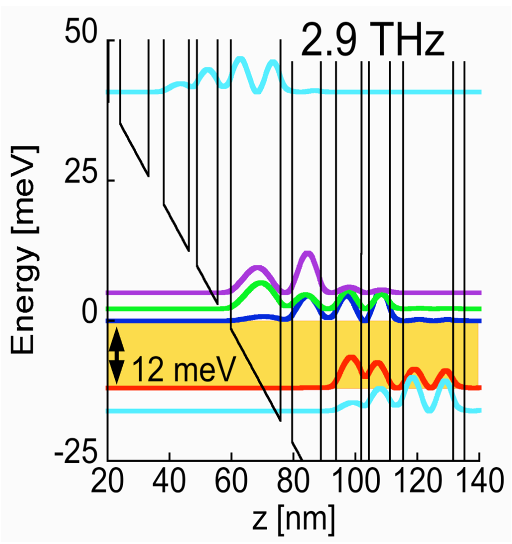
whole lot of ‘different’

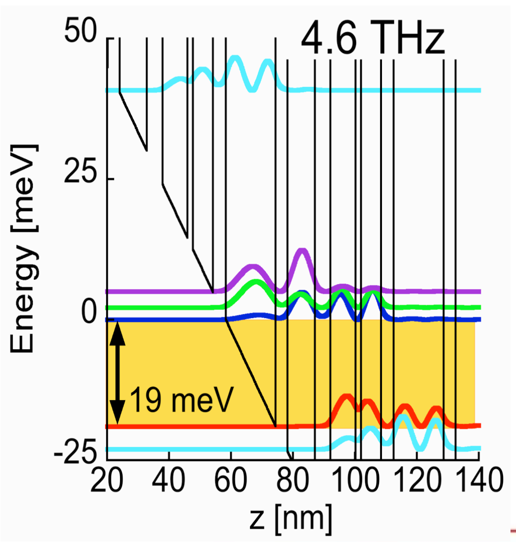
It would be really helpful,

if we could start with one difference first

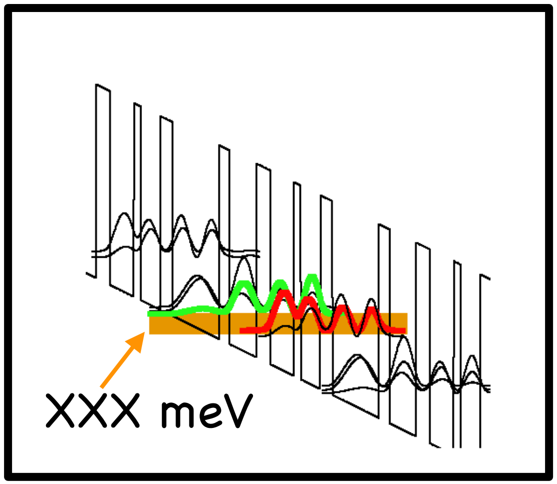
e.g. the photon energy

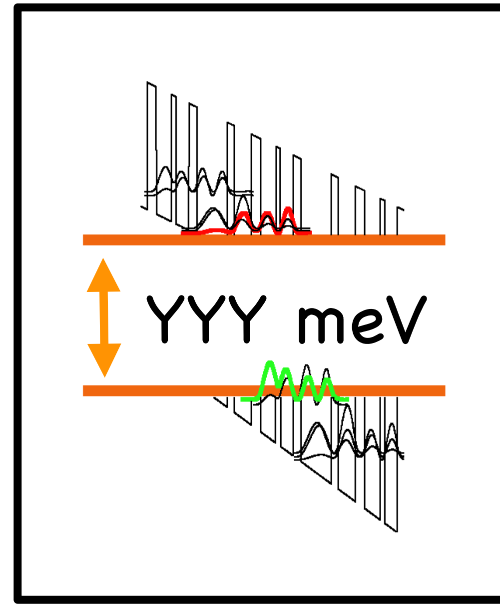






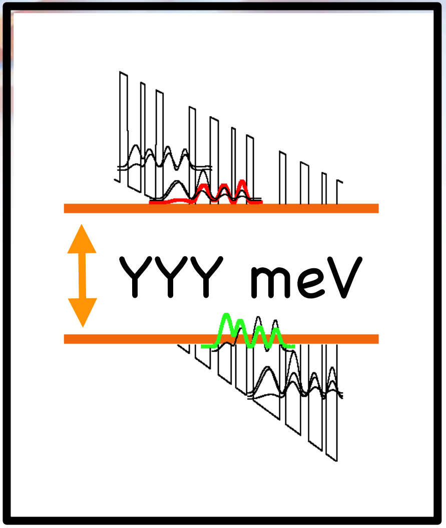
Start with one difference first



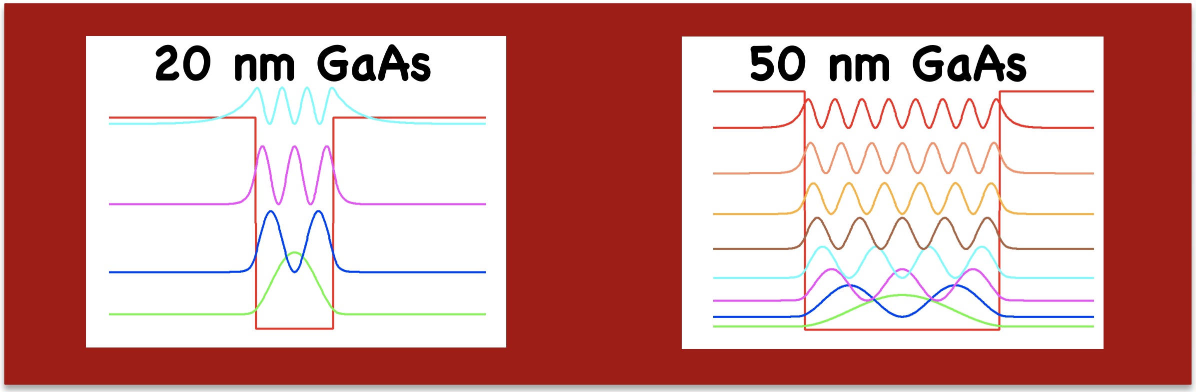


How do we do this?

'Conventional way' (trial and error) won't work here. We need a systematic approach.

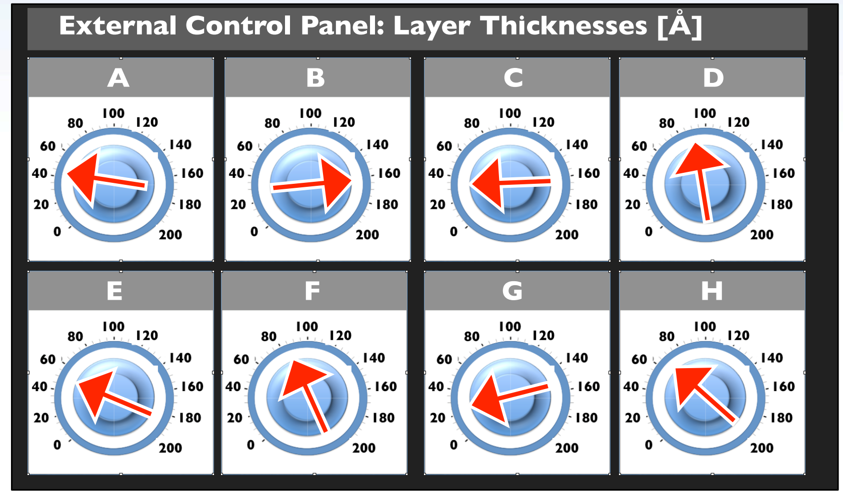


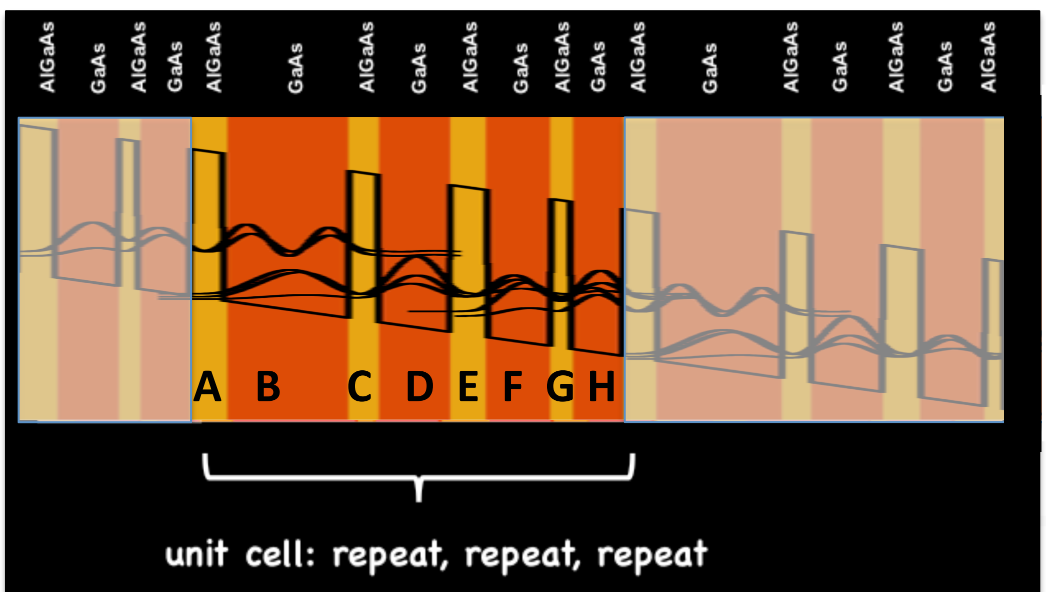
How can we change the photon energy???



eigenstates can be changed over layer thickness

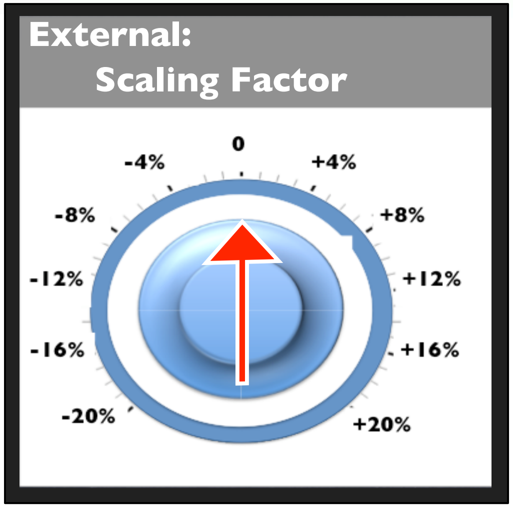
This gives us a number of 'knobs':

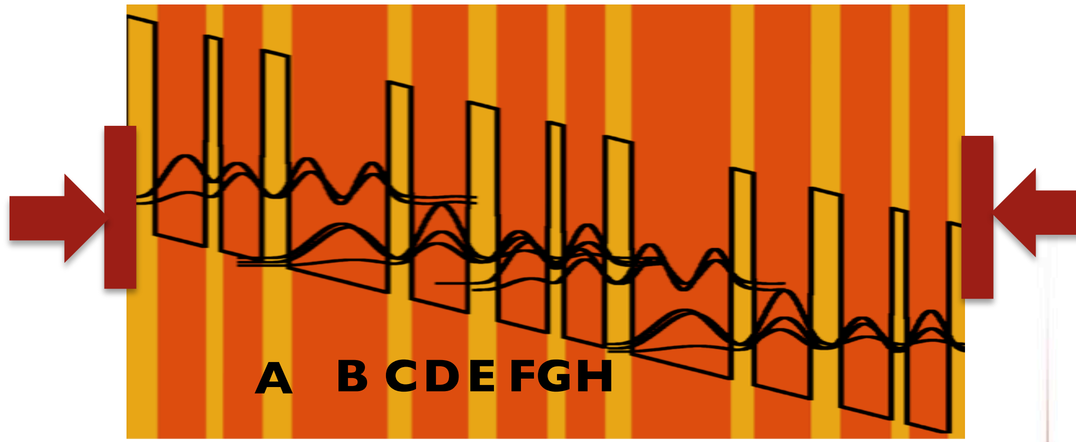


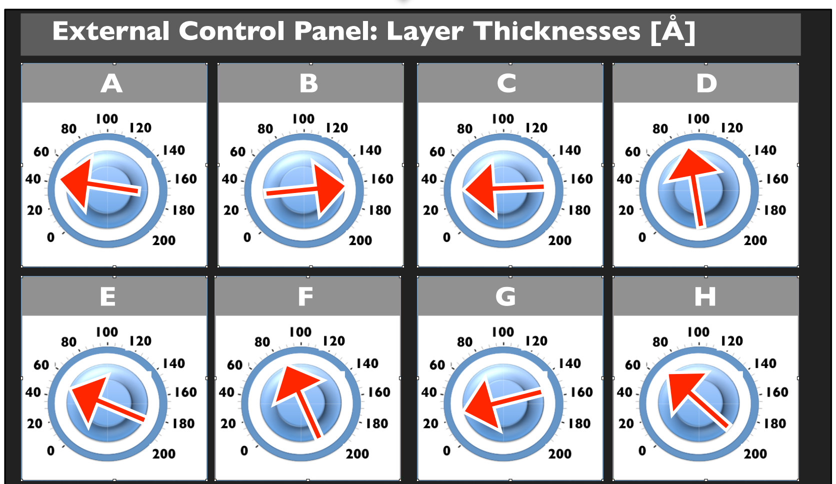


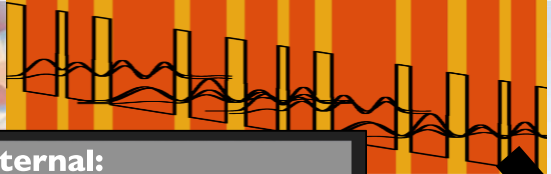
(concept from Beere et al, 2007)

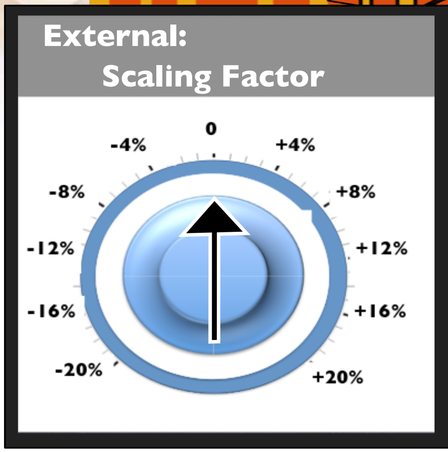
Uniform Thickness Transformation: shrink or stretch whole structure



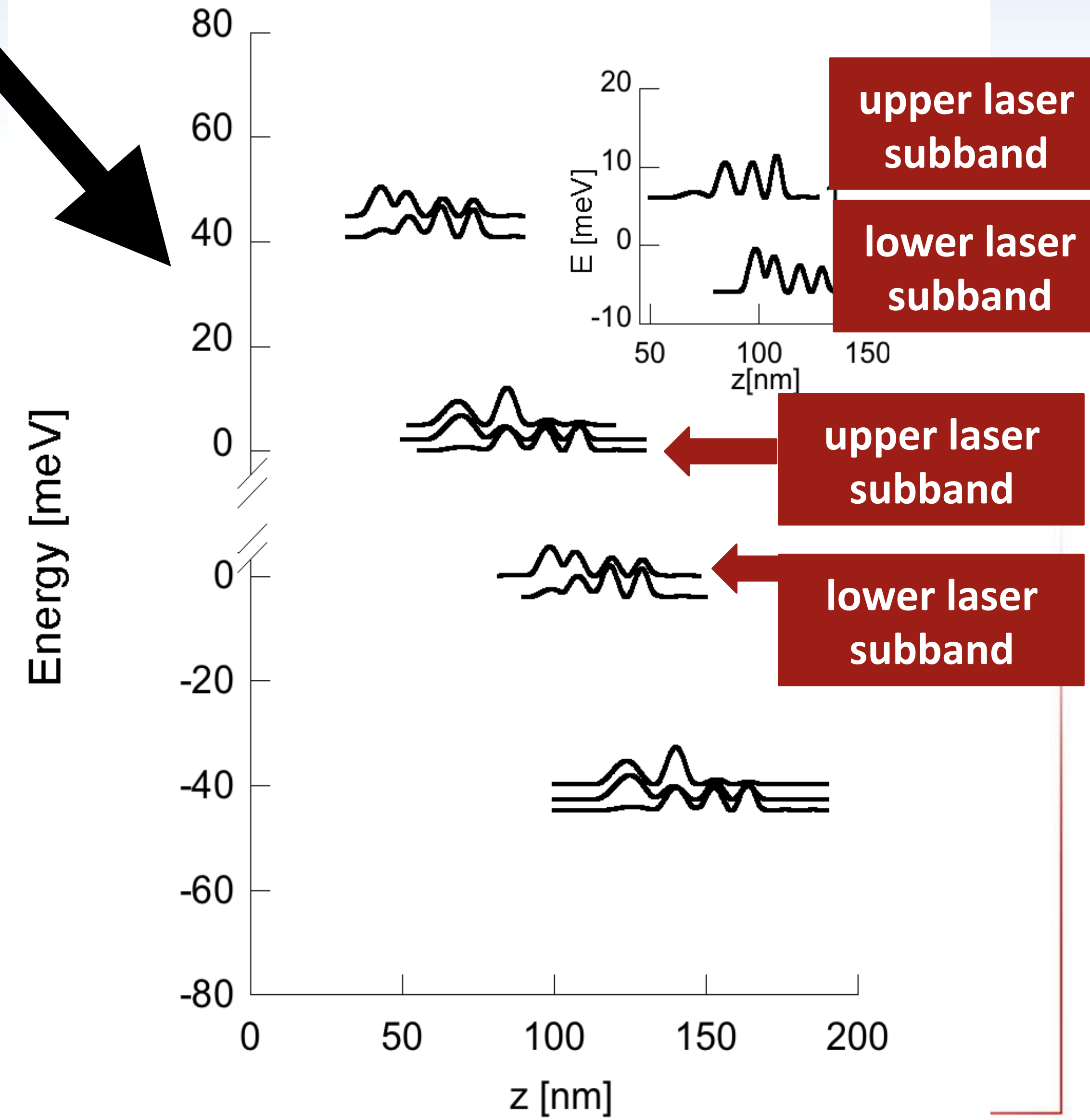








Scaling Factor	Frequency
+ 20%	
+ 16%	
+ 12%	
+ 8%	
+ 4%	
original	2.9 THz
- 4%	
- 8%	
- 12%	
- 16%	
- 20%	



