



# Modeling of Quantum Cascade Laser Sources with Giant Optical Nonlinearities

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- Modeling of quantum cascade lasers
- Inclusion of optical cavity field
- THz difference frequency generation in QCL structures
- Mode-locked QCLs and frequency combs
- Conclusion

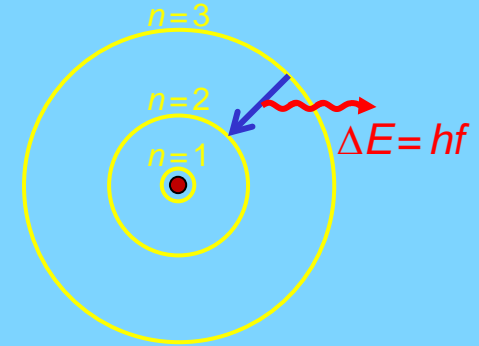


# Quantum Cascade Laser

## Conventional lasers/light sources

Use optical transitions in atoms, molecules, lattices,...

- Usually in infrared, visible or ultraviolet regime
- ⇒ **Scientifically underdeveloped terahertz gap**
- ⇒ **No practical compact diode lasers in mid-infrared**



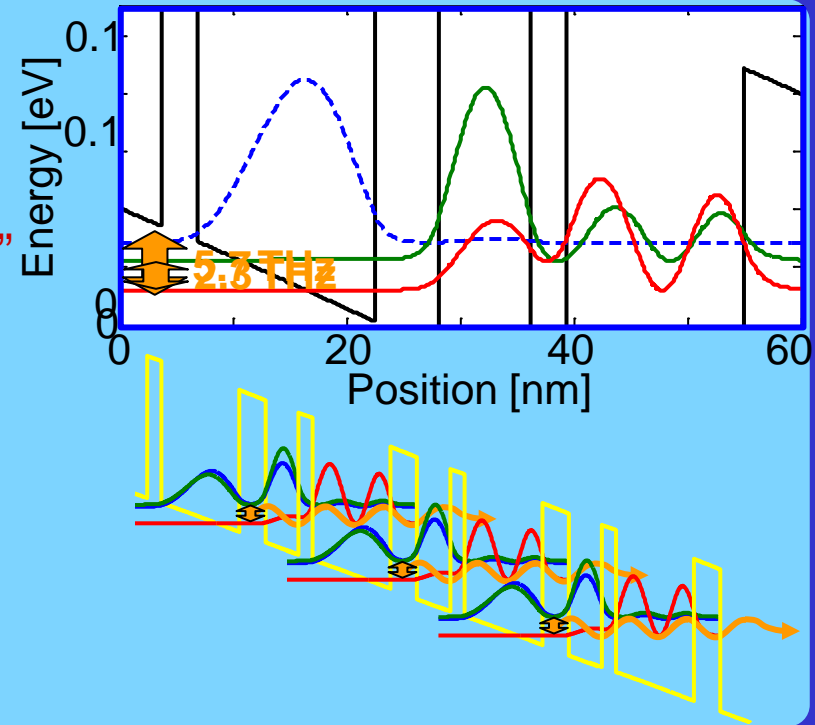
## Quantum cascade laser (QCL)

Use nanostructure as “artificial atom”

- Wavelength does not depend on material, but can be tailored by “quantum engineering”
- ⇒ **QCL covers terahertz and mid-infrared**

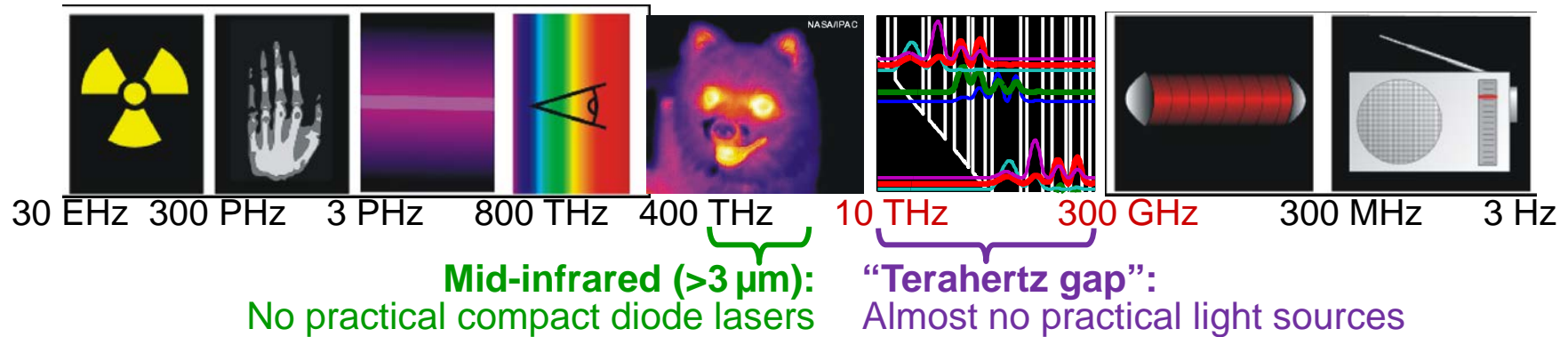
Use many transitions in a series (“cascade”)

- A single electron can emit multiple photons
- ⇒ **Increased optical power and efficiency**



# Quantum Engineering of Active Region

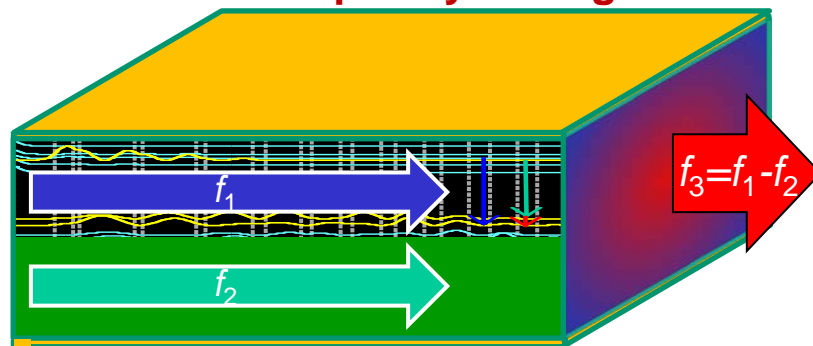
- Optical gain characteristics can be custom-tailored  
 ⇒ Mid-infrared and THz ranges become accessible