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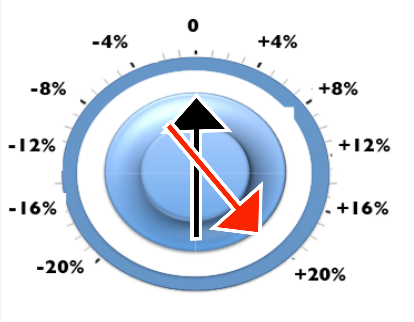
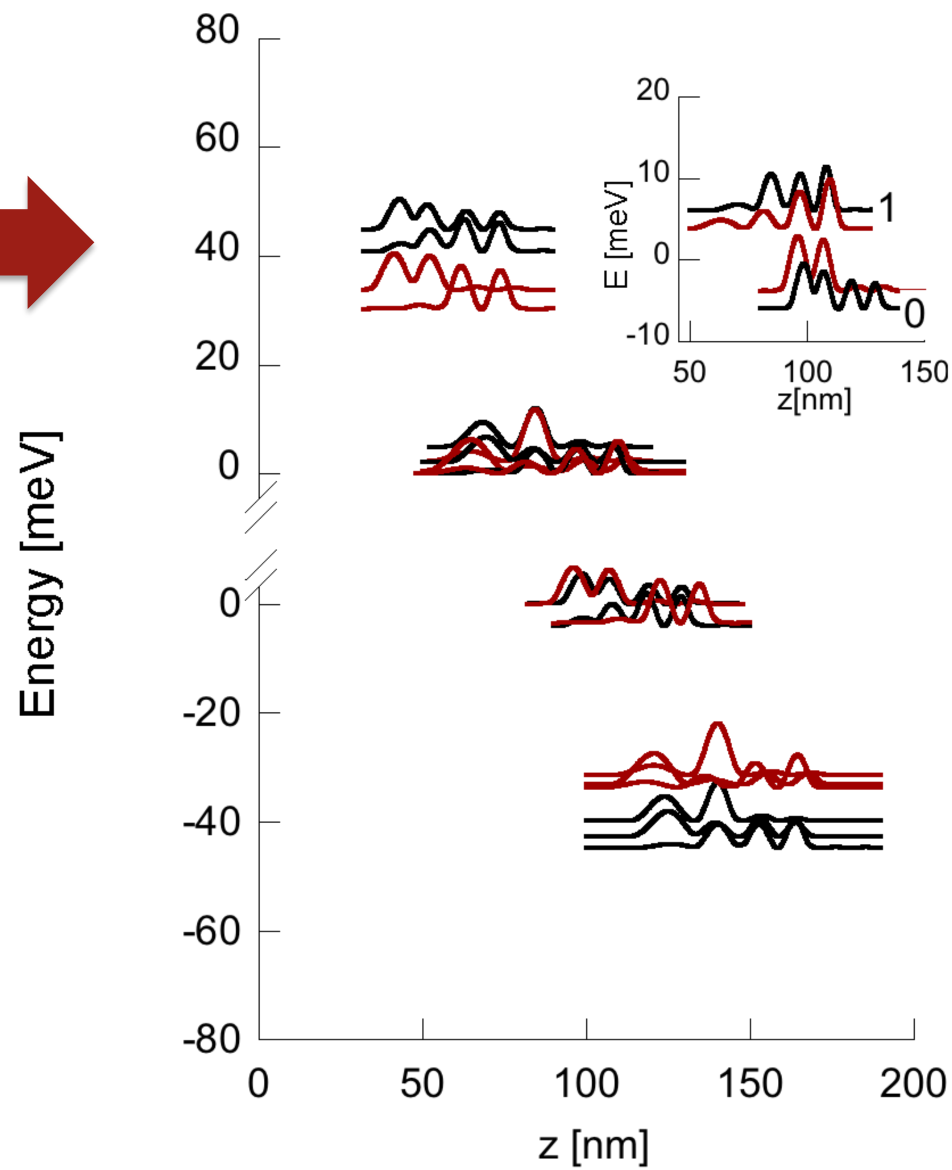
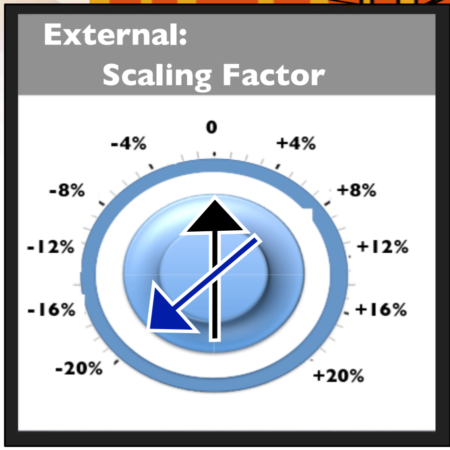
External:
Scaling Factor



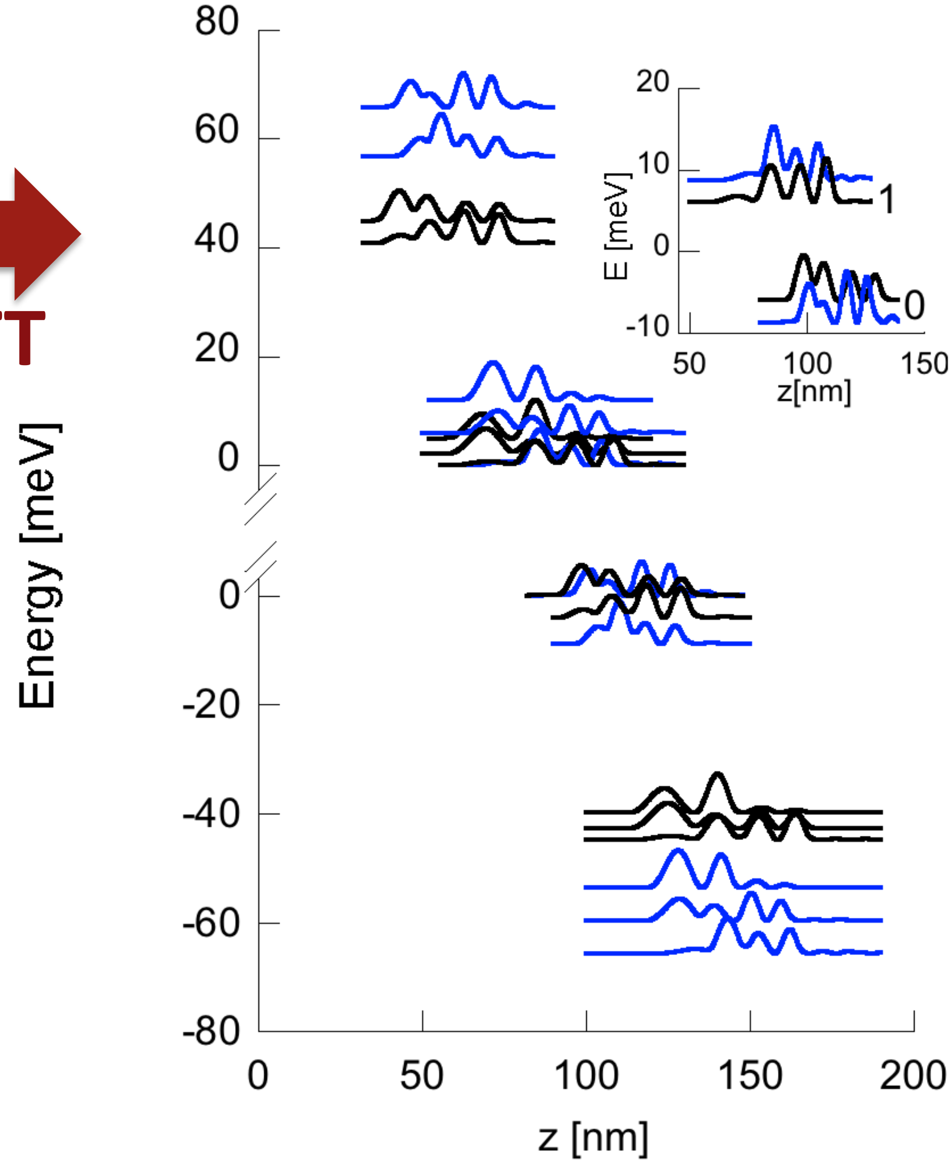
Scaling Factor	Frequency
+ 20%	1.84 THz
+ 16%	
+ 12%	
+ 8%	
+ 4%	
original	2.9 THz
- 4%	
- 8%	
- 12%	
- 16%	
- 20%	





UTT

Scaling Factor	Frequency
+ 20%	
+ 16%	
+ 12%	
+ 8%	
+ 4%	
original	2.9 THz
- 4%	
- 8%	
- 12%	
- 16%	
- 20%	4.23 THz



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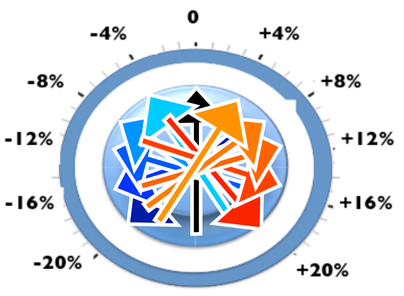
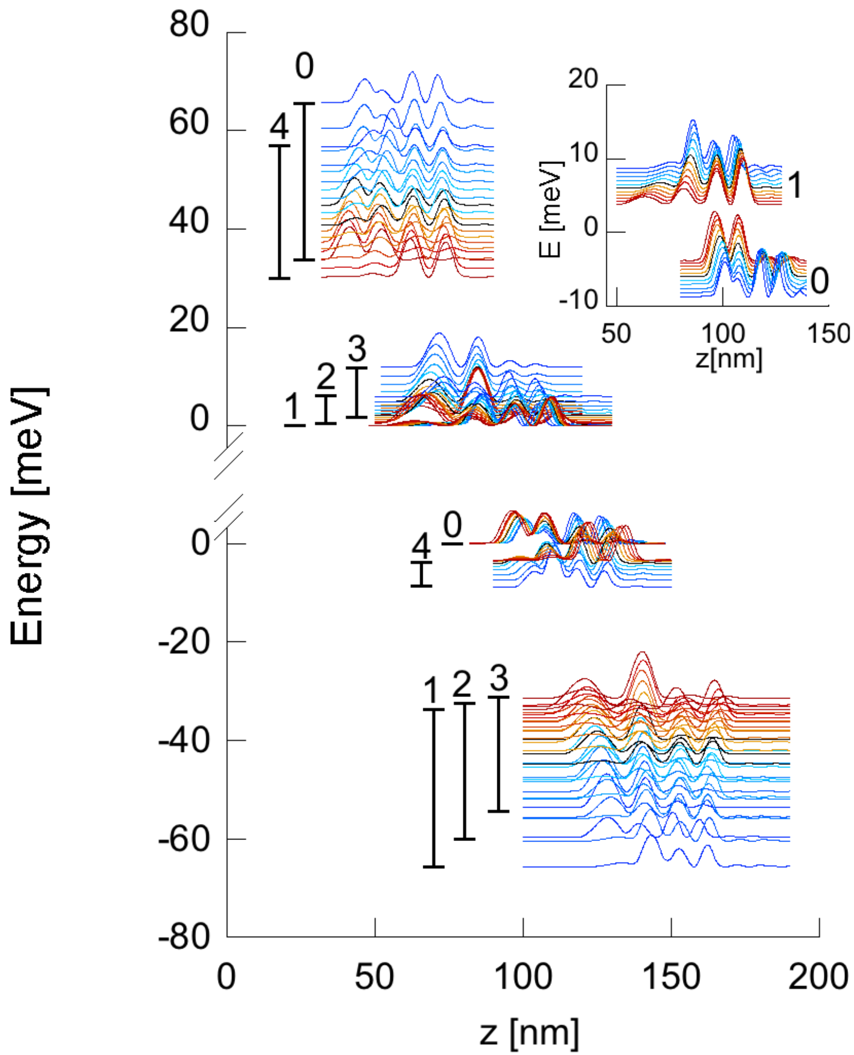
changing ONE structure parameter did not only change the photon energy

External:
Scaling Factor

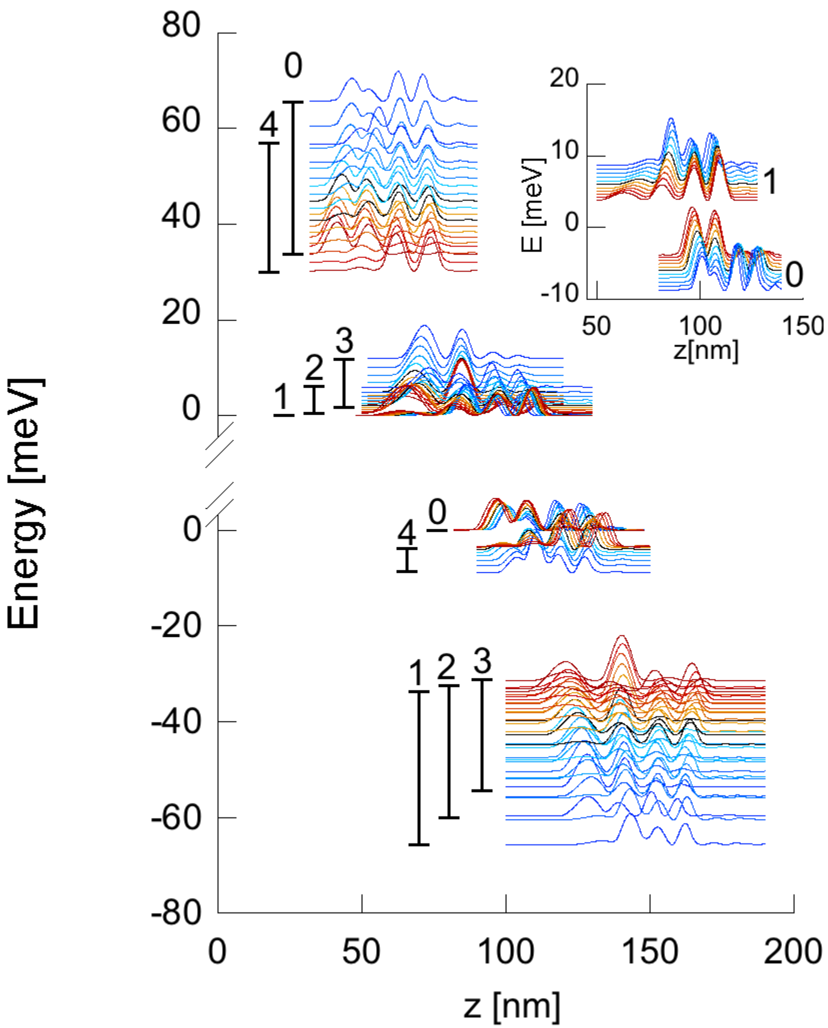


UTT

Scaling Factor	Frequency
+ 20%	1.84 THz
+ 16%	2.03 THz
+ 12%	2.22 THz
+ 8%	2.42 THz
+ 4%	2.66 THz
original	2.9 THz
- 4%	3.14 THz
- 8%	3.38 THz
- 12%	3.683 THz
- 16%	3.95 THz
- 20%	4.23 THz



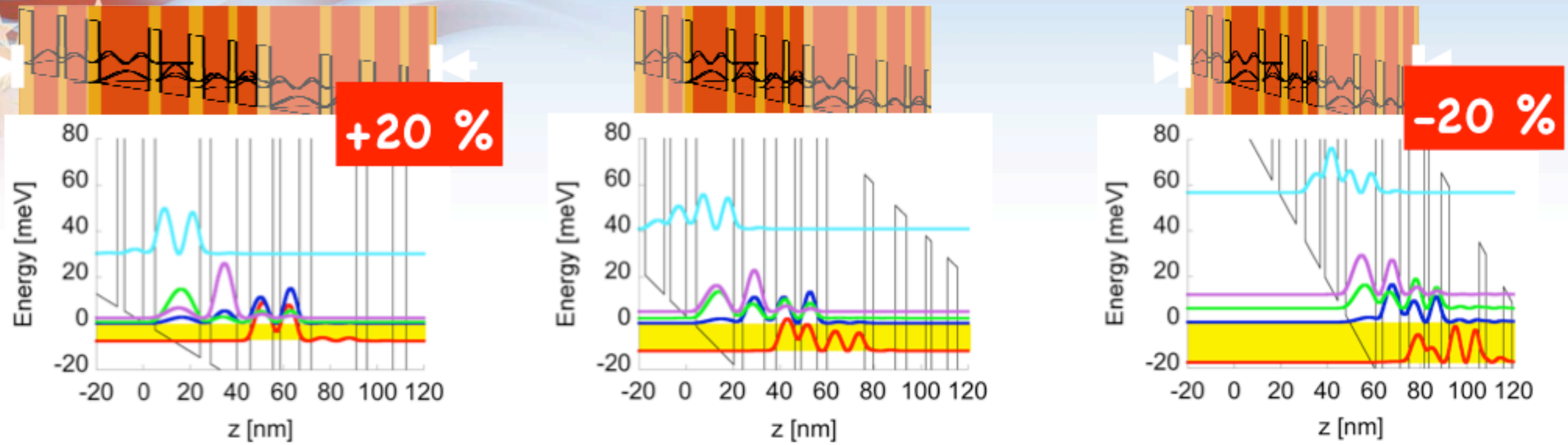
Changing ONE structure parameter changed ALL physical quantities !