- Artificial giant optical nonlinearities can be integrated

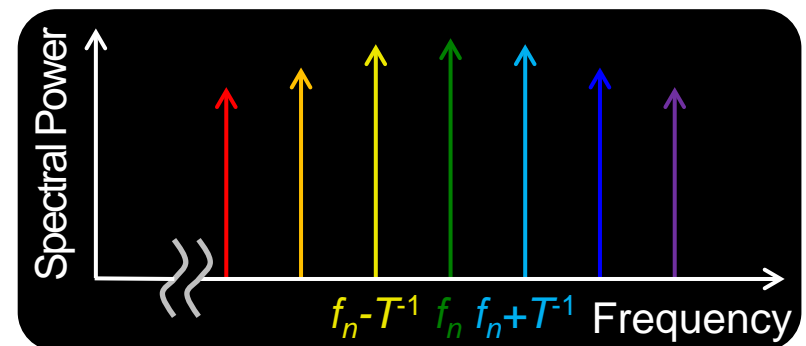
## Frequency conversion structures

- Based on frequency mixing

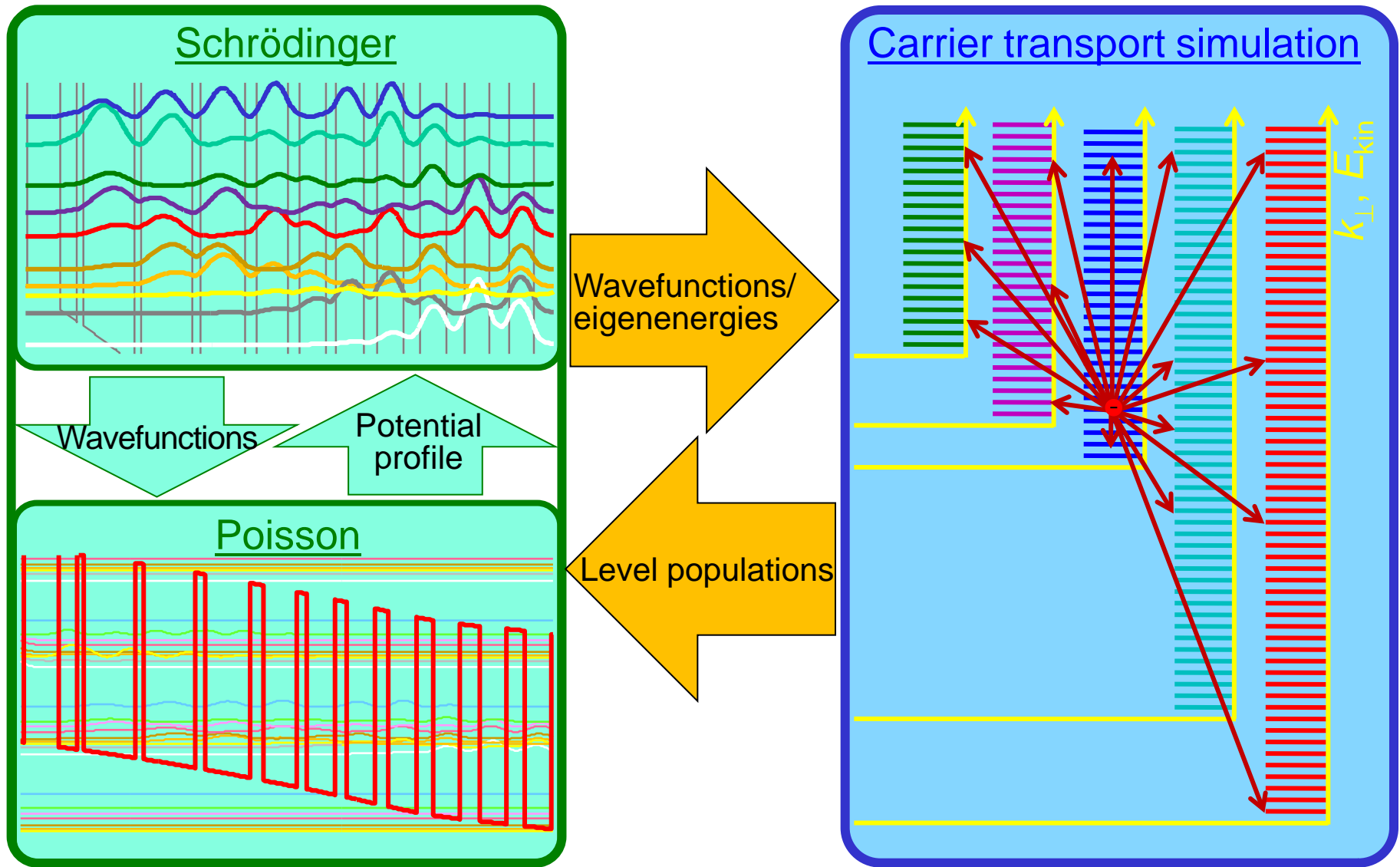


## Mode-locking & frequency combs

- Based on nonlinear coherent interaction



# Ensemble Monte Carlo (EMC)

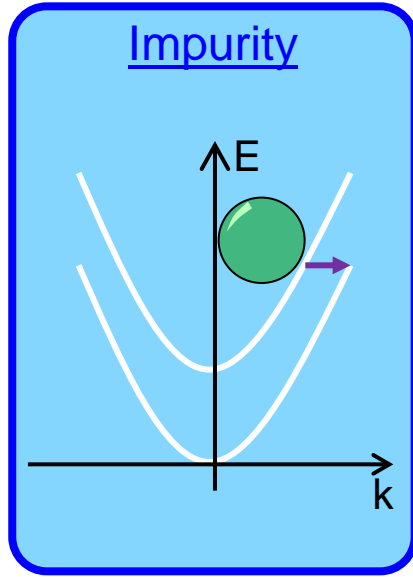
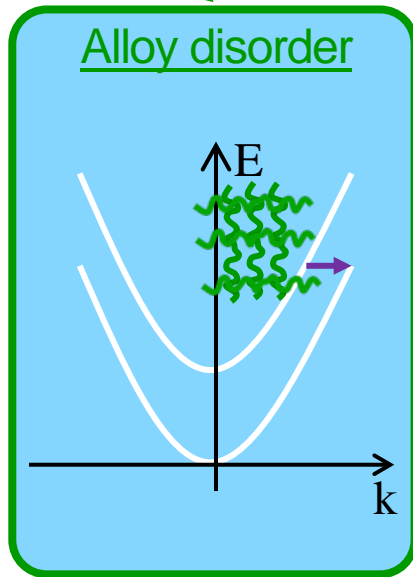
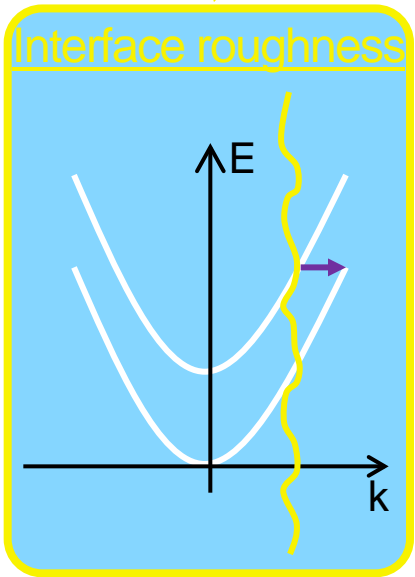
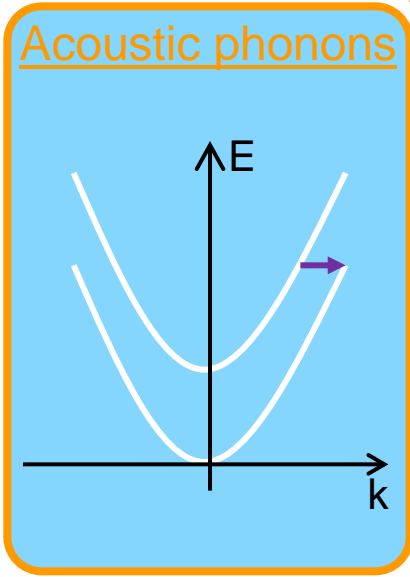
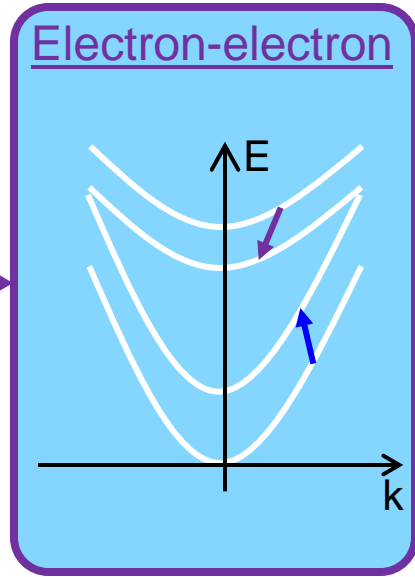
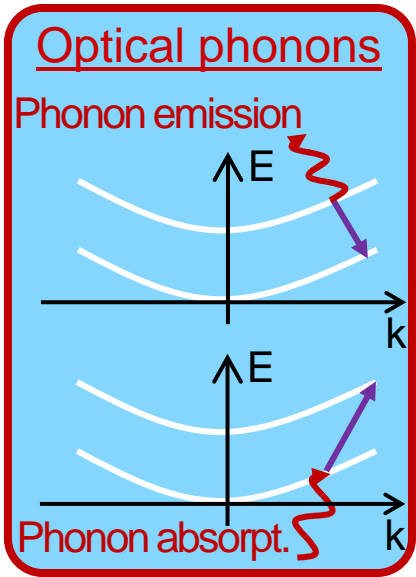


# Boltzmann Equation and Scattering

Boltzmann equation for carrier distribution function  $f_{n,k}(t)$ :

$$\frac{df_{n,k}}{dt} = \sum_s \sum_{m,k'} (W_{mk'nk} f_{m,k'} - W_{nkmk'} f_{n,k})$$

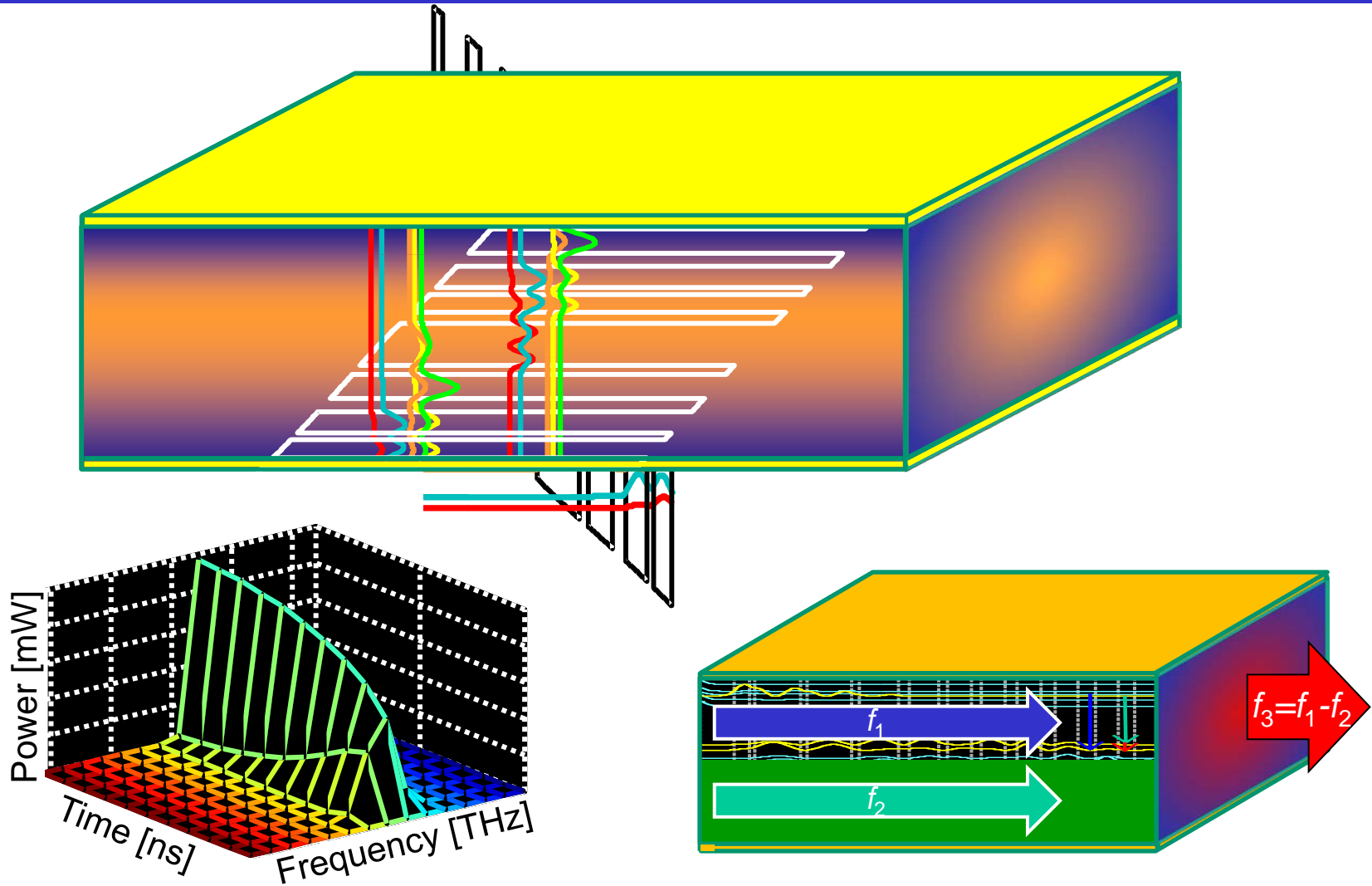
$W_{nkmk'}$



- Modeling of quantum cascade lasers
- **Inclusion of optical cavity field**
- THz difference frequency generation in QCL structures
- Mode-locked QCLs and frequency combs
- Conclusion



# Inclusion of Optical Cavity Field



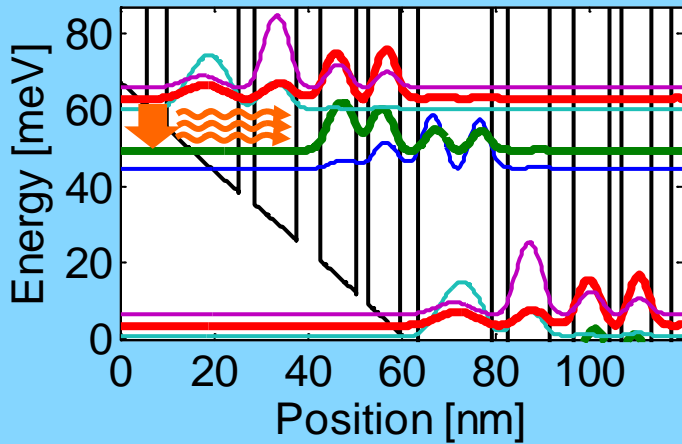
C. Jirauschek, Appl. Phys. Lett. **96**, 011103 (2010)  
A. Mátyás et al., J. Appl. Phys. **110**, 013108 (2011)  
C. Jirauschek, Opt. Express **18**, 25922 (2010)