REALLY? WHY? HOW?

I don't see it...

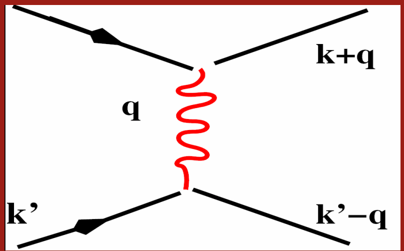
Well,
all the wavefunction shapes
and
all the separation energies
changed.



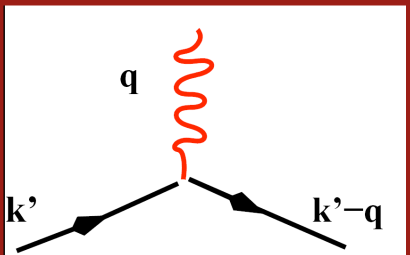
And different wavefunction shapes means:

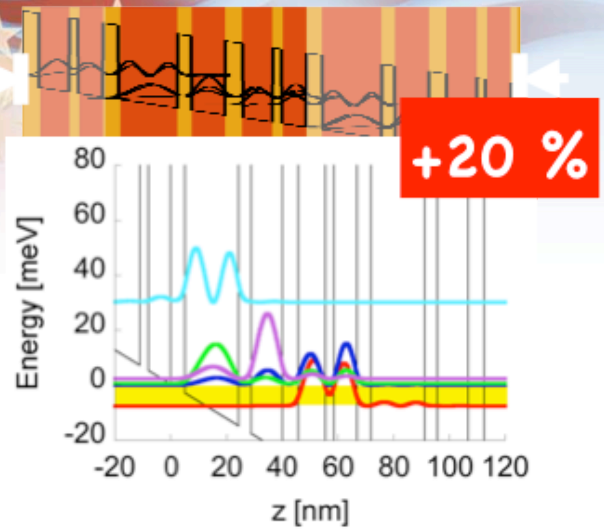
- **diff. Coulomb matrix elements:** $V^{abcd}_{k_{||}} \propto \frac{1}{|k_{||}|} \int dz \int dz' \, \phi_a(z)\phi_b(z')\phi_c(z)\phi_d(z') \, e^{-ik_{||}|z-z'|}$
- **diff. Froehlich matrix elements:** $g^{ab}_q \propto \frac{1}{\sqrt{q_{||}^2 + q_\perp^2}} \int dz \, \phi_a(z)\phi_b(z) \, e^{iq_\perp z}$

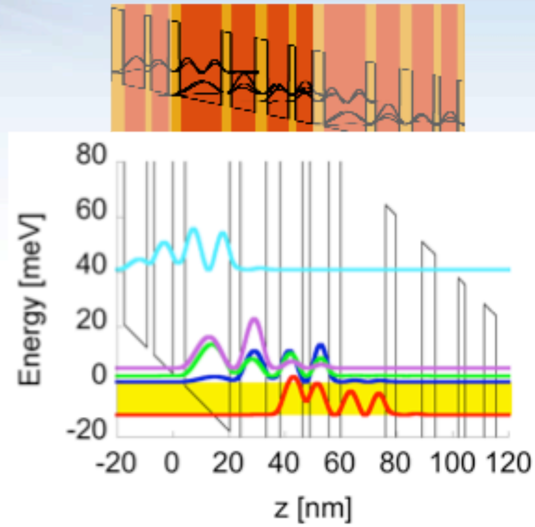
carrier-carrier scattering

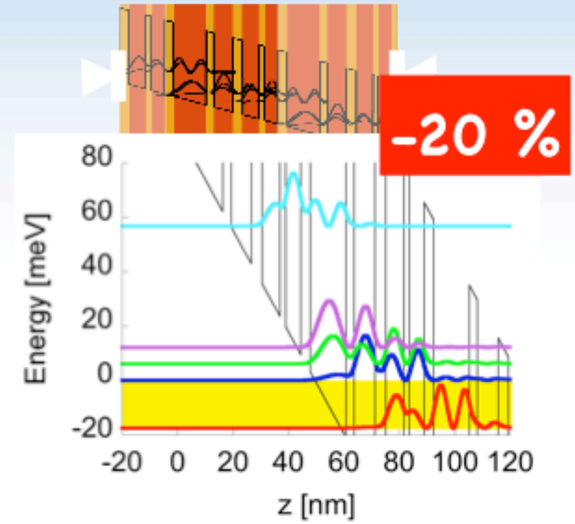


carrier-phonon scattering



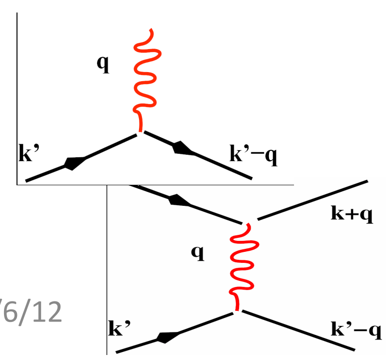


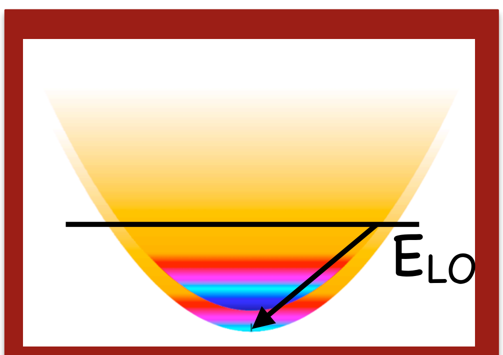


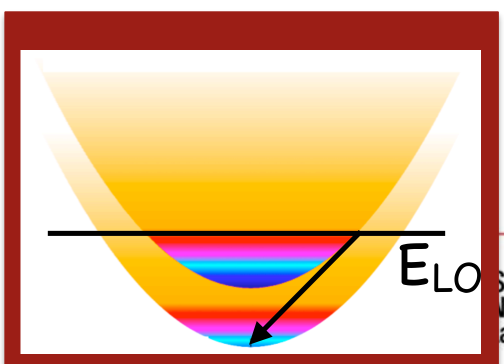


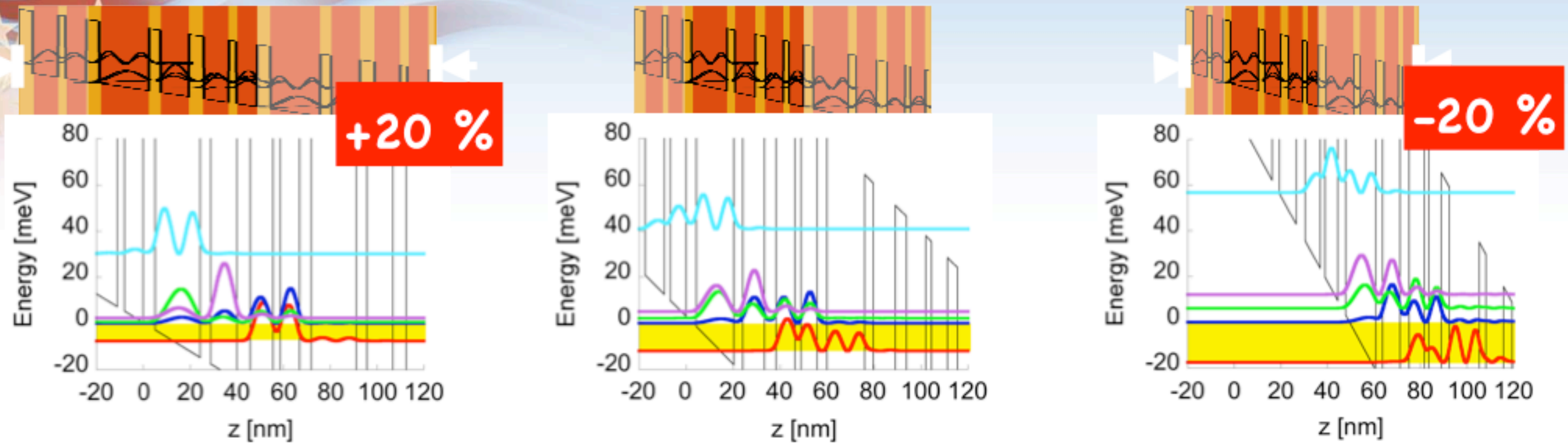
And different separation energies means:

- diff. allowed transitions for cc-scattering: $\delta(\epsilon_{\mathbf{a},\mathbf{k}} + \epsilon_{\mathbf{b},\mathbf{k}'} - \epsilon_{\mathbf{c},\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{d},\mathbf{k}'-\mathbf{q}})$
- diff. allowed transitions for cp-scattering: $\delta(\epsilon_{\mathbf{a},\mathbf{k}} - \epsilon_{\mathbf{b},\mathbf{k}+\mathbf{q}} \pm \hbar\omega_{\mathrm{LO}})$









Different wavefunction shapes

and different separation energies

➡ very different carrier transport!

whole lot of 'different'

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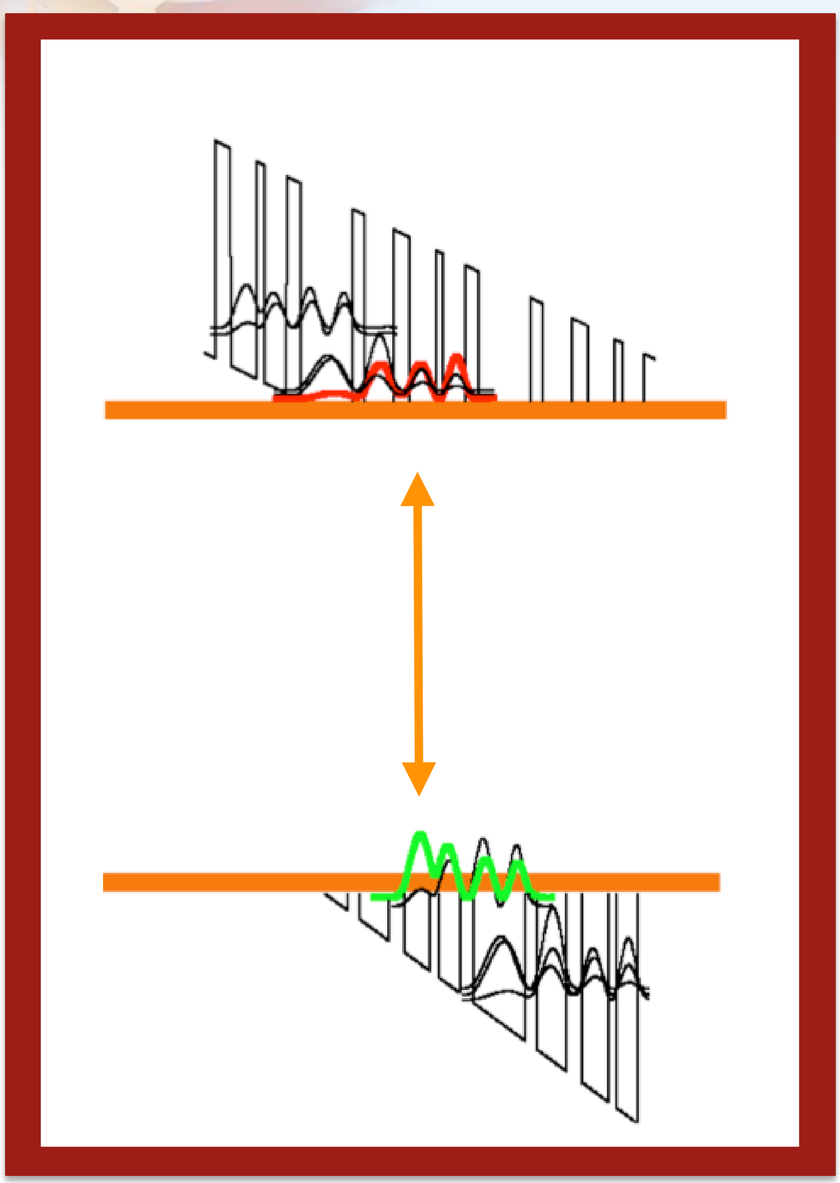
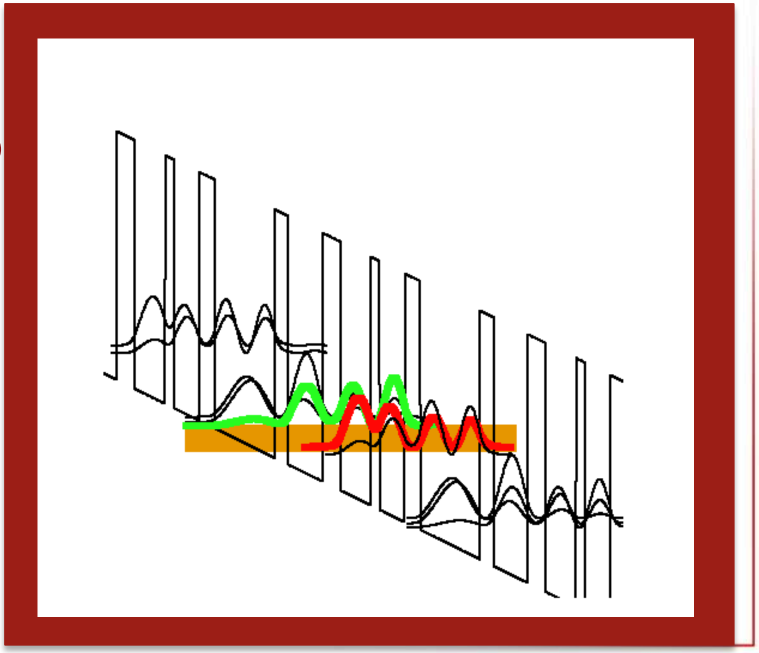
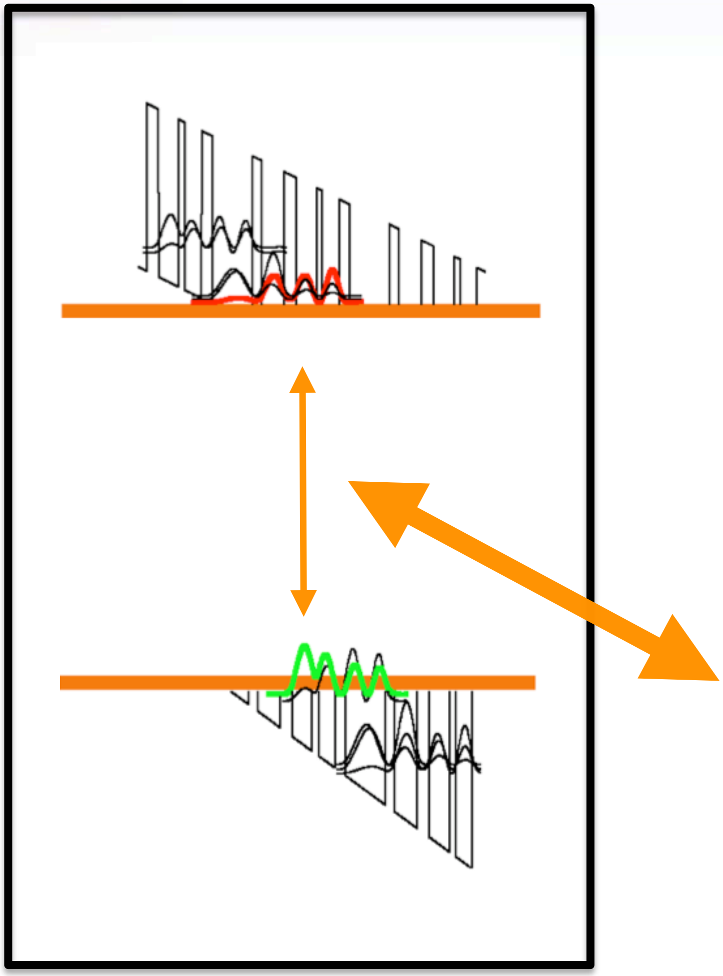
How do we have to change ALL structure parameters so that only 'ONE' physical quantity is changed???

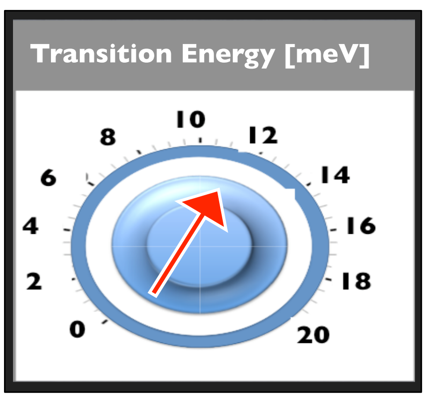


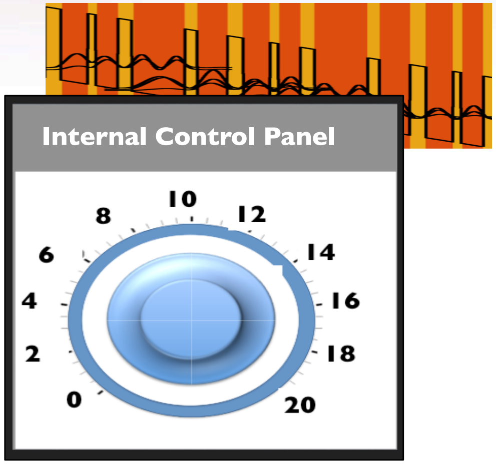
HOW?



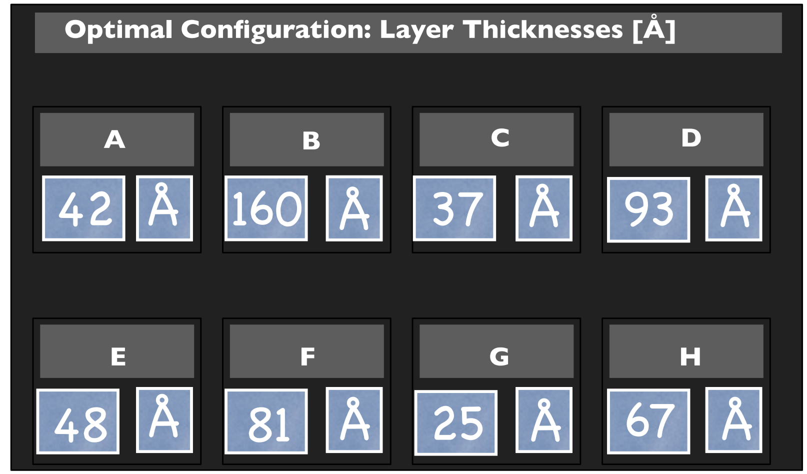


Inverse Quantum Engineering



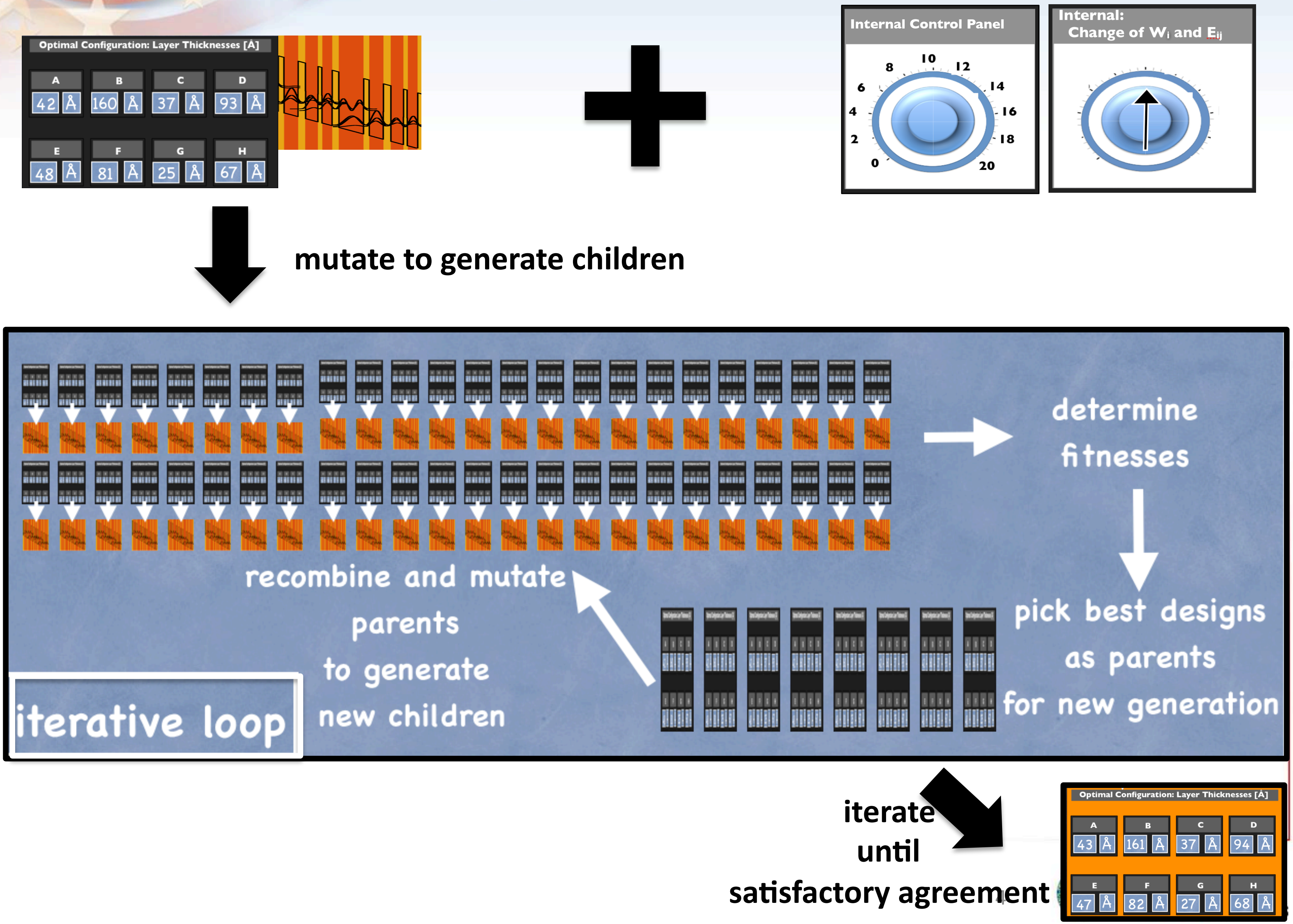


Inverse Quantum Engineering (IQE)

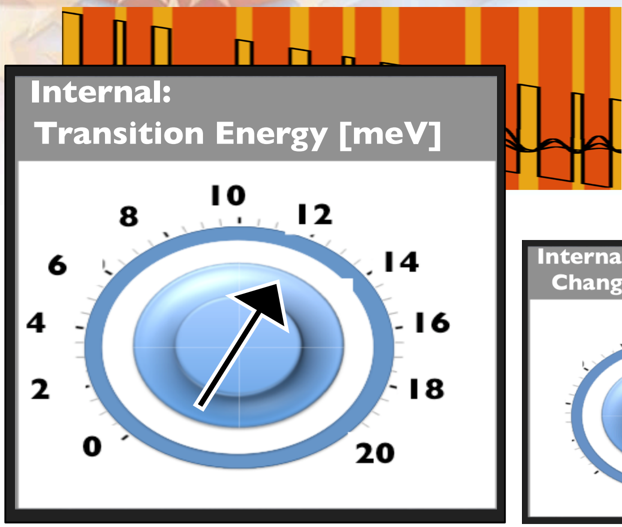


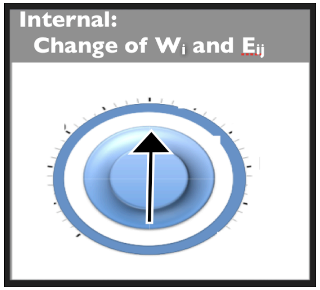
Evolutionary algorithm coupled with Schroedinger-Poisson-Solver: find optimal configuration for specific system under specific constraints

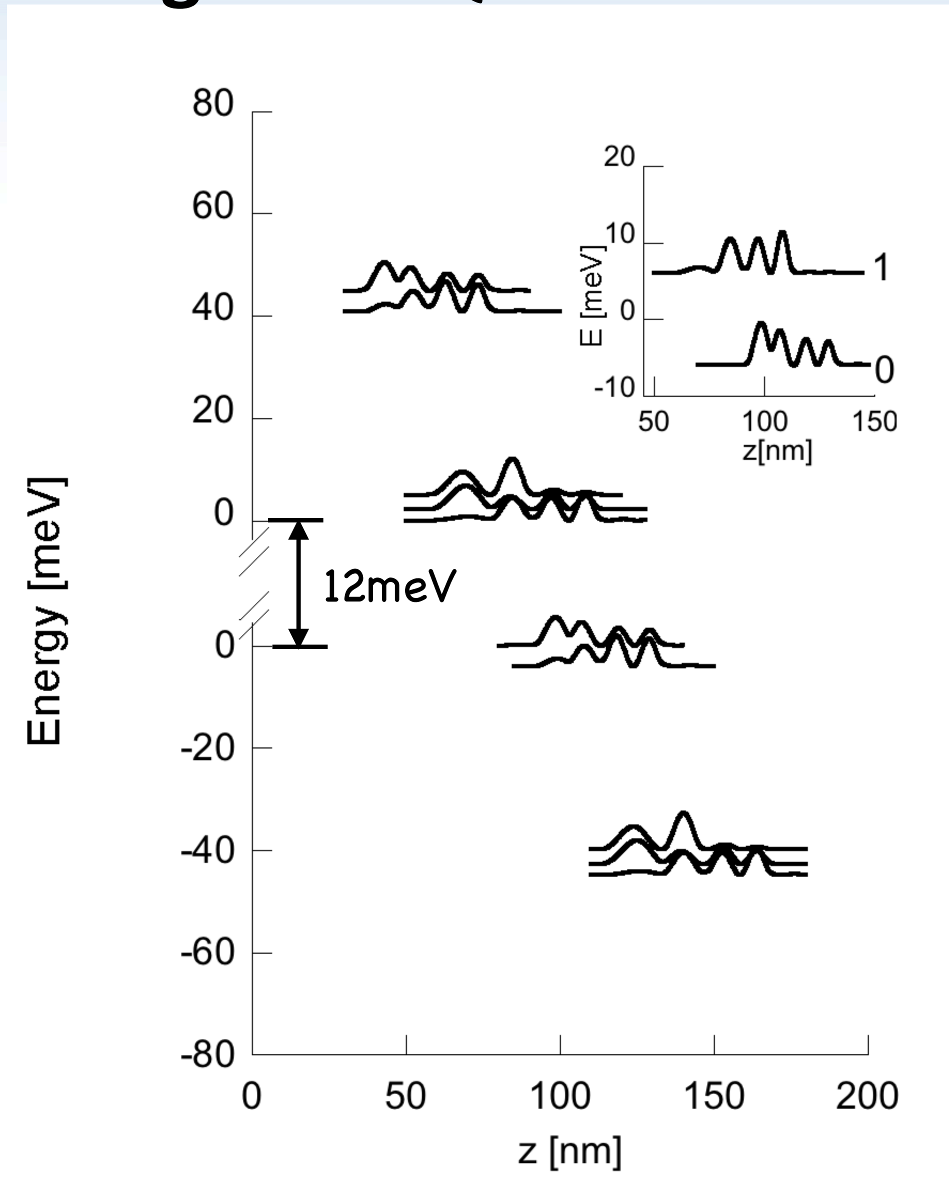
IQE Design Tool !!!



Frequency Tuning with IQE





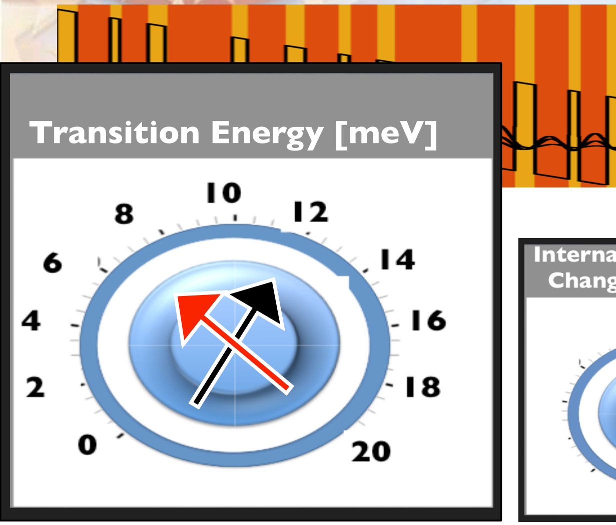


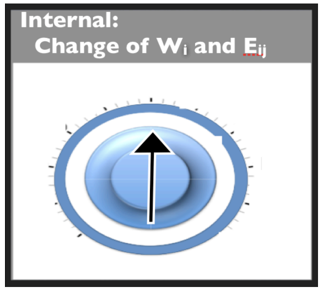
Optimal Configuration: Layer Thicknesses [Å]

A	B	C	D
42 Å	160 Å	37 Å	93 Å

E	F	G	H
48 Å	81 Å	25 Å	67 Å

Frequency Tuning with IQE



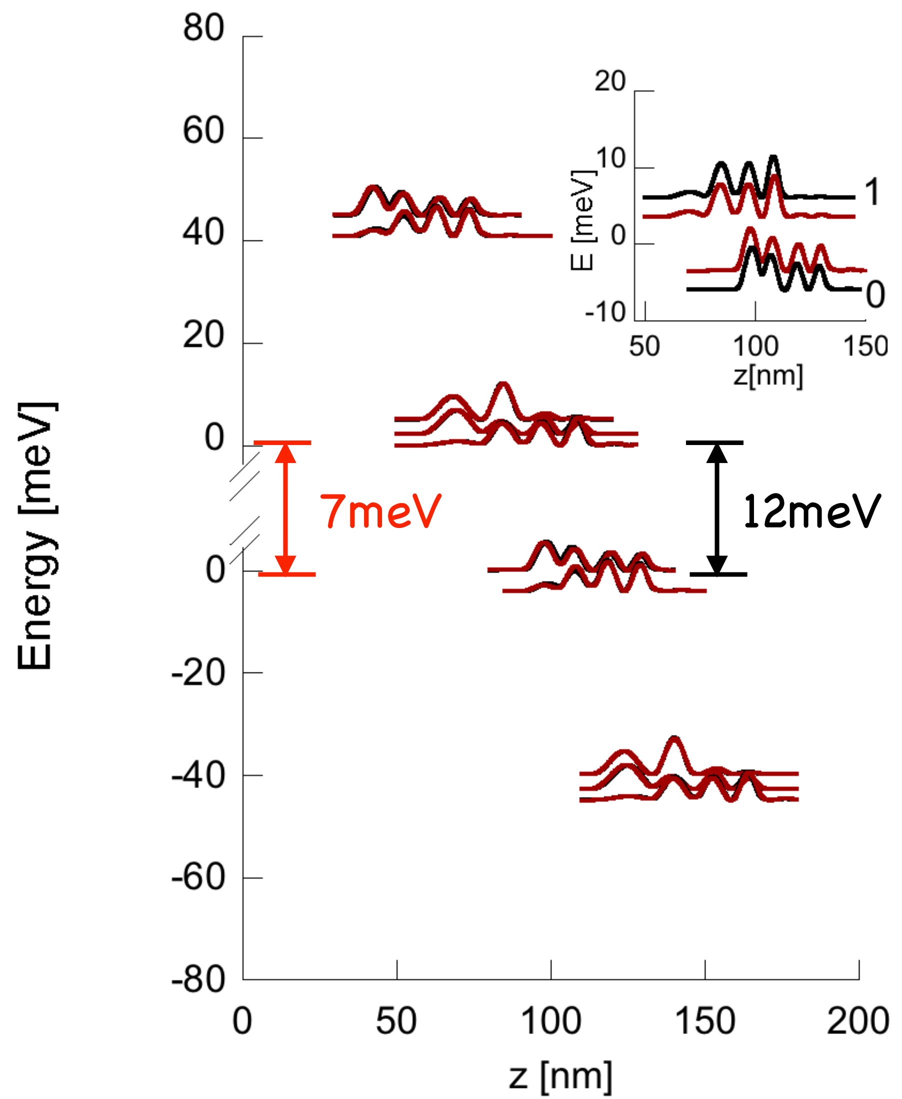


IQE !!!

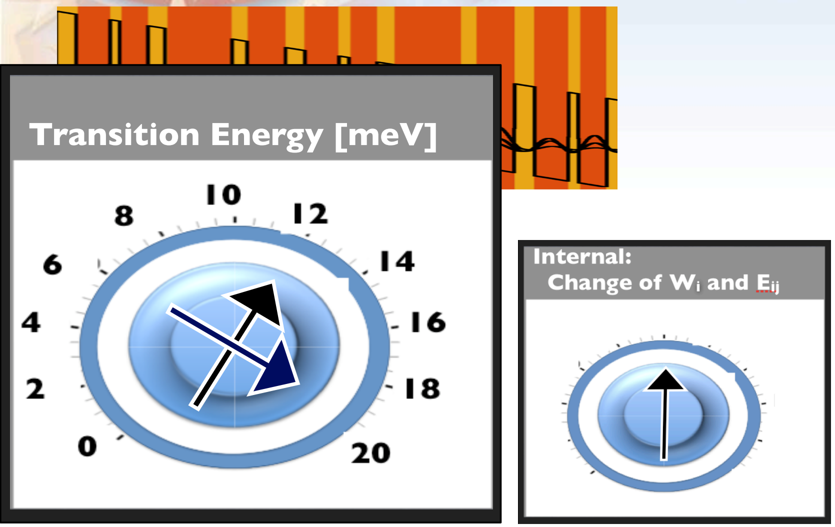
Optimal Configuration: Layer Thicknesses [Å]

A	B	C	D
44 Å	160 Å	36 Å	97 Å

E	F	G	H
46 Å	83 Å	35 Å	69 Å



Frequency Tuning with IQE

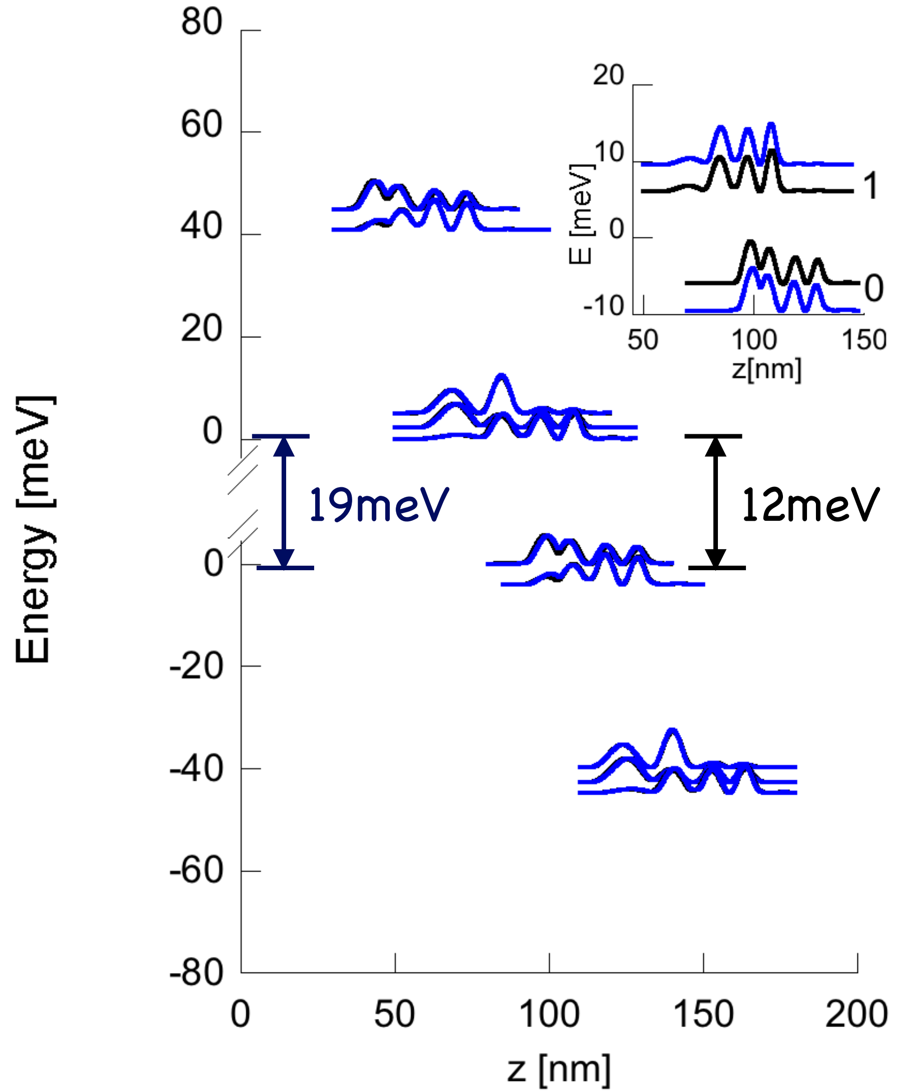


IQE !!!