C. Jirauschek et al., Opt. Express **21**, 6180 (2013)  
C. Jirauschek et al., Opt. Express **23**, 1670 (2015)





# Carrier-Light Coupling in Monte Carlo

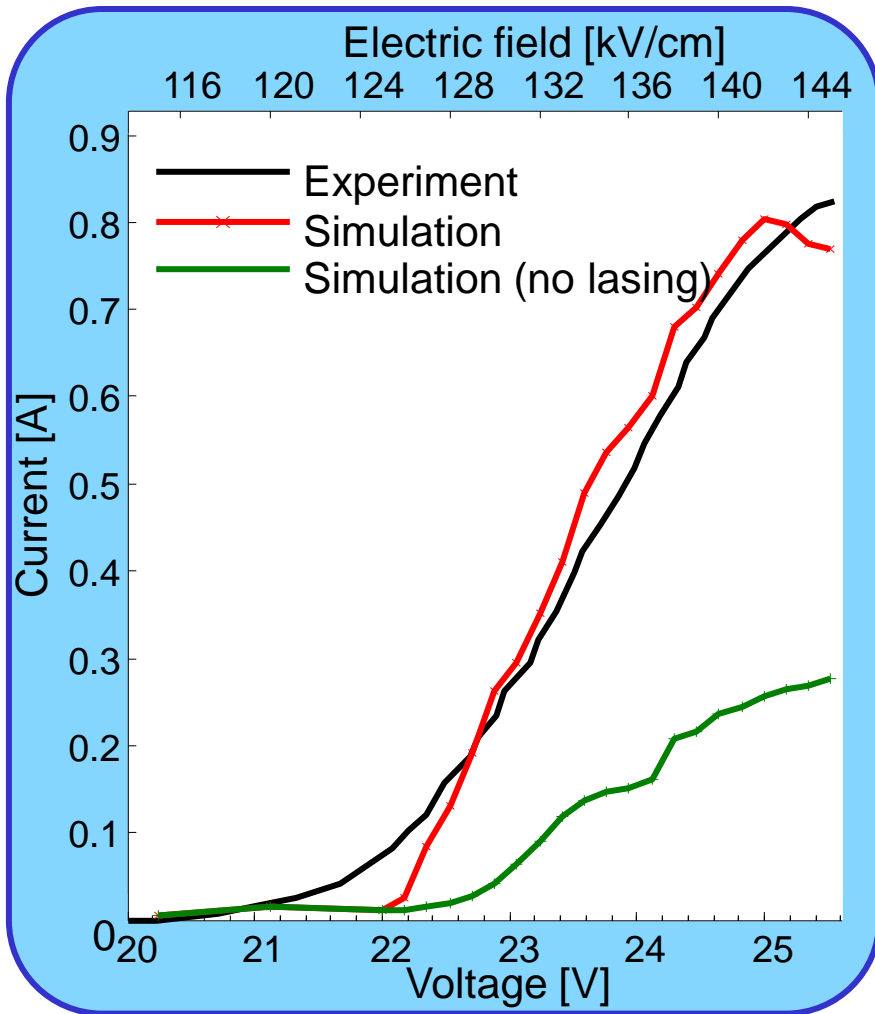


$$g(\omega) = \frac{e^2 \omega}{c \epsilon_0 n_0 \hbar L} n_E^{2D} \sum_{\substack{i,j \\ E_i > E_j}} |z_{ij}|^2$$

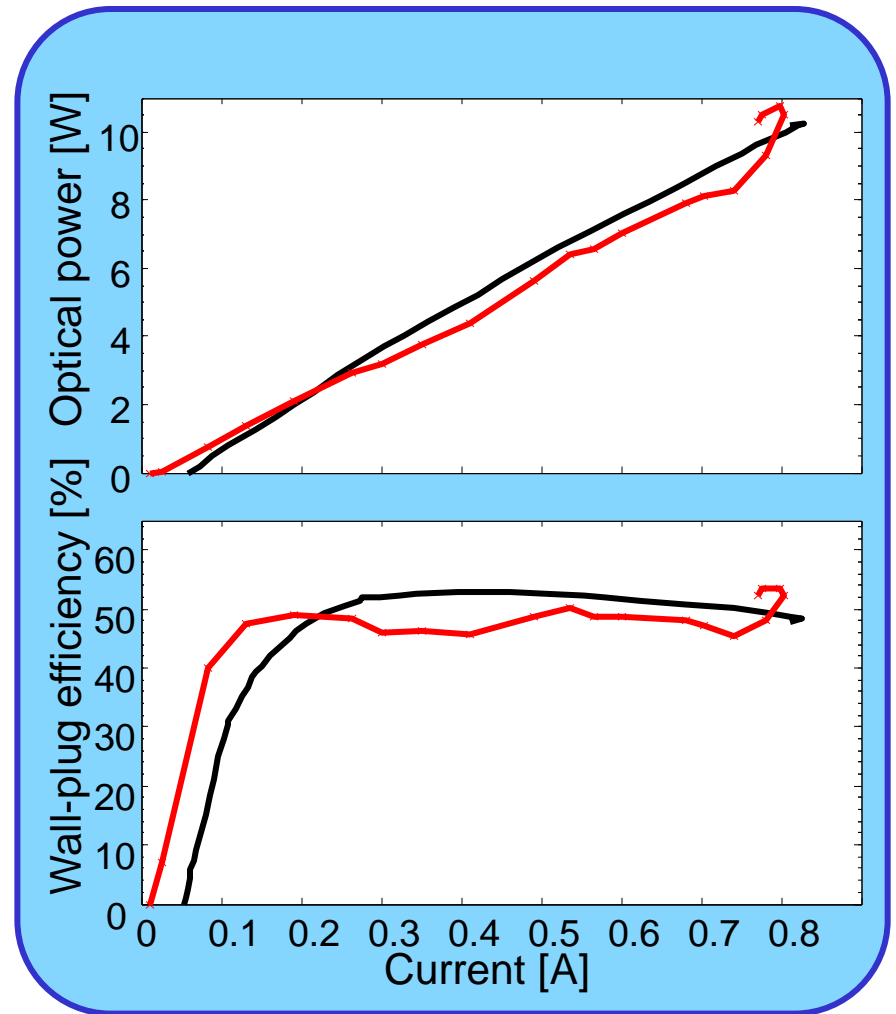
$$\times \int_0^\infty d\varepsilon \frac{[f_i(\varepsilon) - f_j(\varepsilon)] \gamma_{ij}(\varepsilon)}{\gamma_{ij}^2(\varepsilon) + [\omega - (E_i - E_j) / \hbar]^2}$$



# Simulation of High Efficiency Mid-Infrared QCL



Design: Y. Bai et al., Nat. Photonics 4, 99 (2010)



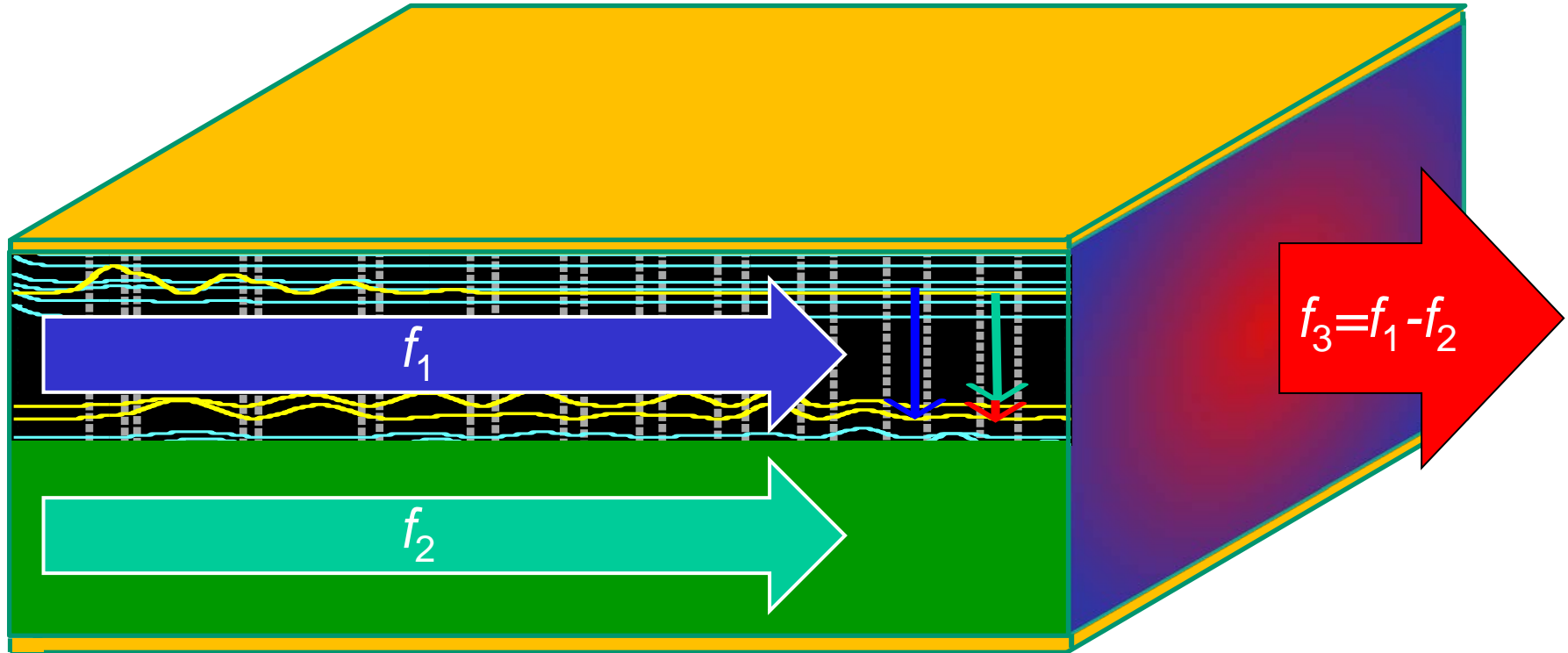
A. Matyas et al., J. Appl. Phys. 110, 013108 (2011)



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# THz Difference Frequency Generation QCL Structure