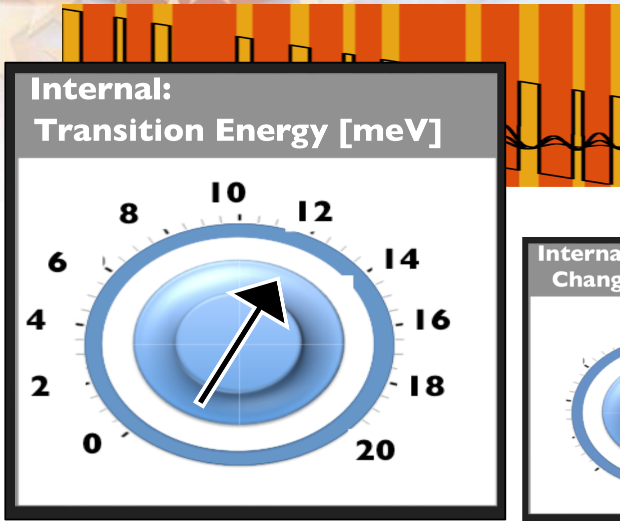
Optimal Configuration: Layer Thicknesses [Å]

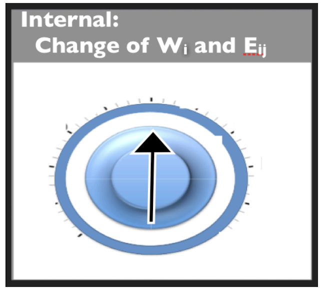
A	B	C	D
41 Å	162 Å	38 Å	88 Å

E	F	G	H
51 Å	81 Å	17 Å	65 Å

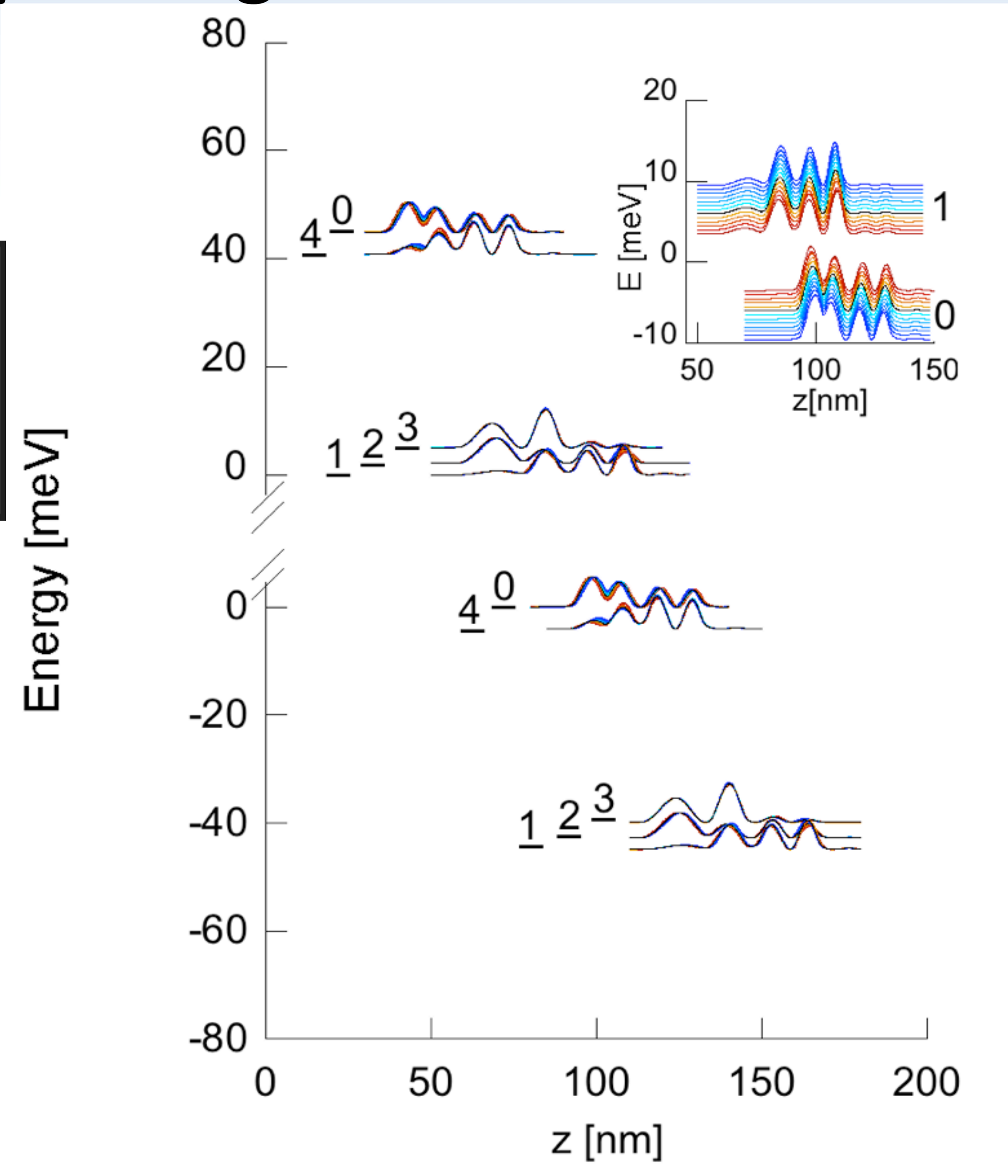


Frequency Tuning with IQE



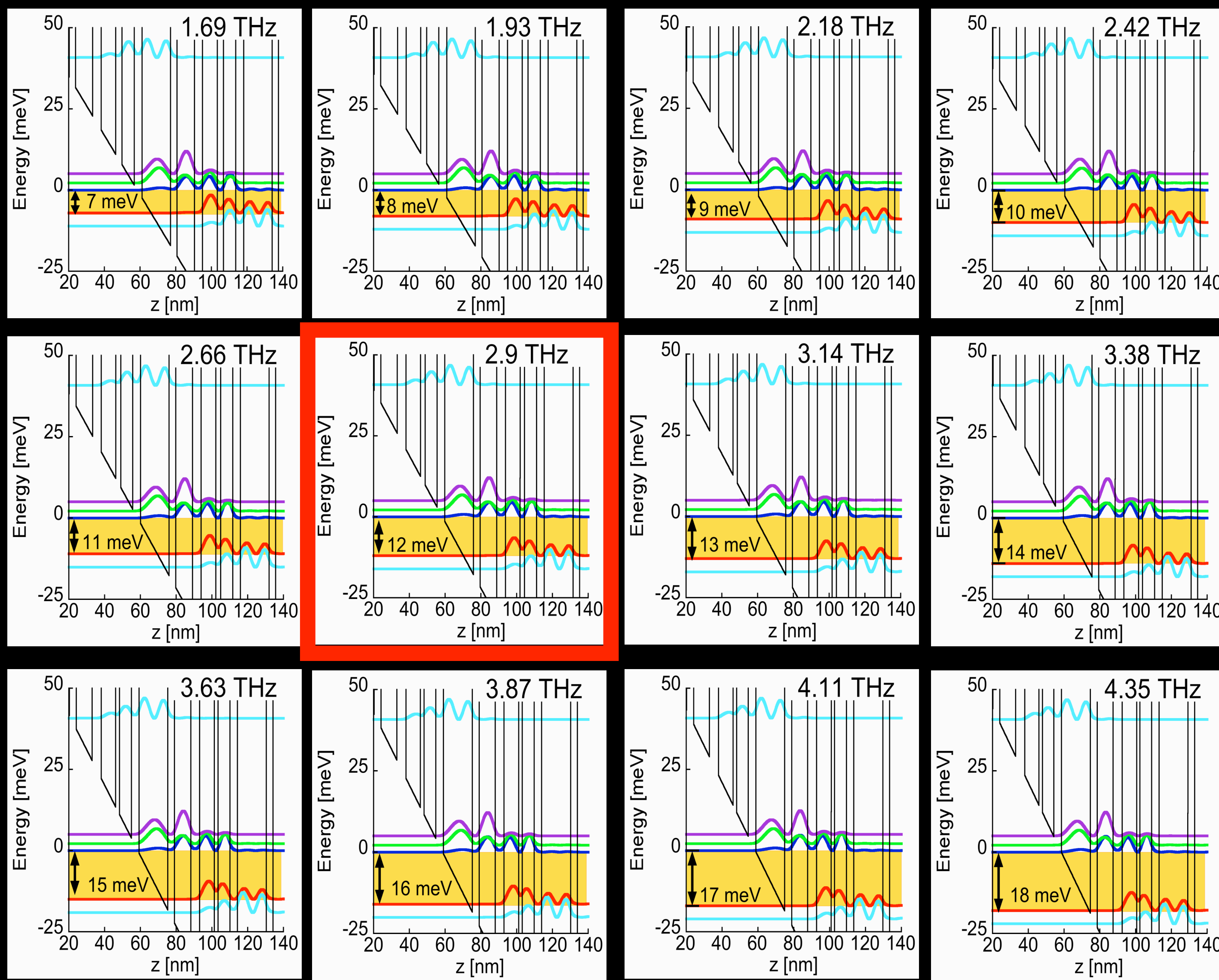


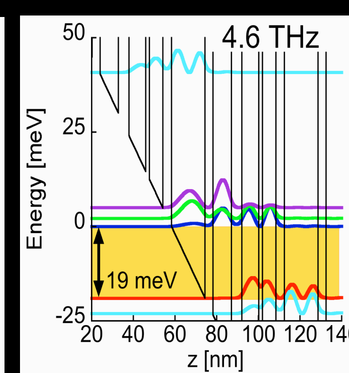
Frequency
1.69 THz
1.93 THz
2.18 THz
2.42 THz
2.66 THz
2.9 THz
3.14 THz
3.38 THz
3.63 THz
3.87 THz
4.11 THz
4.35 THz
4.6 THz

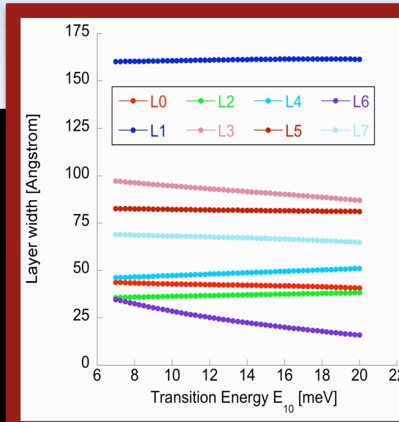


changed ONLY targeted transition energy !

Tuning the emission frequency of a THz QCL with IQE

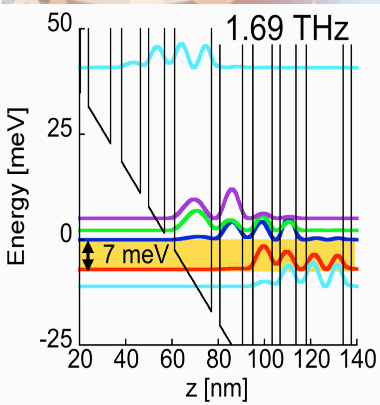


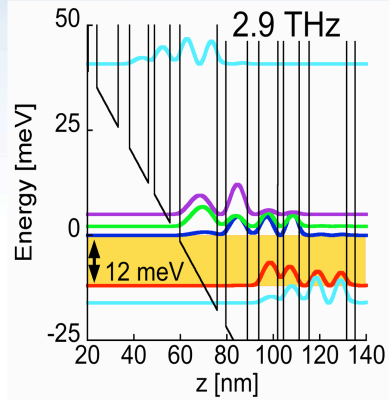


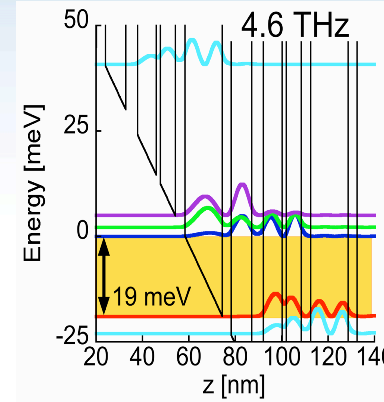


1.69 THz to 4.6 THz

"Inverse-Quantum-Engineering: a new methodology for designing quantum cascade lasers", IEEE JQE 46, 1414 (2010)







And same wavefunction shapes means:

- same Coulomb matrix elements: $V^{abcd}_{k_{||}} \propto \frac{1}{|k_{||}|} \int dz \int dz' \, \phi_a(z)\phi_b(z')\phi_c(z)\phi_d(z') \, e^{-ik_{||}|z-z'|}$
- same Froehlich matrix elements: $g^{ab}_{q} \propto \frac{1}{\sqrt{q^2_{||} + q^2_{\perp}}} \int dz \, \phi_a(z)\phi_b(z) \, e^{iq_{\perp} z}$

And same separation energies means:

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

ONE difference: photon energy (laser frequency!)

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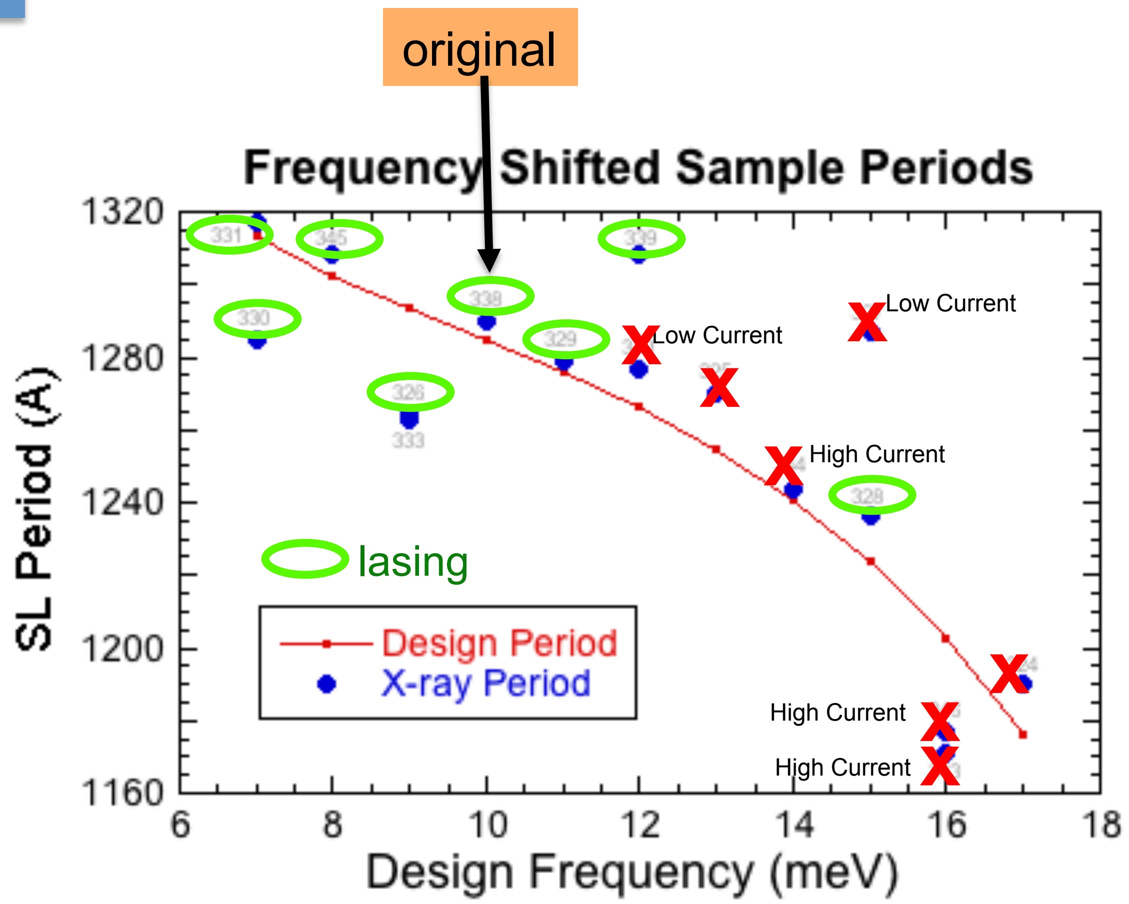
Growth

Fabrication

Experiment

Series of IQE-designed lasers at 11 frequencies



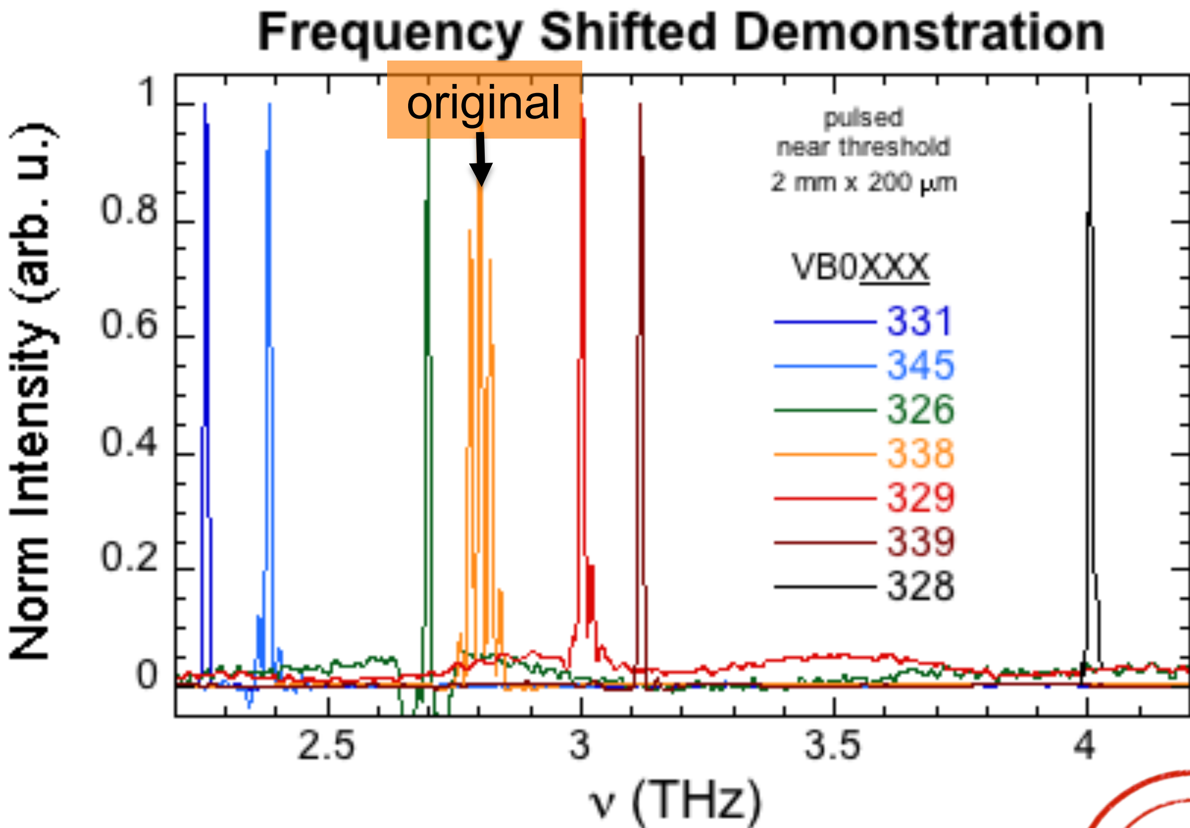
Sandia National Laboratories

Growth

Fabrication

Experiment

Observed lasing at 7 frequencies

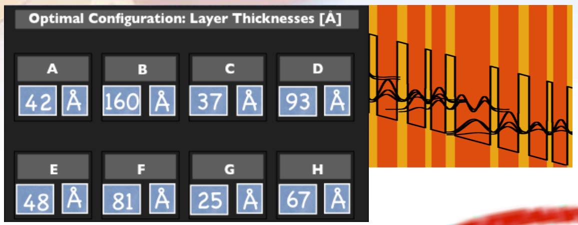


VALIDATED!!

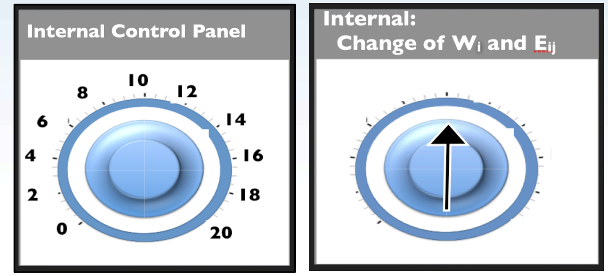
PROOF: IQE Design Tool WORKS !!

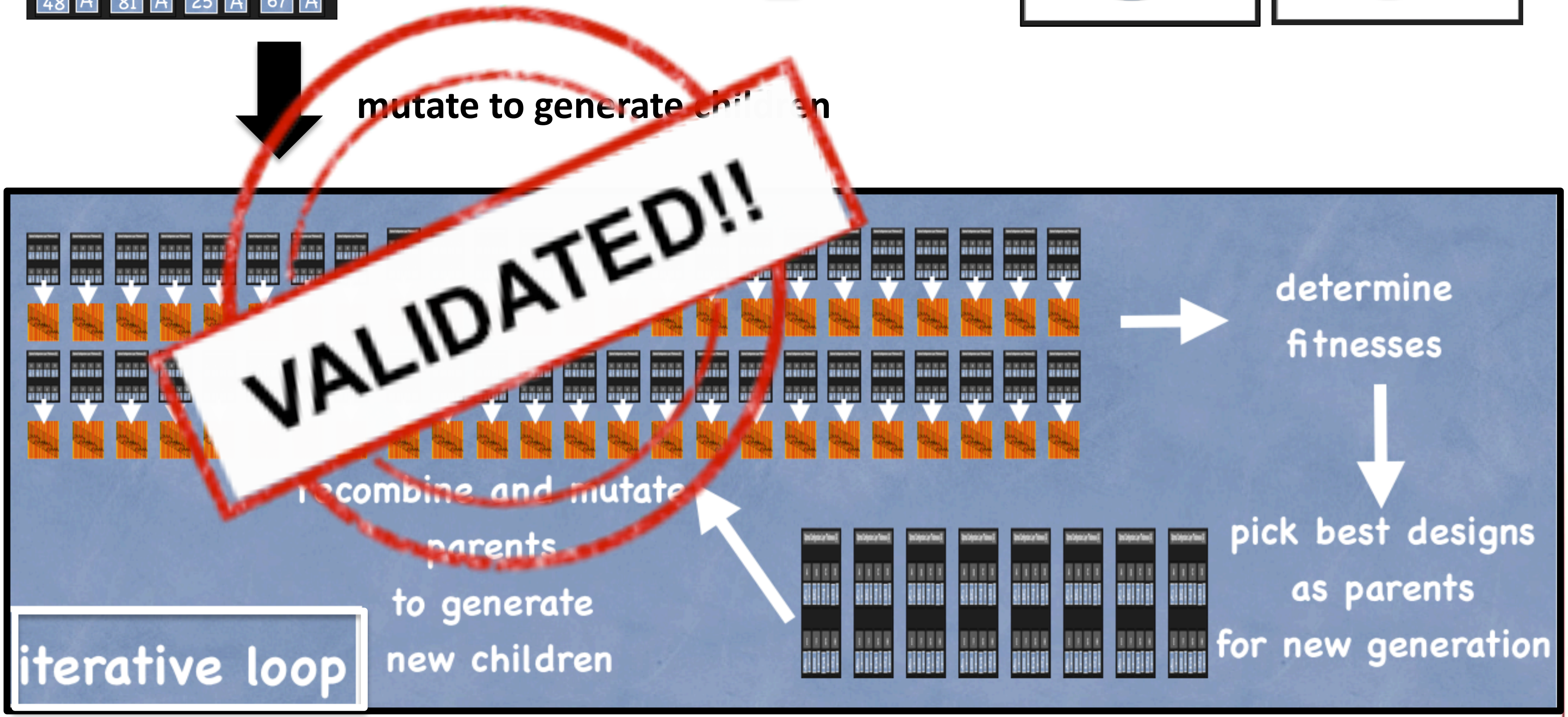
Sandia National Laboratories

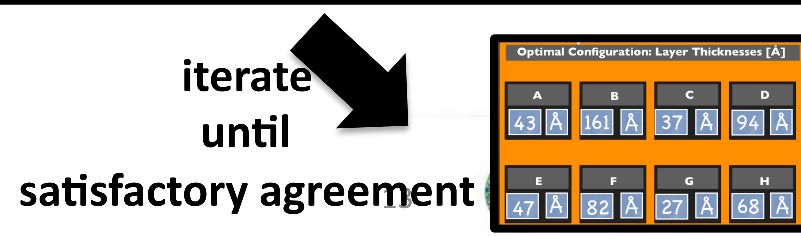
IQE Design Tool !!!



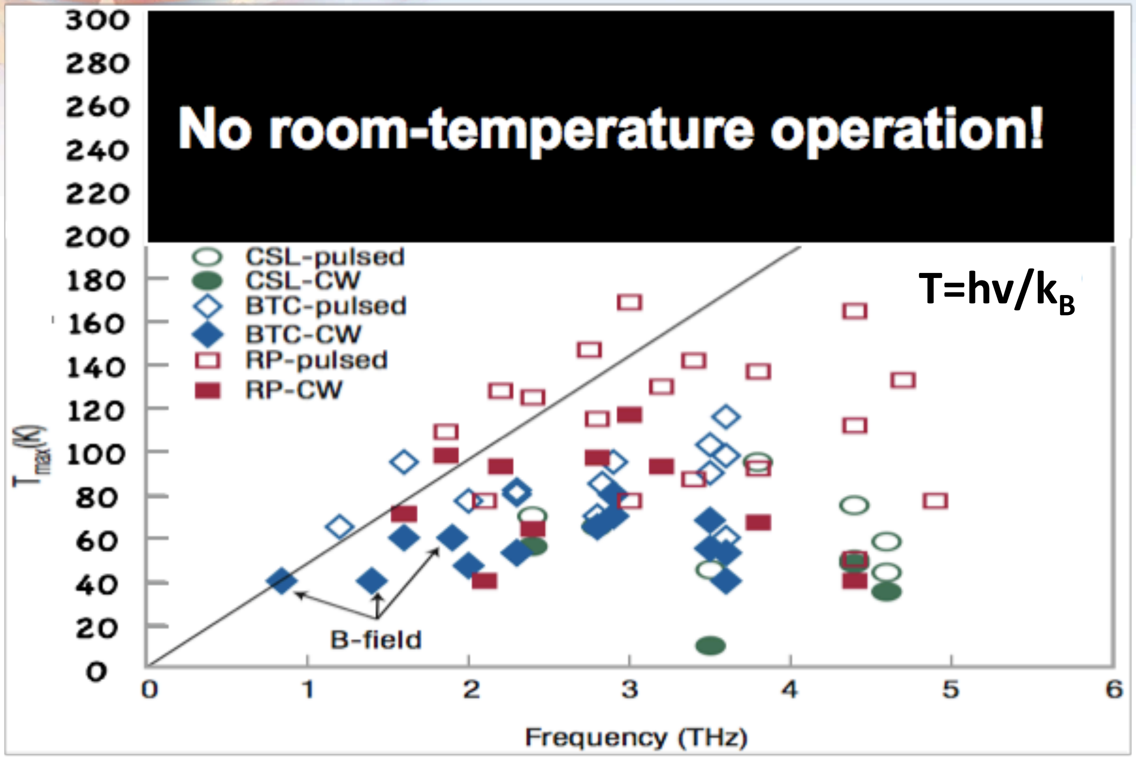
+







**Already proven useful for
Qswitch RTBF and 4-wave mixing LDRD!
Just starting to also use for GaN LDRD!**

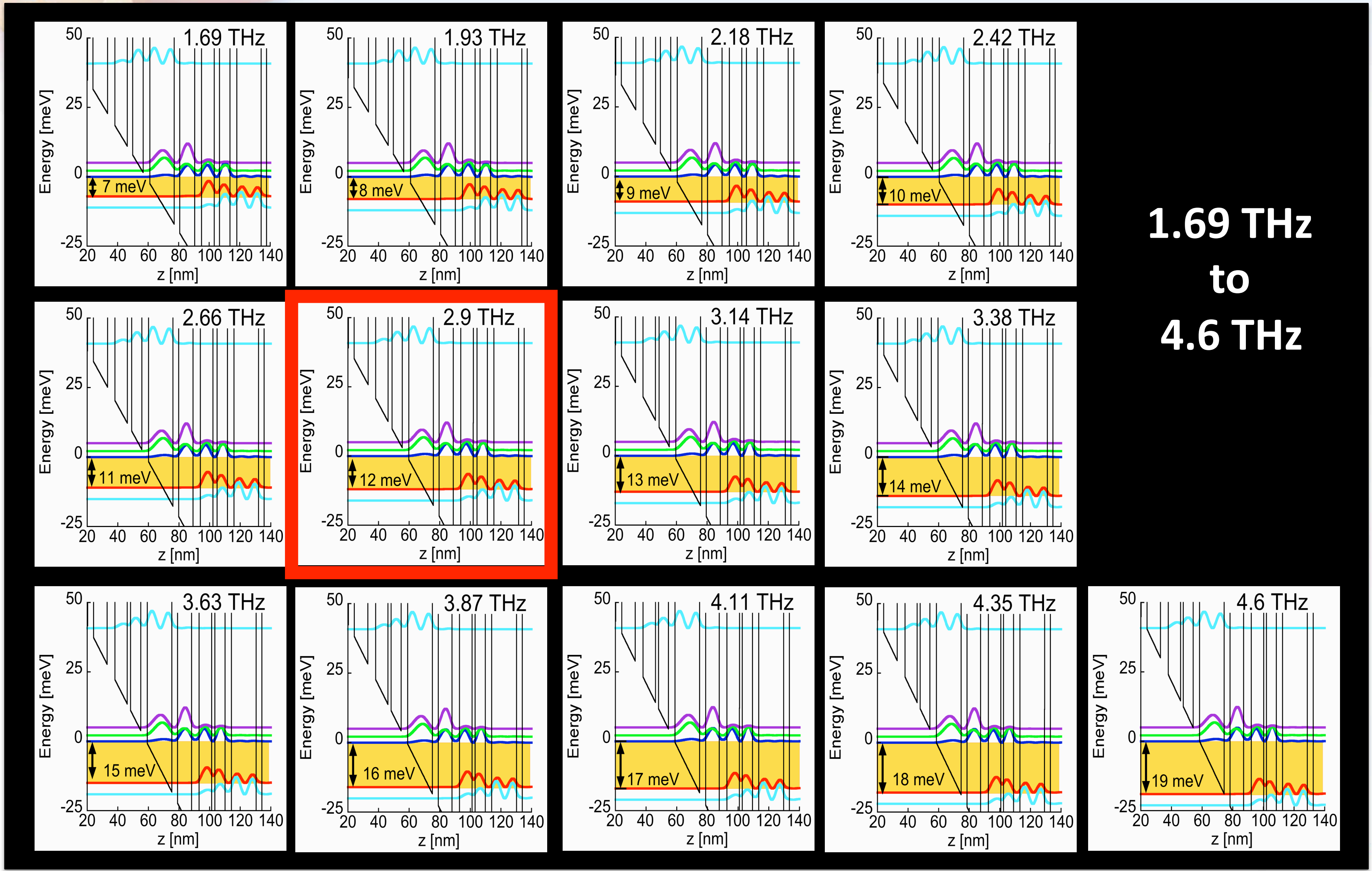


But why?
Is there a fundamental limit?
$T_{MAX} \leq h\nu/k_B$?

Question from all potential sponsors:

"Can I get a room temperature THz QCL?"

Tuning the emission frequency of a THz QCL with IQE



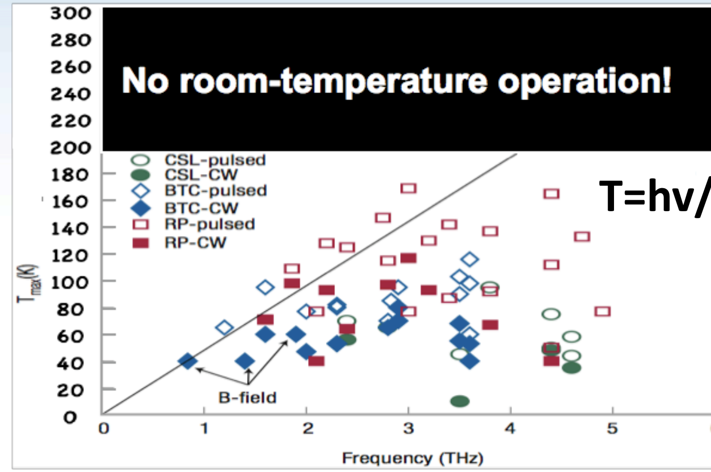
"Inverse-Quantum-Engineering: a new methodology for designing quantum cascade lasers", IEEE JQE 46, 1414 (2010)

Growth

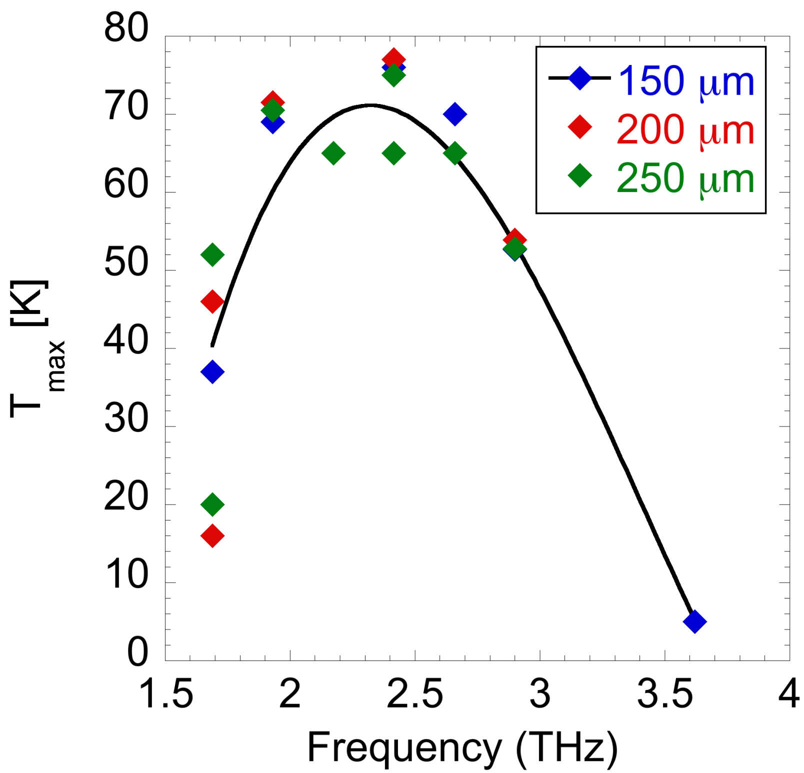
Fabrication

Experiment

QUESTION: Is T_{max} limited by 1/kT ????