## Ideal THz source

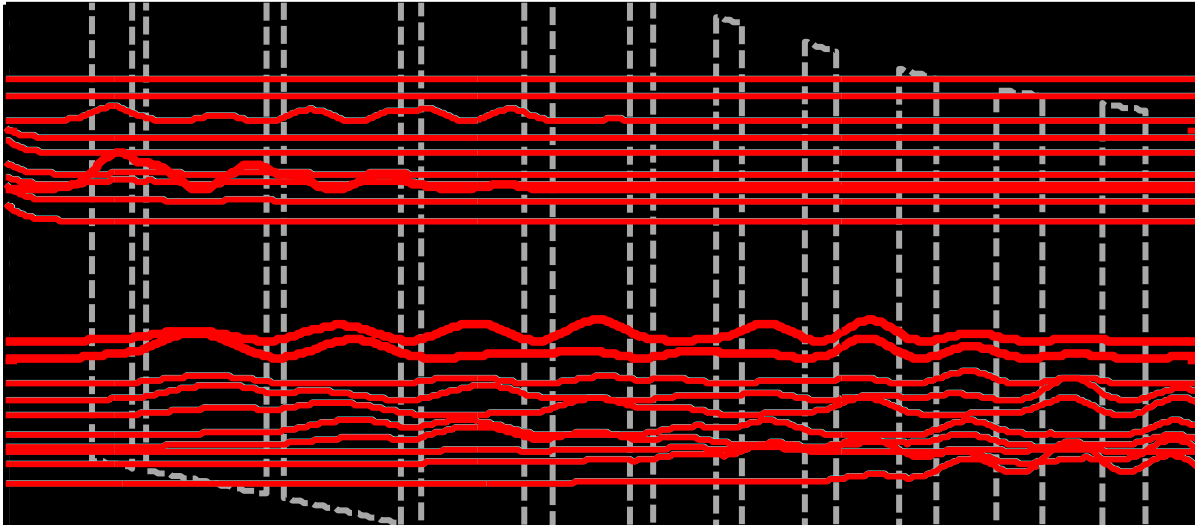
- Room temperature operation
- Broadband tunability
- THz output power in mW range

## THz DFG QCL source

- M. Belkin et al., Appl. Phys. Lett. **92**, 201101 (2008)  
**1.0-4.6 THz**
- Q.Y. Lu et al., Appl. Phys. Lett. **101**, 251121 (2012)  
**1.7-5.25 THz**
- K. Vijayraghava et al., Nature Comm. **4**, 2021 (2013)  
**1.9 mW pulsed, 3  $\mu$ W cw (at room temperature)**
- M. Razeghi et al., Opt. Express **23**, 8462 (2015)



# Modeling of Nonlinear Susceptibility



$$\chi^{(2)} = \frac{1}{\hbar^2 \epsilon_0 L_P} \sum_{\ell, m, n} d_{\ell m} d_{m n} d_{n \ell} n_E^{2D} \int_0^\infty f_\ell (K_{\ell m n} - K_{m \ell n}) d\varepsilon,$$

$$K_{\ell m n} = \left( \frac{1}{\omega_{n \ell} - i\gamma_{n \ell} - \omega} + \frac{1}{\omega_{n m} + i\gamma_{n m} + \omega} \right) \left( \frac{1}{\omega_{m \ell} - i\gamma_{m \ell} + \omega_2} + \frac{1}{\omega_{m \ell} - i\gamma_{m \ell} - \omega_1} \right)$$

$L_P$ : Period length  
 $\varepsilon$ : Kinetic energy  
 $f_m(\varepsilon)$ : Distribution function  
 $n_E^{2D} = m^* / (\pi \hbar^2)$ : 2D density of states

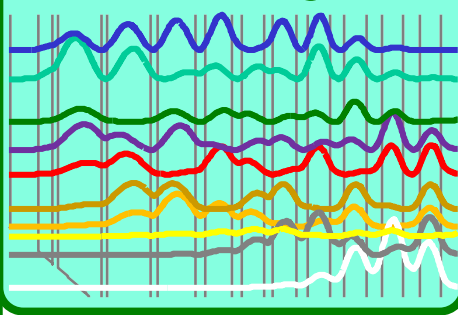
$\gamma_{mn}(\varepsilon)$ : Optical linewidth  
 $d_{mn}$ : Dipole matrix element  
 $\omega_{mn}$ : Resonance frequency  
 $\omega_{1,2}/\omega$ : Mid-IR/THz frequencies



# Multi-Domain Simulation Approach

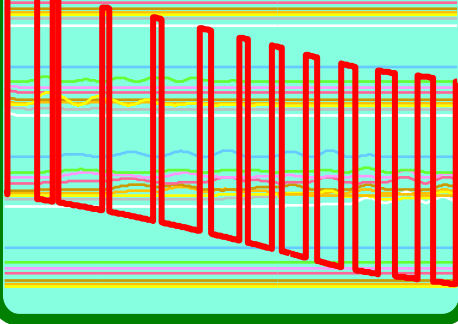
## Quantized energy states

### Schrödinger



Wave functions  
Potential profile

### Poisson

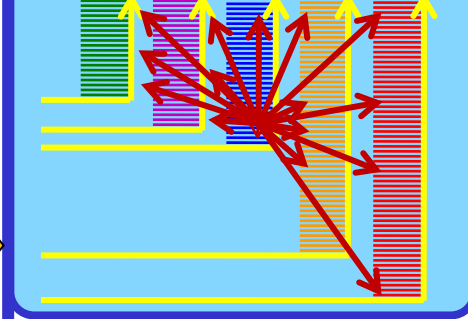


Wave functions/  
energies

Subband  
populations

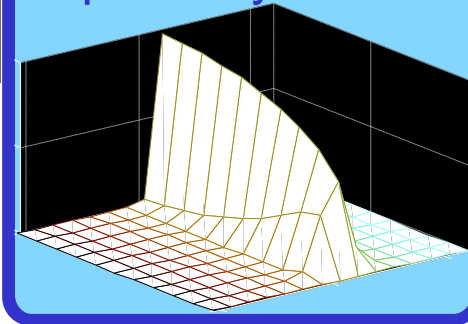
## Carrier and photon dynamics

### Monte Carlo



Gain Intensity

### Optical dynamics



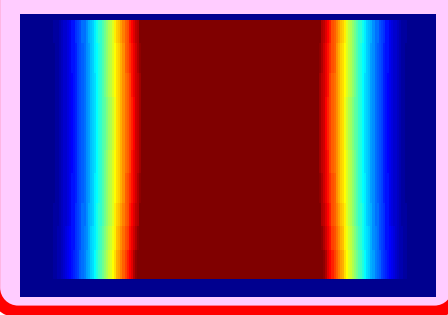
Suscep-  
tibility

Cavity loss  
Overlap  
factor

Subband  
populations  
Linewidth

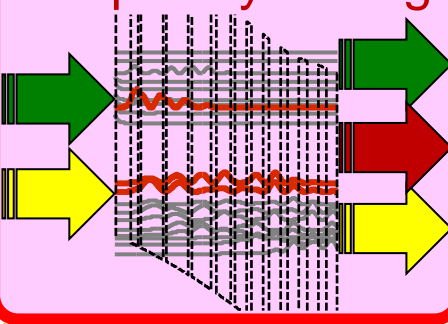
## Resonator and optical nonlinearity

### Mode solver



Mode  
profiles

### Frequency mixing

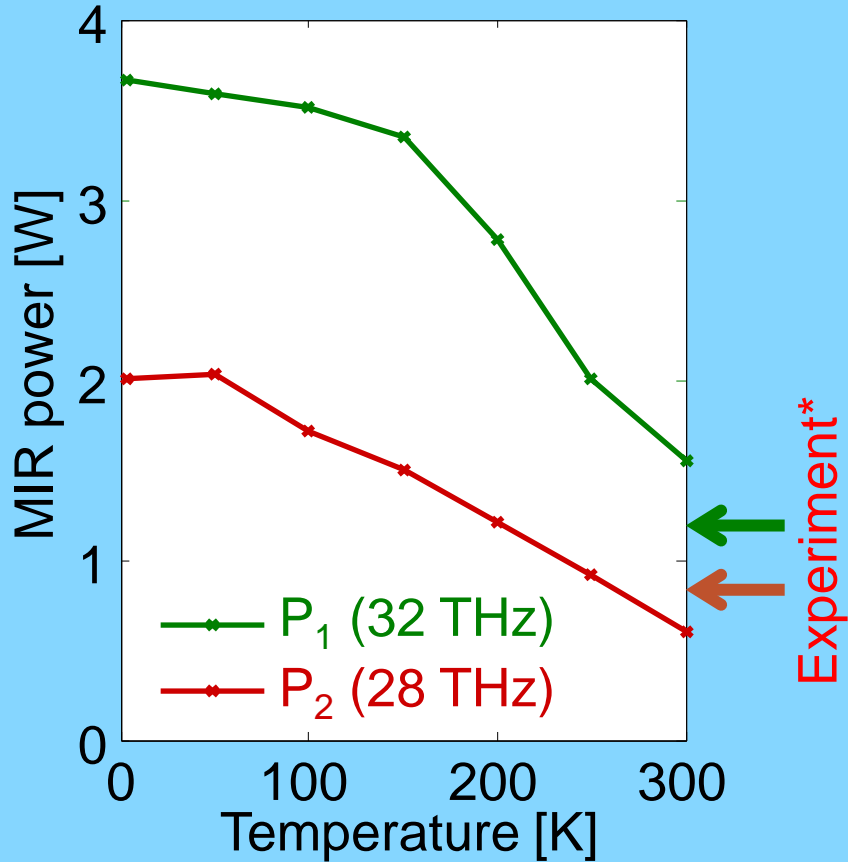


Wave functions, energies

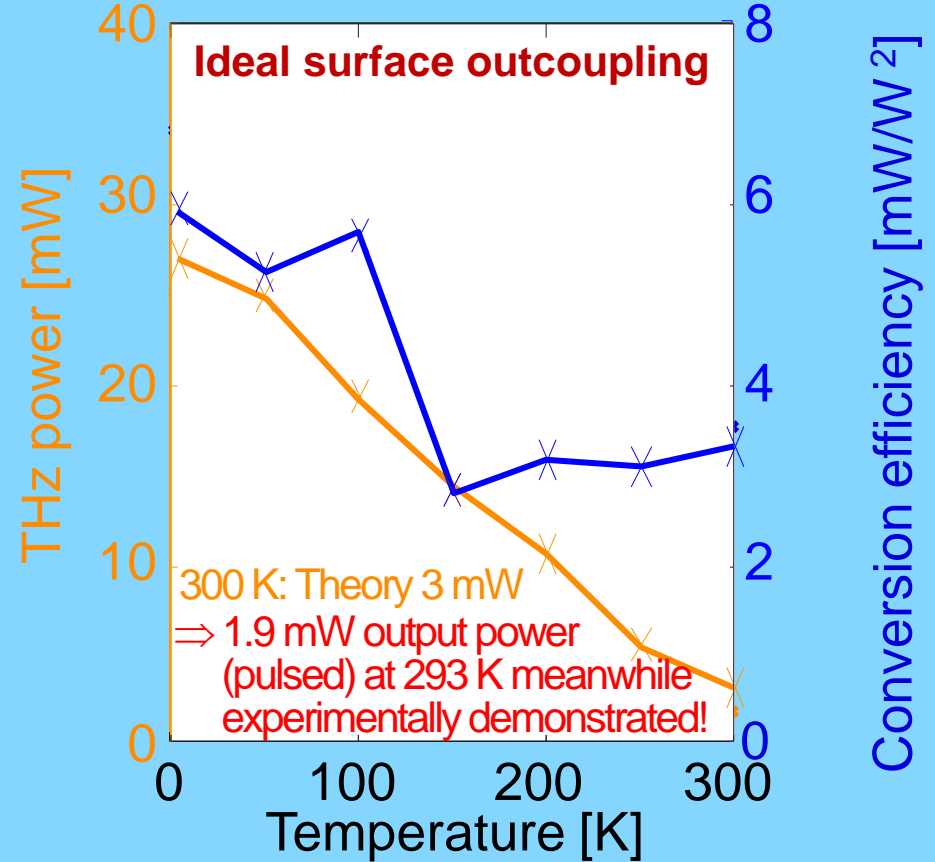


# Comparison Simulation - Experiment

## Mid-infrared results



## THz results



\*Q. Y. Lu et al., Appl. Phys. Lett. **99**, 131106 (2011)