$T=h\nu/k_B$



Experimental Result: 1/kT NOT true !!!

"Index Tuning for Precise Frequency Selection of Terahertz Quantum Cascade Lasers", IEEE Photonics Technology Letters 23, 30 (2011)

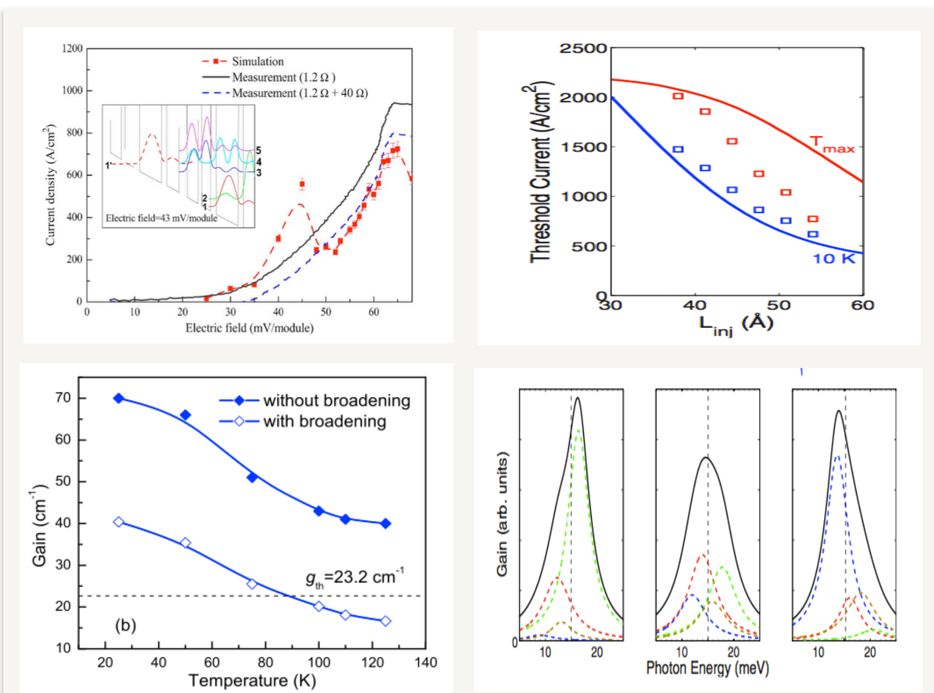
"Optical bistability from domain formation in terahertz quantum cascade lasers", IEEE JSTQE 17, 222 (2011)

Simulation

Code

Needed:
Performance simulator to study 1/kT limit theoretically

Variety of performance simulators described in literature*



* Taken from: Appl. Phys. 42, 025101 (2009), PRB 81, 205311 (2010), JAP 103, 103113 (2008)

Status quo of Performance Simulators

I. rate equation model

$$\frac{d}{dt}n_i = -\sum_a \gamma_{ia} n_i + \sum_a \gamma_{ai} n_a$$

???

$$G = \frac{\Delta N_{ij} e^2 f_{ij}}{2\pi L_p c n \epsilon_0 m^* \Delta\nu}$$

$$J = e\sum_{a,a^+}[\gamma_{a,a^+} n_a - \gamma_{a^+,a} n_{a^+}]$$

II. ensemble Monte-Carlo model

$$\frac{d}{dt}\sigma^{ii}_{\mathbf{k}}|_{scatt,ci} = -\sum_a \gamma^{i,a}_{\mathbf{k}} \sigma^{ii}_{\mathbf{k}} + \sum_a \gamma^{a,i}_{\mathbf{k}} (1-\sigma^{ii}_{\mathbf{k}})$$

III. simplified density matrix approach

$$\frac{d}{dt}n_i = -\sum_a \gamma_{ia} n_i + \sum_a \gamma_{ai} n_a$$

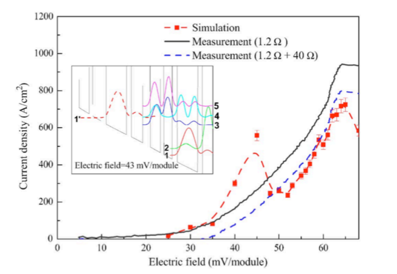
$$\begin{aligned}\frac{d}{dt}\sigma^{ij}| = {} & \frac{i}{\hbar}(\epsilon_i-\epsilon_j)\sigma^{ij} - \gamma_{ij}\sigma^{ij} \\ & -\frac{i}{\hbar}\sum_a \left[d_{j,i}\sigma^{jj} - d_{j,i}\sigma^{ii}\right]E(t) \\ & -\frac{i}{\hbar}\sum_{a\neq j} d_{a,i}\sigma^{aj}E(t) + \frac{i}{\hbar}\sum_{a\neq i} d_{j,a}\sigma^{ia}E(t)\end{aligned}$$

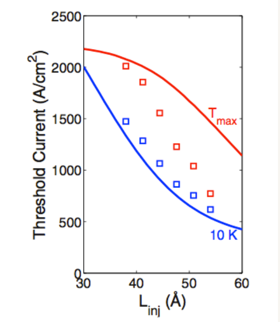
$$g(\omega) = \frac{\omega}{n_b c}\Im\left[\frac{P(\omega)}{\epsilon_0 E(\omega)}\right]$$

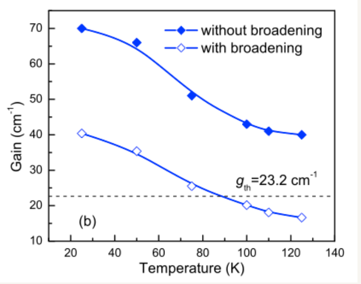
$$J = -\frac{1}{L_p}\sum_{i,j} \mathrm{i}(\epsilon_j-\epsilon_i)P_{ij}(t)$$

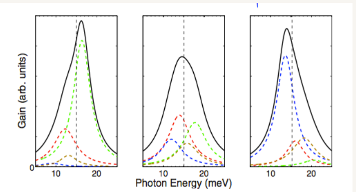
???

Literature results*:





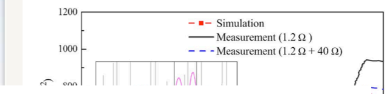




* Taken from: Appl. Phys. 42, 025101 (2009), PRB 81, 205311 (2010), JAP 103, 103113 (2008)

Status quo of Performance Simulators

Literature results*:



I. rate equation

$$\frac{d}{dt}n_i = -\sum$$

$$\sum_a \gamma_{\mathbf{k}}^{i,a}\sigma_{\mathbf{k}}^{ii} + \sum$$

III. simplified density m

$$\frac{d}{dt}n_i = -\sum_a \gamma_{ia}n_i + \sum_a \gamma_{ai}n_a$$

$$\frac{d}{dt}\sigma^{ij}| = \frac{\mathrm{i}}{\hbar}(\epsilon_i - \epsilon_j)\sigma^{ij} - \gamma_{ij}\sigma^{ij}$$
$$-\frac{\mathrm{i}}{\hbar}\sum_a \left[d_{j,i}\sigma^{jj} - d_{j,i}\sigma^{ii}\right]E(t)$$
$$-\frac{\mathrm{i}}{\hbar}\sum_{a\neq j} d_{a,i}\sigma^{aj}E(t) + \frac{\mathrm{i}}{\hbar}\sum_{a\neq i} d$$

Crude approximations

Fit parameters

* Taken from: Appl. Phys. 42, 025101 (2009), PRB 81, 205311 (2010), JAP 103, 103113 (2008)

Simulation

Code

Needed: Performance simulator without fit parameters !!!

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

$$\frac{d}{dt}\sigma^{ij}_{\mathbf{k}} = \frac{d}{dt}\langle a^\dagger_{j,\mathbf{k}} a_{j',\mathbf{k}}\rangle = \frac{\mathrm{i}}{\hbar}\langle [H, a^\dagger_{j,\mathbf{k}} a_{j',\mathbf{k}}]\rangle$$

carrier-field

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

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

+

$$\frac{d}{dt}\sigma^{ij}_{\mathbf{k}} = -\frac{\mathrm{i}}{\hbar}\sum_a \left[d_{j,i}\sigma^{jj}_{\mathbf{k}} - d_{j,i}\sigma^{ii}_{\mathbf{k}}\right]E(t) - \frac{\mathrm{i}}{\hbar}\sum_{a\neq j} d_{a,i}\sigma^{aj}_{\mathbf{k}}E(t) + \frac{\mathrm{i}}{\hbar}\sum_{a\neq i} d_{j,a}\sigma^{ia}_{\mathbf{k}}E(t)$$

carrier-phonon

$$H_{\mathrm{cp}} = \sum_{a,b,\mathbf{k}}\sum_{\mathbf{Q}} [g^{ab}_{\mathbf{Q}}\, a^\dagger_{a\mathbf{k}}\, b_{\mathbf{Q}}\, a_{b\mathbf{k}-\mathbf{Q}_{||}} + h.a.]$$

$$\begin{aligned}
\frac{d}{dt}\sigma^{ii}_{\mathbf{k}}|_{cp} = &\mp\frac{2\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{a,b,c} Re[g^{bc,ia}_{\hat{\mathbf{q}}_{||}}\sigma^{ac}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}\sigma^{bi}_{\mathbf{k}}]\delta(\epsilon^b_{\mathbf{k}} - \epsilon^c_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}}) \\
&-\frac{2\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{a,b} Re[g^{ba,ia}_{\hat{\mathbf{q}}_{||}}\sigma^{bi}_{\mathbf{k}}]\delta(\epsilon^b_{\mathbf{k}} - \epsilon^a_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}})(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \mp \frac{1}{2}) \\
&+\frac{2\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{a,b} Re[g^{ib,ia}_{\hat{\mathbf{q}}_{||}}\sigma^{ab}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}]\delta(\epsilon^i_{\mathbf{k}} - \epsilon^b_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}})(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \pm \frac{1}{2})
\end{aligned}$$

+

$$\begin{aligned}
\frac{d}{dt}\sigma^{ij}_{\mathbf{k}}|_{cp} = &\frac{\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{b,c}[\mp\sum_a g^{bc,ia}_{\hat{\mathbf{q}}_{||}}\sigma^{ac}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}\sigma^{bj}_{\mathbf{k}} - g^{bc,ic}_{\hat{\mathbf{q}}_{||}}(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \mp \frac{1}{2})\sigma^{bj}_{\mathbf{k}} \\
&\mp\sum_a g^{ja,bc}_{\hat{\mathbf{q}}_{||}}\sigma^{ca}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}\sigma^{ib}_{\mathbf{k}} - g^{jc,bc}_{\hat{\mathbf{q}}_{||}}(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \mp \frac{1}{2})\sigma^{ib}_{\mathbf{k}}]\delta(\epsilon^b_{\mathbf{k}} - \epsilon^c_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}}) \\
&+\frac{\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{c,b} g^{jb,ic}_{\hat{\mathbf{q}}_{||}}\sigma^{cb}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}\delta(\epsilon^j_{\mathbf{k}} - \epsilon^b_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}})(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \pm \frac{1}{2}) \\
&+\frac{\pi}{\hbar}\sum_{\hat{\mathbf{q}}}\sum_{c,b} g^{jc,ib}_{\hat{\mathbf{q}}_{||}}\sigma^{bc}_{\mathbf{k}+\hat{\mathbf{q}}_{||}}\delta(\epsilon^i_{\mathbf{k}} - \epsilon^b_{\mathbf{k}+\mathbf{Q}_{||}} \pm \hbar\omega_{\mathrm{LO}})(n_{\hat{\mathbf{q}}_{||}} + \frac{1}{2} \pm \frac{1}{2})
\end{aligned}$$

carrier-impurity

$$H_{ci} = \sum_{c,d}\sum_{l}\sum_{\mathbf{q},\mathbf{k}} V^l_{cd}(\mathbf{q}) a^\dagger_{c,\mathbf{k}+\mathbf{q}} a_{d,\mathbf{k}}$$

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

+

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

carrier-carrier

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

$$\begin{aligned}
\frac{d}{dt}\sigma^{ii}_{\mathbf{k}}|_{scatt(cc)} = &\frac{4\pi}{\hbar}\sum_{\mathbf{k}',\mathbf{q}}\sum_{w,x,y,z,g}\Re[V^{iywz}_{\mathbf{q}}\sigma^{wx}_{\mathbf{k}+\mathbf{q}}\sigma^{zg}_{\mathbf{k}'-\mathbf{q}}(V^{iyxg}_{\mathbf{q}} - \sum_o \sigma^{oy}_{\mathbf{k}'}V^{ioxg}_{\mathbf{q}}) \\
&\times\delta(\epsilon_{i,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\
&+\sum_o V^{xywz}_{\mathbf{q}}\sigma^{xi}_{\mathbf{k}}(-\sigma^{gz}_{\mathbf{k}'-\mathbf{q}}\sigma^{ow}_{\mathbf{k}+\mathbf{q}}V^{iyog}_{\mathbf{q}} + \sigma^{yo}_{\mathbf{k}'}(\sigma^{gw}_{\mathbf{k}+\mathbf{q}}V^{iogz}_{\mathbf{q}} + \sigma^{gz}_{\mathbf{k}'-\mathbf{q}}V^{iowg}_{\mathbf{q}} \\
&-V^{iowz}_{\mathbf{q}})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}})]
\end{aligned}$$

+

$$\begin{aligned}
\frac{d}{dt}\sigma^{ij}_{\mathbf{k}}|_{scatt(cc)} = &\frac{2\pi}{\hbar}\sum_{\mathbf{k}',\mathbf{q}}\sum_{w,x,y,z,g}[V^{iywz}_{\mathbf{q}}\sigma^{wx}_{\mathbf{k}+\mathbf{q}}\sigma^{zg}_{\mathbf{k}'-\mathbf{q}}(V^{jyxg}_{\mathbf{q}} - \sum_o \sigma^{oy}_{\mathbf{k}'}V^{joxg}_{\mathbf{q}}) \\
&\times\delta(\epsilon_{i,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\
&+V^{jywz}_{\mathbf{q}}\sigma^{xw}_{\mathbf{k}+\mathbf{q}}\sigma^{gz}_{\mathbf{k}'-\mathbf{q}}(V^{iyxq}_{\mathbf{q}} - \sum_o \sigma^{yo}_{\mathbf{k}'}V^{ioxg}_{\mathbf{q}}) \\
&\times\delta(\epsilon_{j,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\
&+\sum_o V^{xywz}_{\mathbf{q}}\sigma^{xj}_{\mathbf{k}}(-\sigma^{gz}_{\mathbf{k}'-\mathbf{q}}\sigma^{ow}_{\mathbf{k}+\mathbf{q}}V^{iyog}_{\mathbf{q}} + \sigma^{yo}_{\mathbf{k}'}(\sigma^{gw}_{\mathbf{k}+\mathbf{q}}V^{iogz}_{\mathbf{q}} + \sigma^{gz}_{\mathbf{k}'-\mathbf{q}}V^{iowg}_{\mathbf{q}} \\
&-V^{iowz}_{\mathbf{q}})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}}) \\
&+\sum_o V^{xywz}_{\mathbf{q}}\sigma^{ix}_{\mathbf{k}}(-\sigma^{zg}_{\mathbf{k}'-\mathbf{q}}\sigma^{wo}_{\mathbf{k}+\mathbf{q}}V^{jyog}_{\mathbf{q}} + \sigma^{oy}_{\mathbf{k}'}(\sigma^{wg}_{\mathbf{k}+\mathbf{q}}V^{jogz}_{\mathbf{q}} + \sigma^{zg}_{\mathbf{k}'-\mathbf{q}}V^{jowg}_{\mathbf{q}} \\
&-V^{jowz}_{\mathbf{q}})) \times \delta(\epsilon_{x,\mathbf{k}} + \epsilon_{y,\mathbf{k}'} - \epsilon_{z,\mathbf{k}+\mathbf{q}} - \epsilon_{w,\mathbf{k}'-\mathbf{q}})
\end{aligned}$$

Simulation

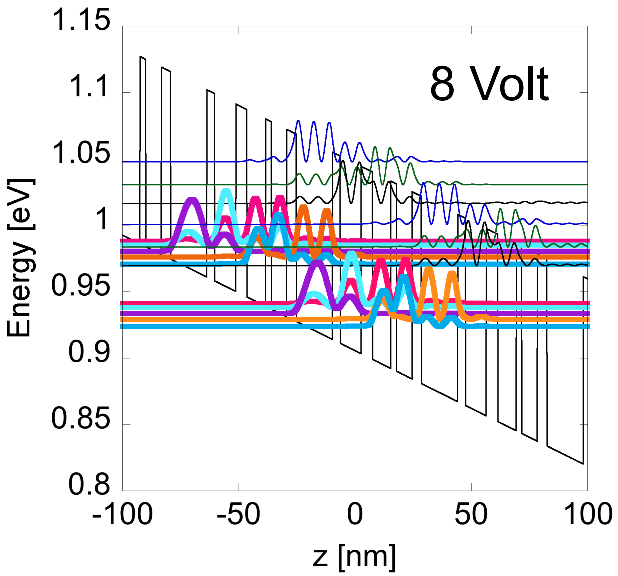
Code

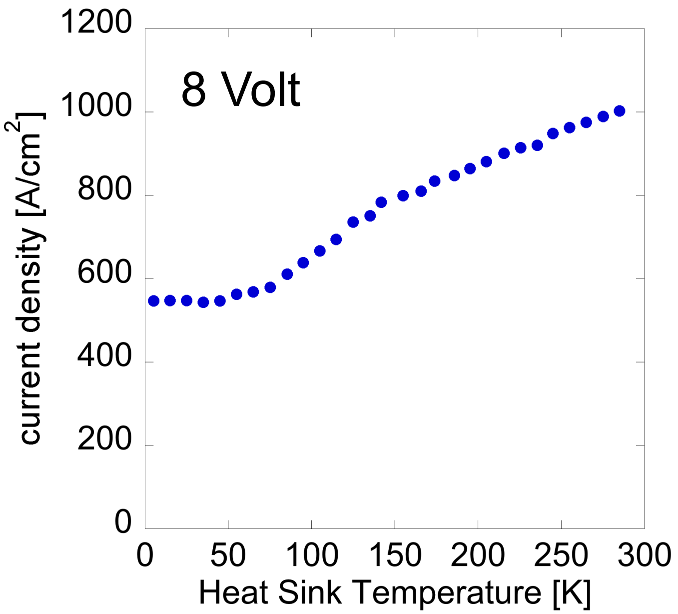
Needed: Performance simulator

without fit parameters !!!

VALIDATED

Experiment





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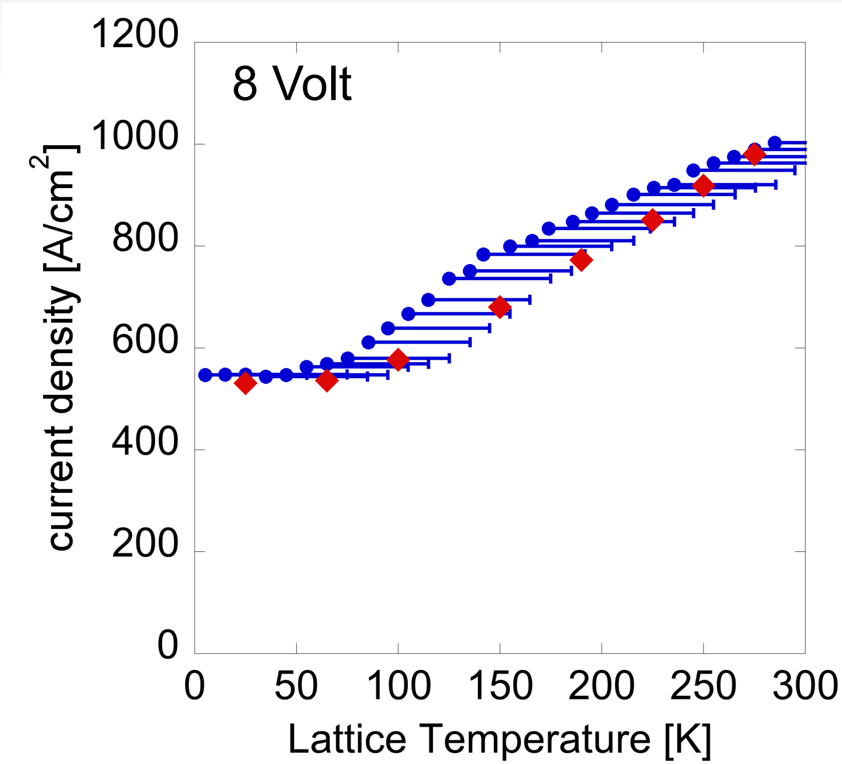
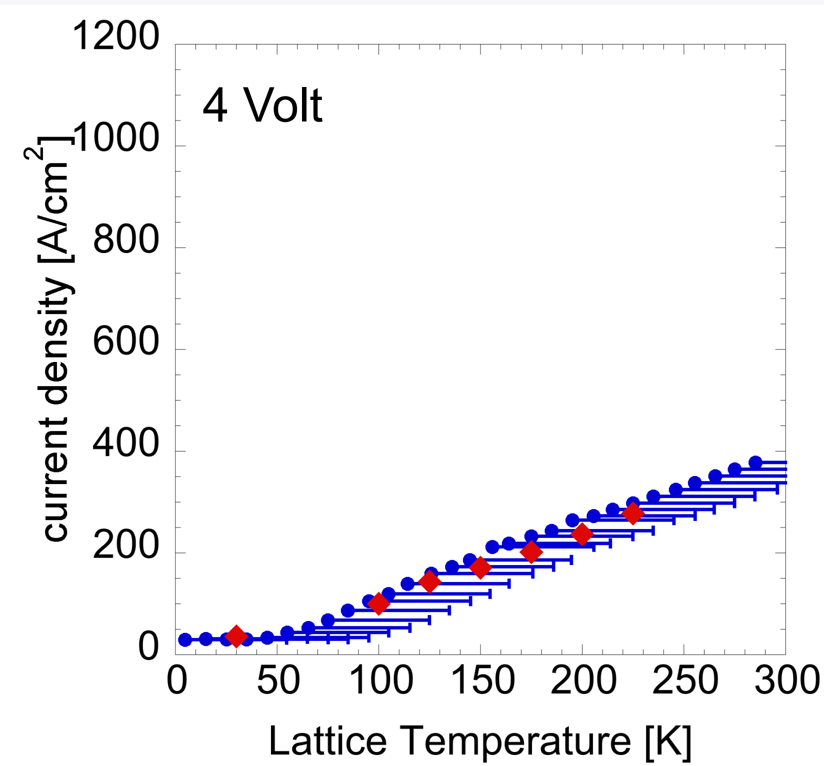
Experiment Simulation

Experiment Simulation





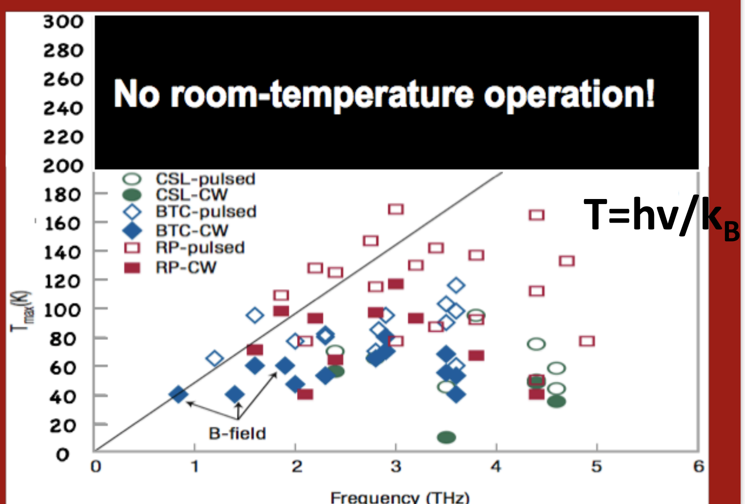
Performance Simulator

NO fit parameters !!!

(confirms exp. results by Vitiello et al on bias-depending Joule heating)

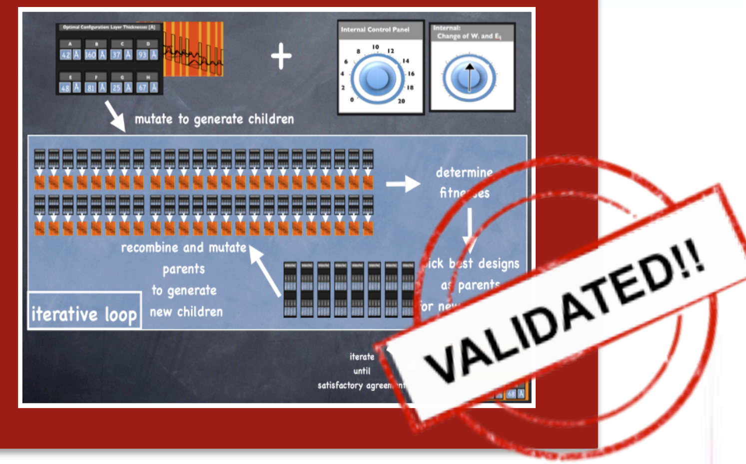
Understanding the high temperature limits of THz QCLs

I.



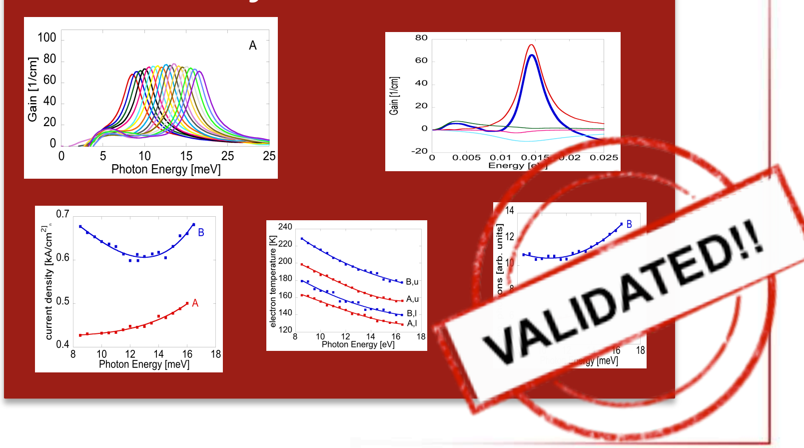
II.

IQE Design Tool



III.

No-Fit Performance Simulator



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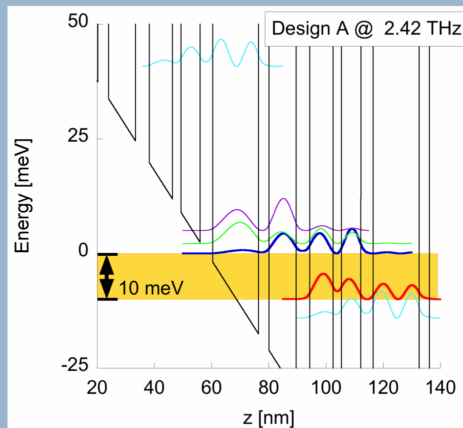
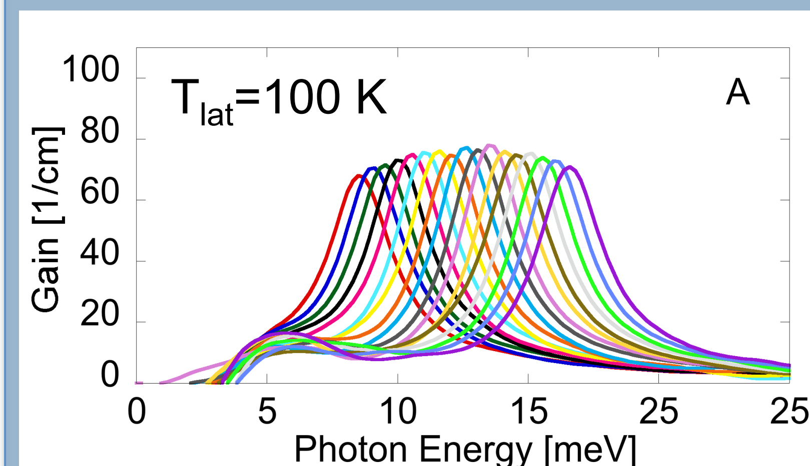
Extras

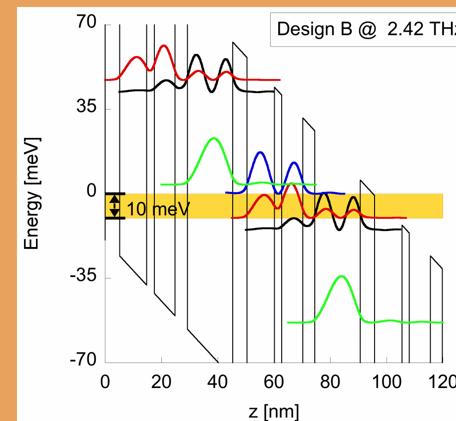
Use quantum kinetic performance simulator to investigate 1/kt

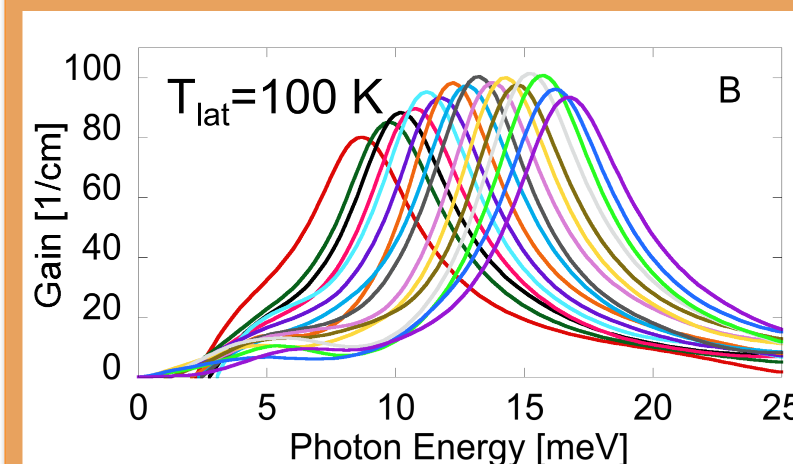
Frequency-shift design A

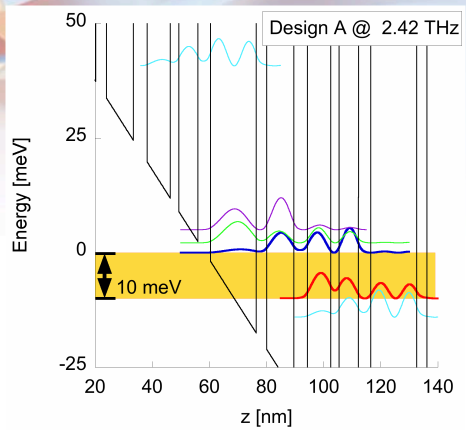




Frequency-shift design B

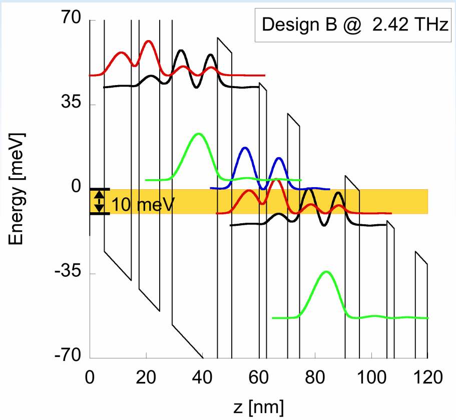




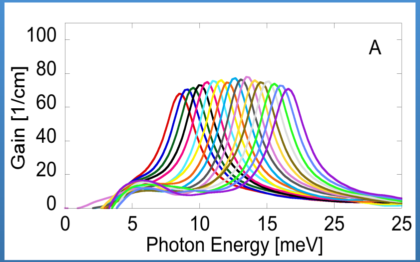


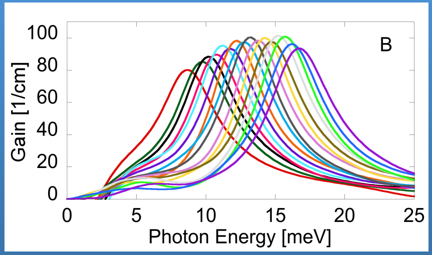
Which design is better???

And WHY ???

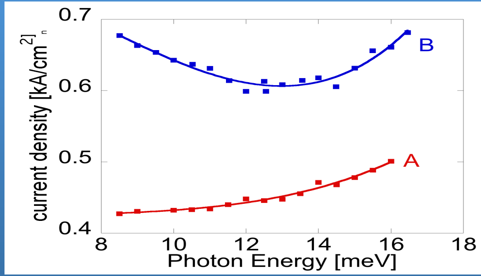


gain…

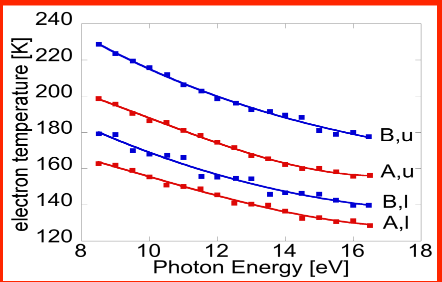




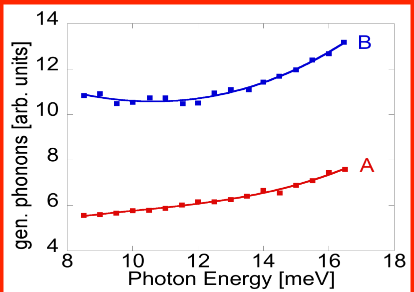
current density…



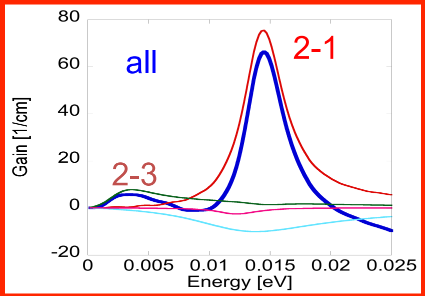
electrons…



phonons…



diff. gain contrib.…



Cannot "simply" simulate… can actually start understanding…

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