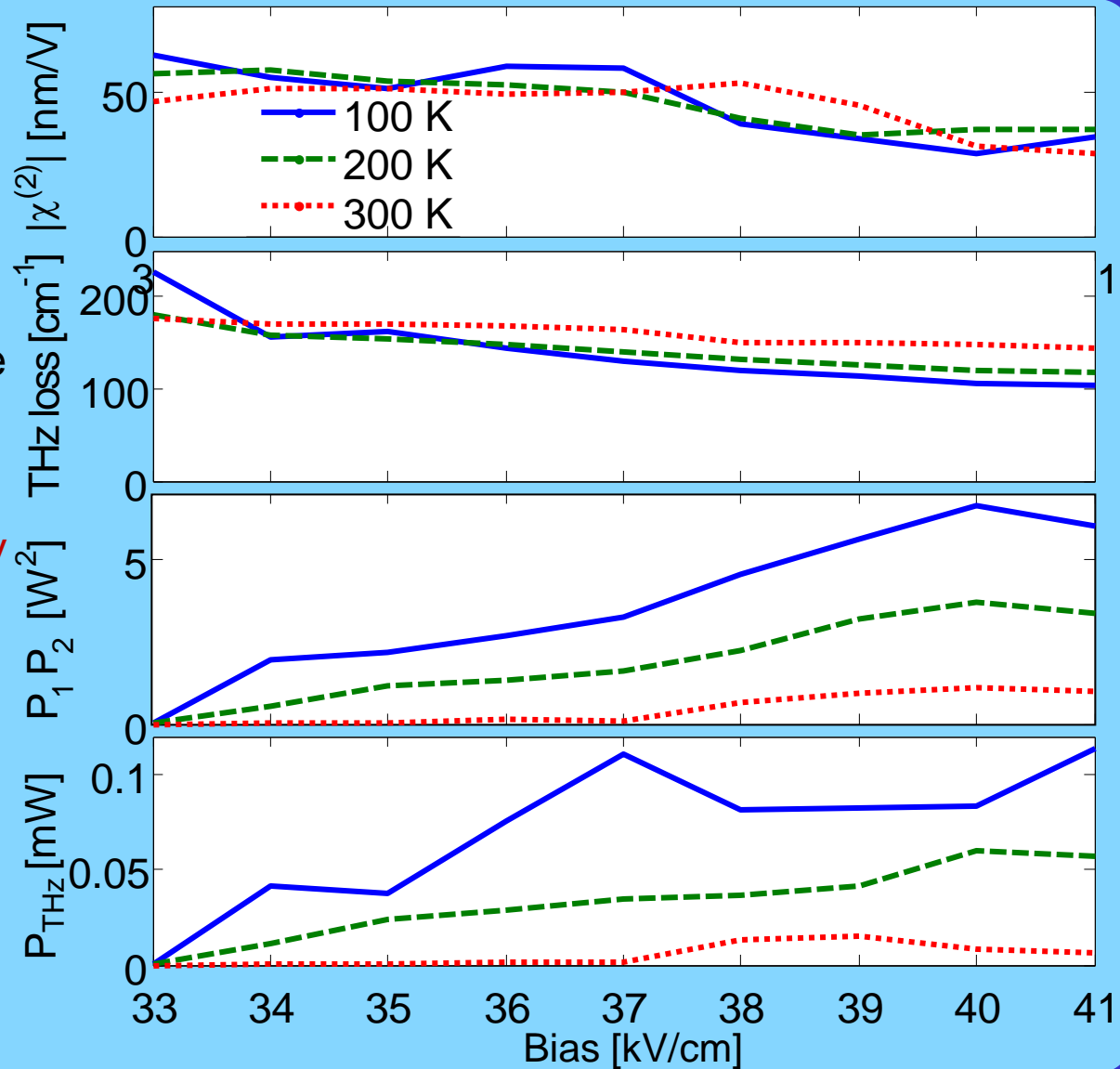
Extracted parameters in good agreement with experimental estimates:

- Nonlinear susceptibility  $|\chi^{(2)}| = 44 \text{ nm/V}$
- THz waveguide loss  $a = 150 \text{ cm}^{-1}$  C. Jirauschek et al., Opt. Express **21**, 6180 (2013)



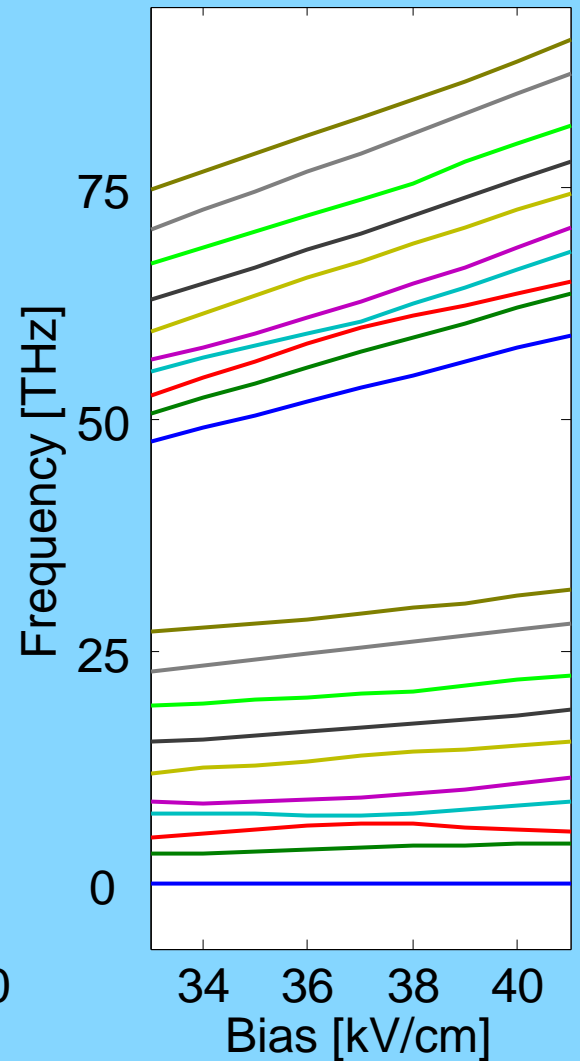
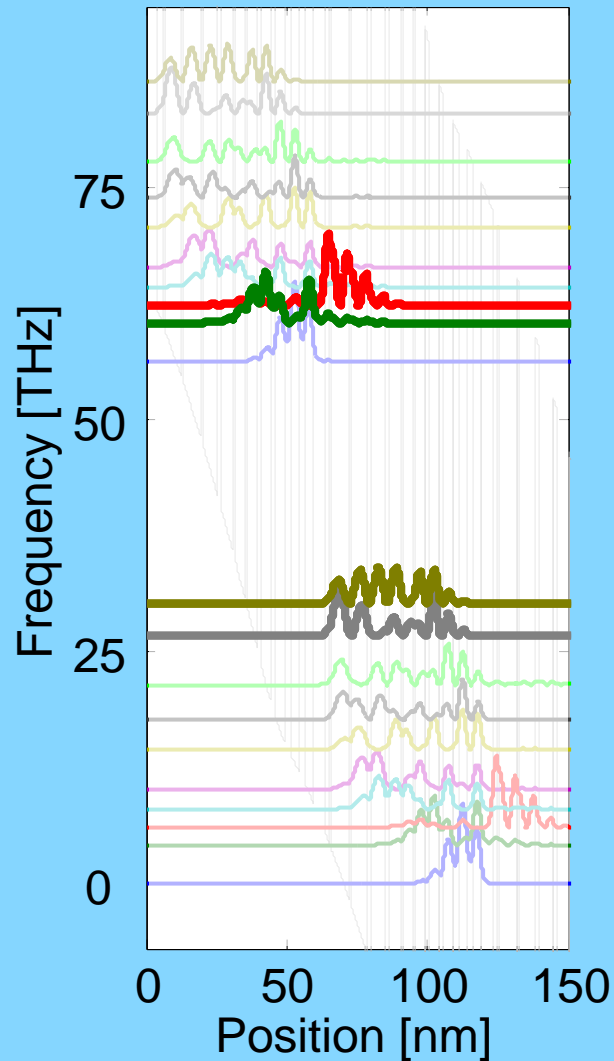
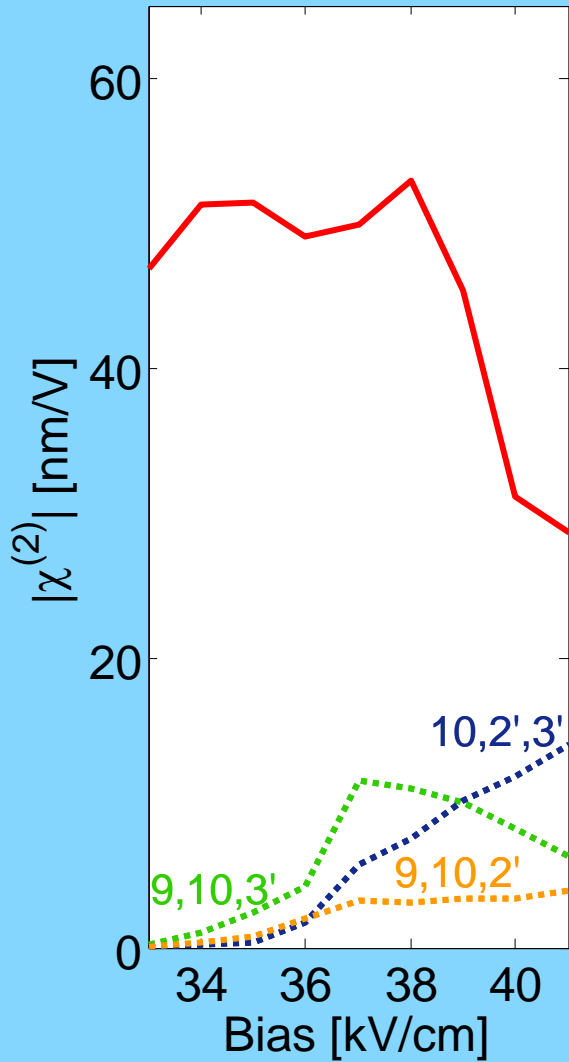
# Temperature Degradation of THz Power

- Susceptibility  $\chi^{(2)}$  does not degrade with temperature
- THz loss  $a_{\text{THz}}$  moderately increases with temperature
- MIR powers  $P_1, P_2$  strongly decrease with temperature
- THz power  $P_{\text{THz}}$  strongly degrades with temperature





# Contributions of Individual Subband Triplets

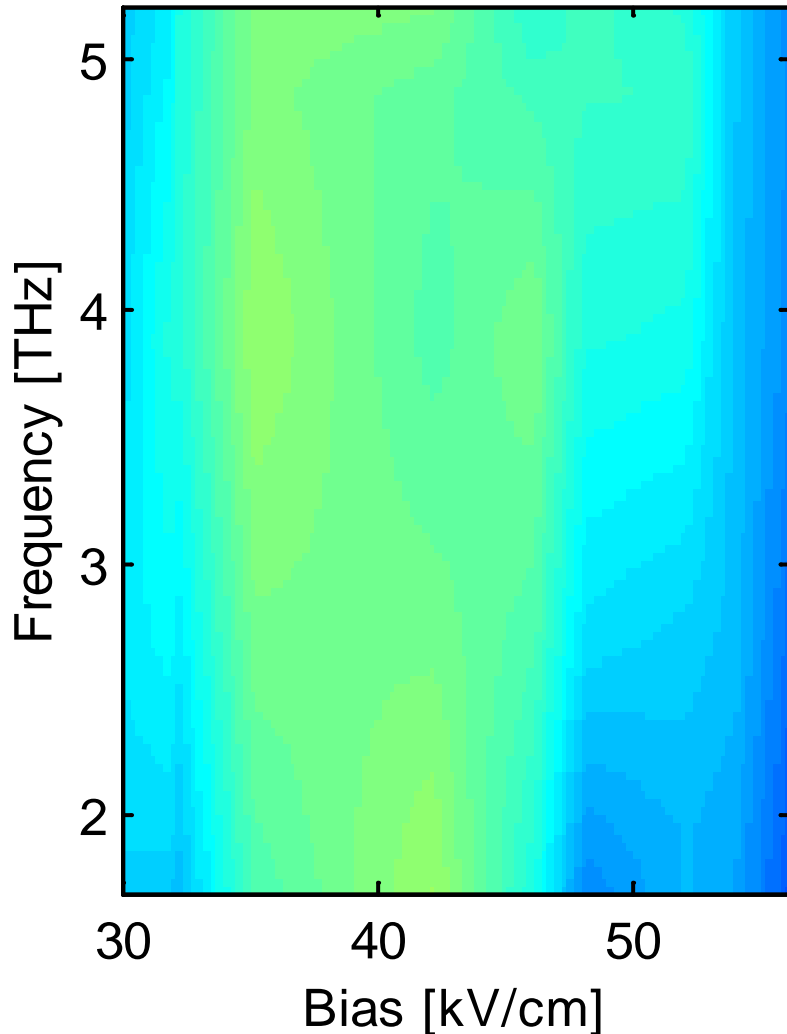


C. Jirauschek et al., Opt. Express **23**, 1670 (2015)

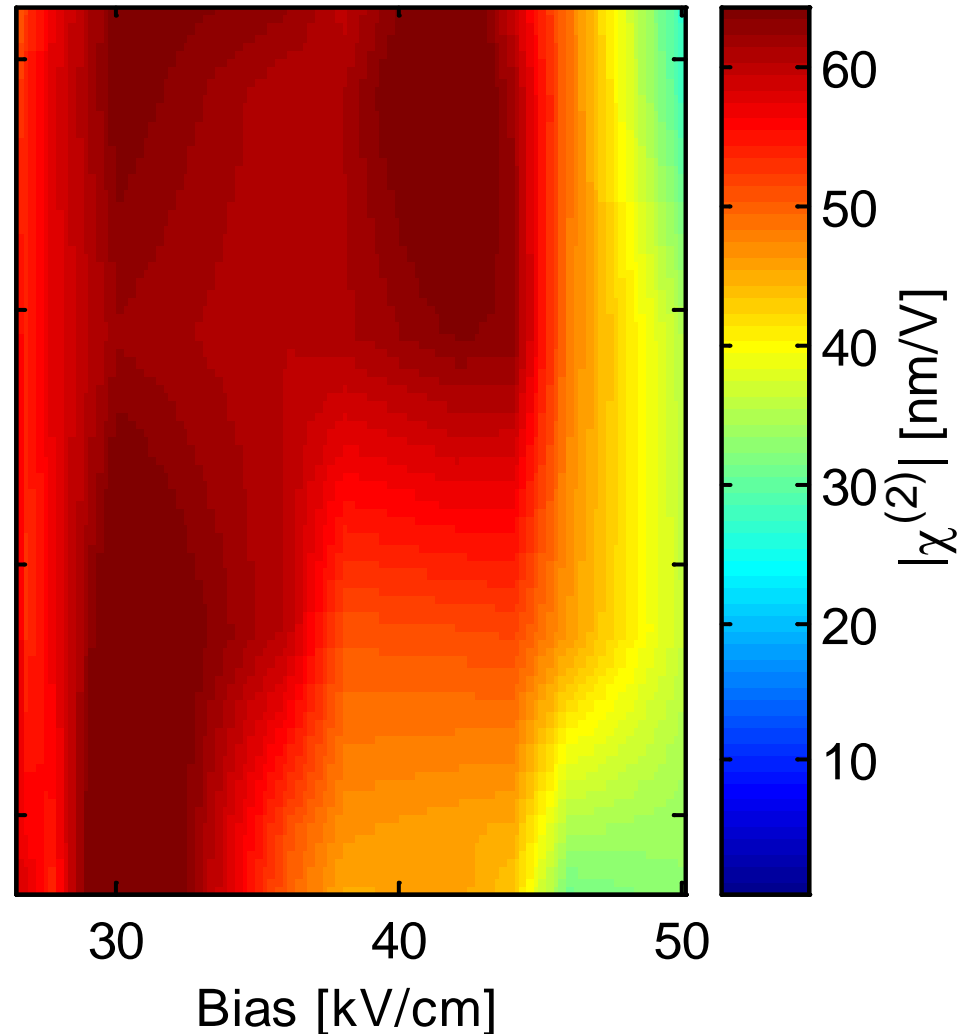


# Susceptibility of Widely Tunable THz DFG Structure

**8.2  $\mu\text{m}$  design**



**9.2  $\mu\text{m}$  design**



Design: K. Vijayraghava et al., Nature Comm. 4, 2021 (2013)



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# Extended Maxwell-Bloch Equations

Field: 
$$\frac{n}{c} \partial_t \mathbf{E} = -\partial_z \mathbf{E} - i \frac{k N \mu \Gamma}{2 \epsilon_0 n^2} \eta - \frac{1}{2} \ell (\mathbf{E}) \mathbf{E}$$

Polarization: 
$$\partial_t \eta = \frac{i \mu}{2 \hbar} \mathbf{E} \Delta - \frac{\eta}{T_2}$$

Inversion: 
$$\partial_t \Delta = \frac{\Delta_p - \Delta}{T_1} + \frac{i \mu}{\hbar} (\mathbf{E}^* \eta - c.c.)$$

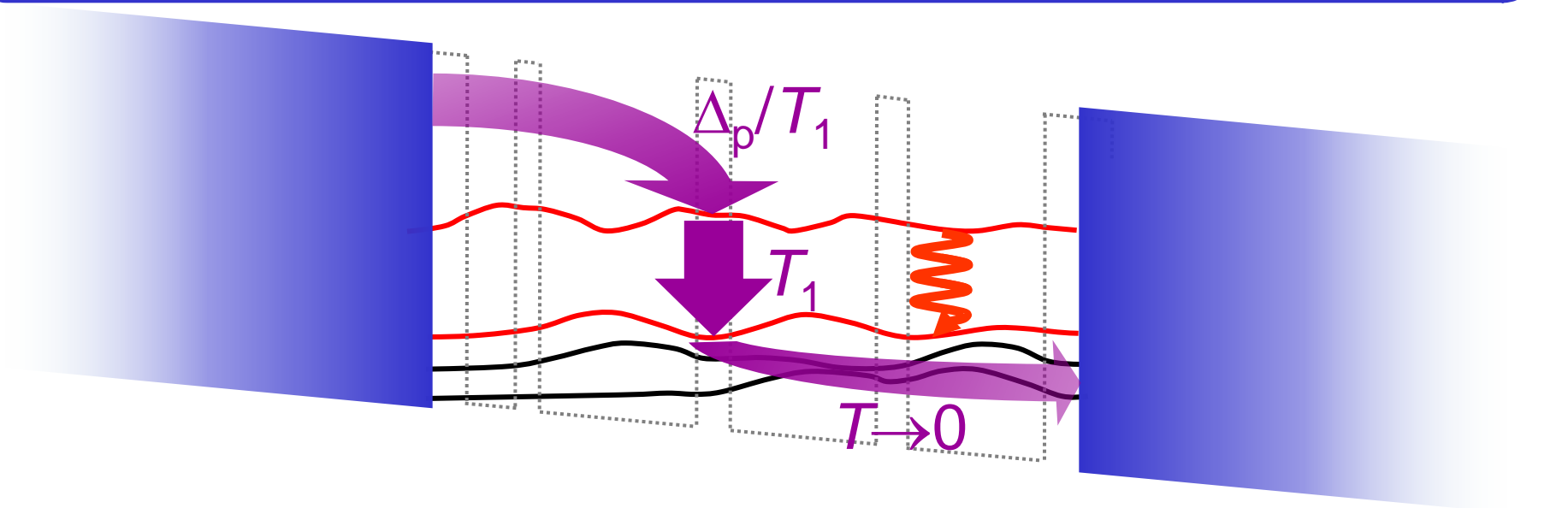


# Rate Equations

Field:  $\frac{n}{c} \partial_t E = -\partial_z E - i \frac{k N \mu \Gamma}{2 \epsilon_0 n^2} \eta - \frac{1}{2} \ell(E) E$

Polarization:  $\partial_t \eta = \frac{i \mu}{2 \hbar} E \Delta - \frac{\eta}{T_2}$

Inversion:  $\partial_t \Delta = \frac{\Delta_p - \Delta}{T_1} + \frac{i \mu}{\hbar} (E^* \eta - c.c.)$

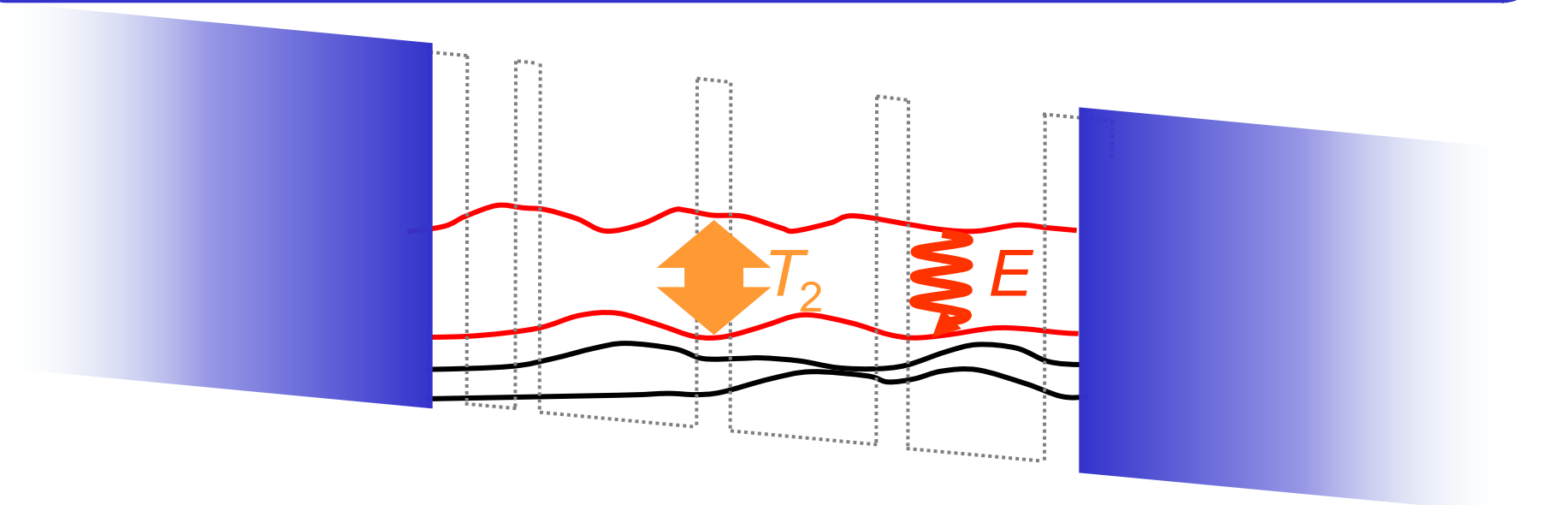


# Coherent Effects

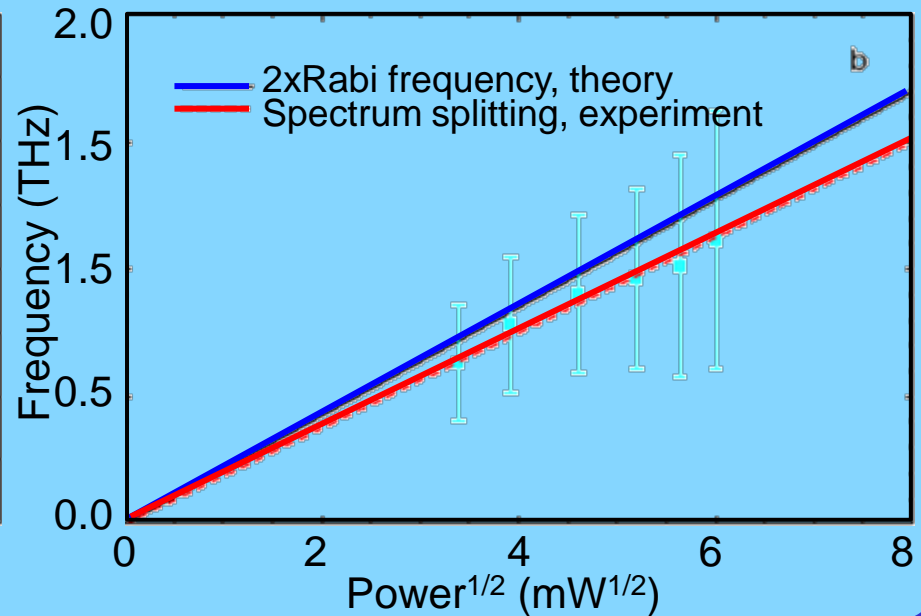
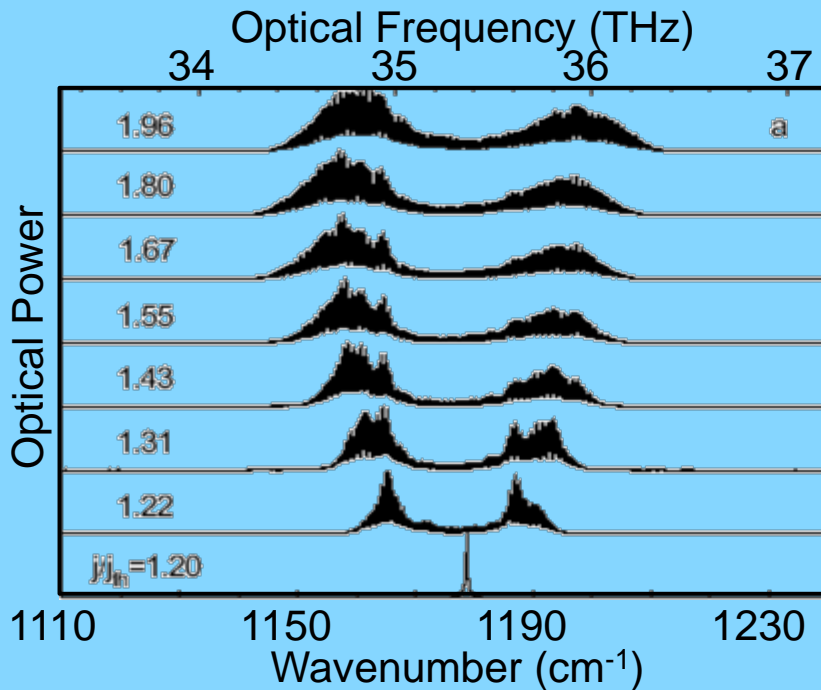
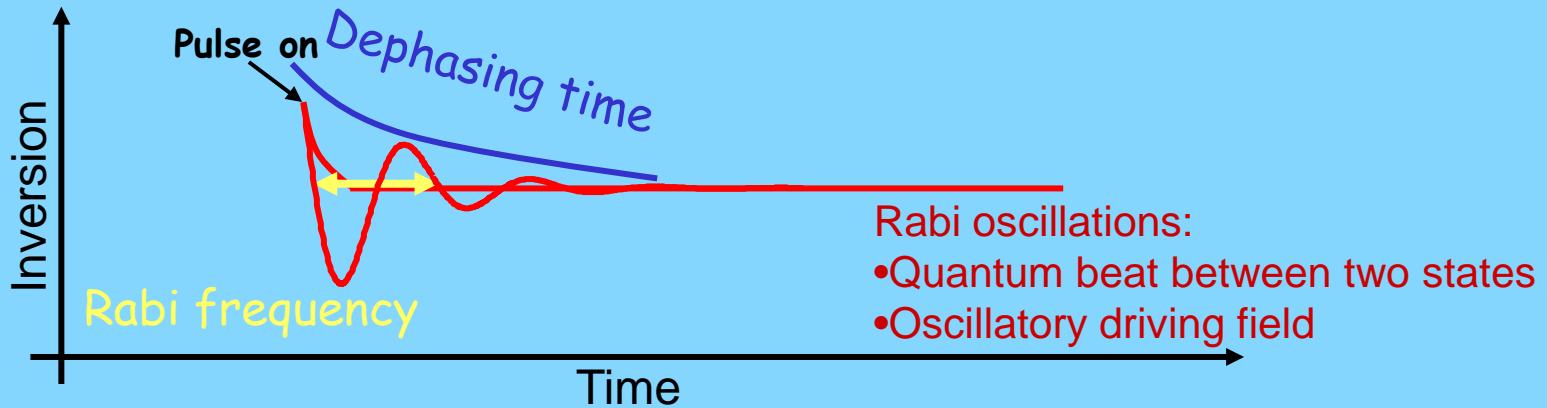
Field:  $\frac{n}{c} \partial_t E = -\partial_z E - i \frac{k N \mu \Gamma}{2 \epsilon_0 n^2} \eta - \frac{1}{2} \ell(E) E$

Polarization:  $\partial_t \eta = \frac{i \mu}{2 \hbar} E \Delta - \frac{\eta}{T_2}$

Inversion:  $\partial_t \Delta = \frac{\Delta_p - \Delta}{T_1} + \frac{i \mu}{\hbar} (E^* \eta - c.c.)$



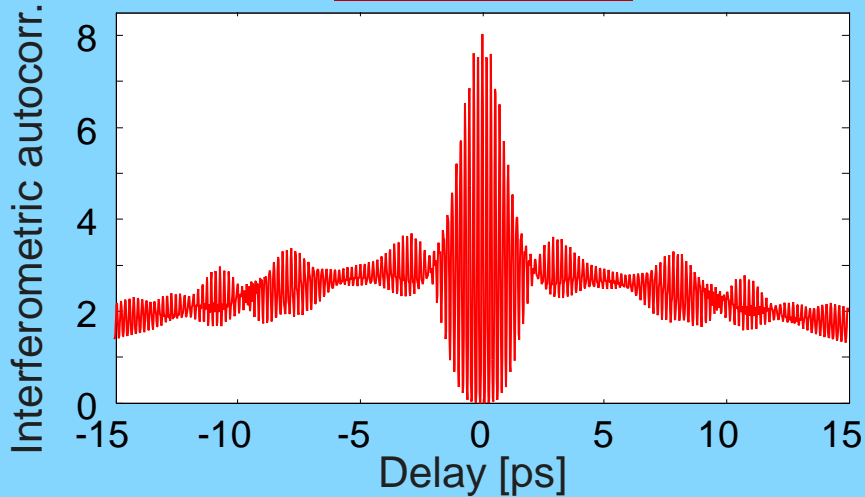
# Manifestation of Coherent Effects



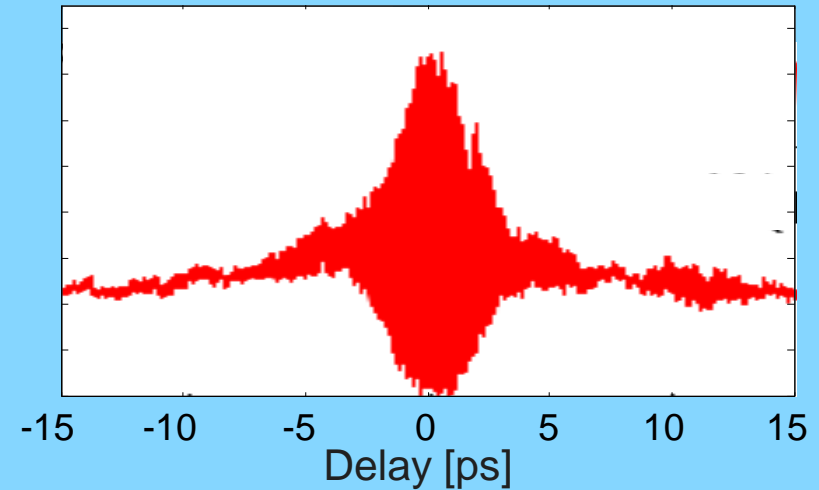
C. Y. Wang et al., Phys. Rev. A **75**, 031802(R) (2007)

# Simulation of Actively Mode-Locked QCLs

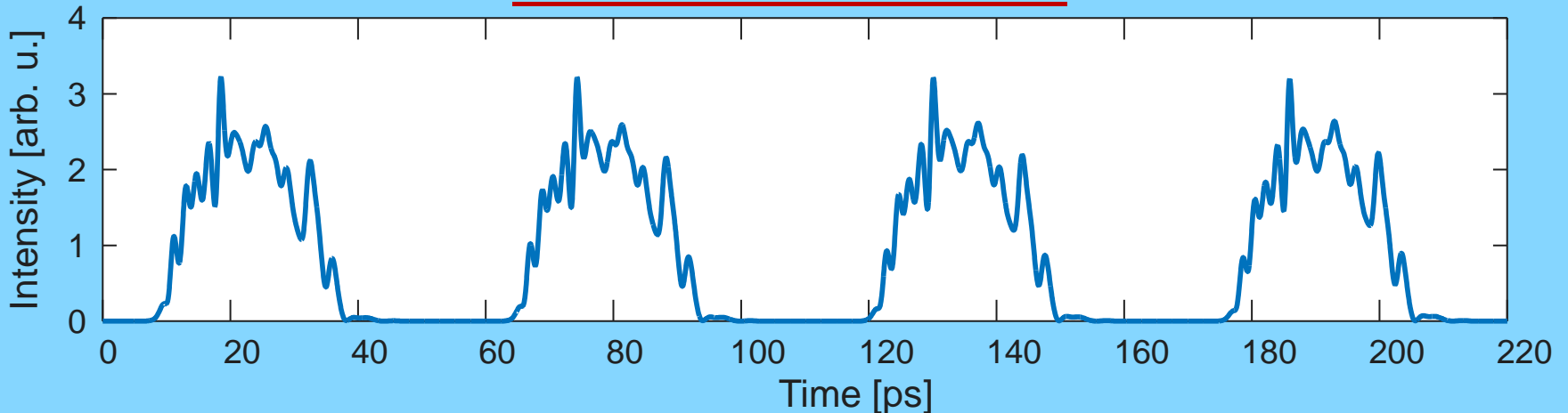
Simulation



Experiment



Simulated Pulse Train



V.-M. Gkortsas et al., Opt. Express **18**, 13616 (2010)





# Multi-Domain Simulation Approach

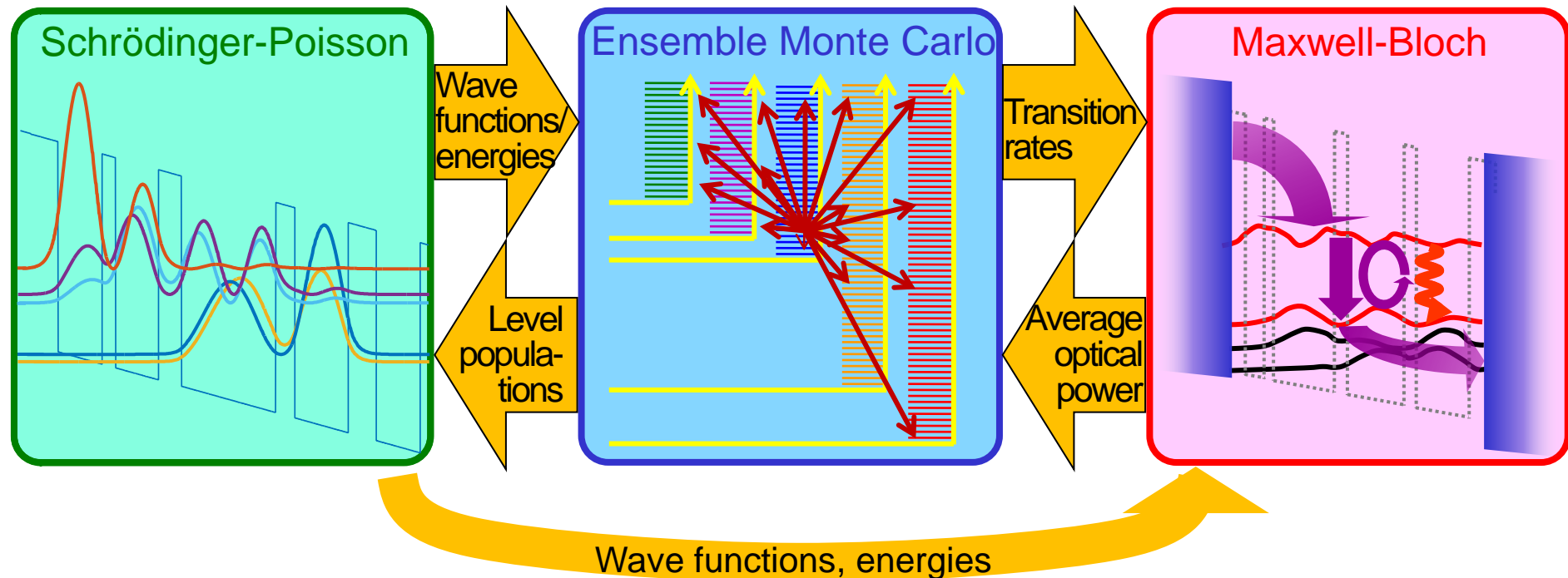
Maxwell-Bloch approach requires lifetimes/  
transition rates as input parameters

- Empirical or guessed values are used,  
affecting the quantitative accuracy

EMC self-consistently evaluates scattering  
based on the corresponding Hamiltonians

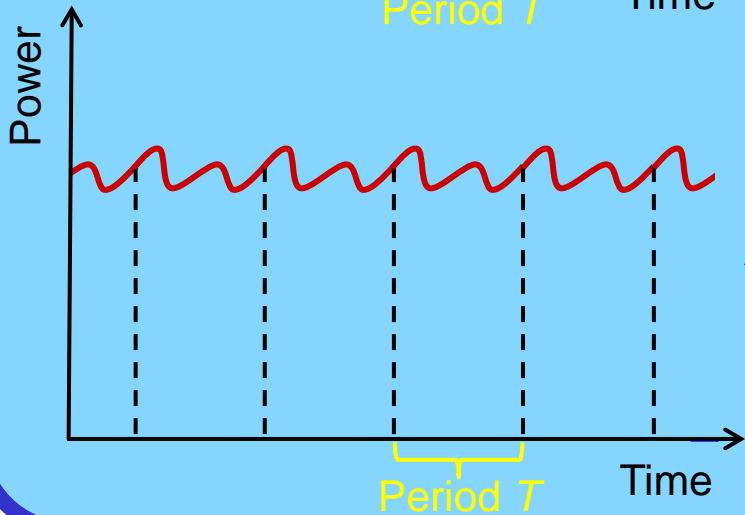
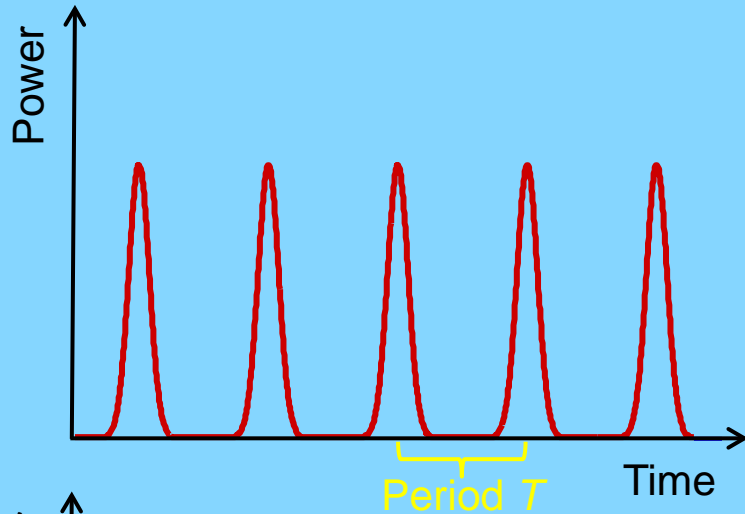
- Computational burden impedes inclusion  
of the full spatiotemporal dynamics

## Coupled Maxwell-Bloch/EMC approach

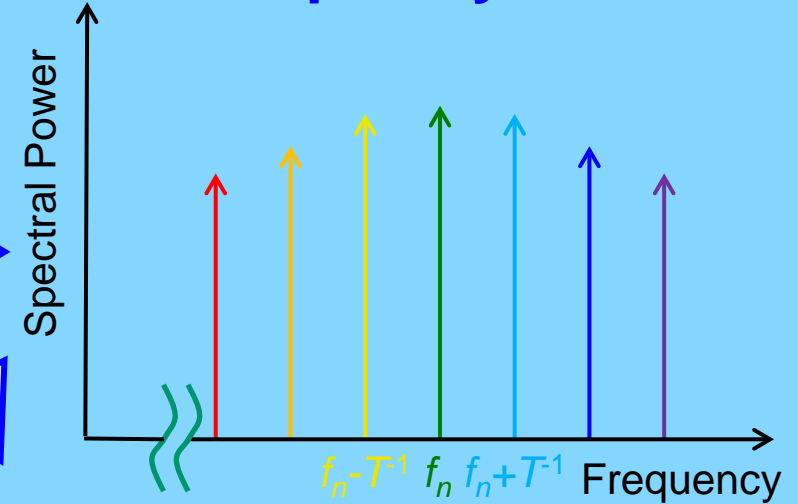


# QCL-Based Frequency Combs

## Periodic waveform



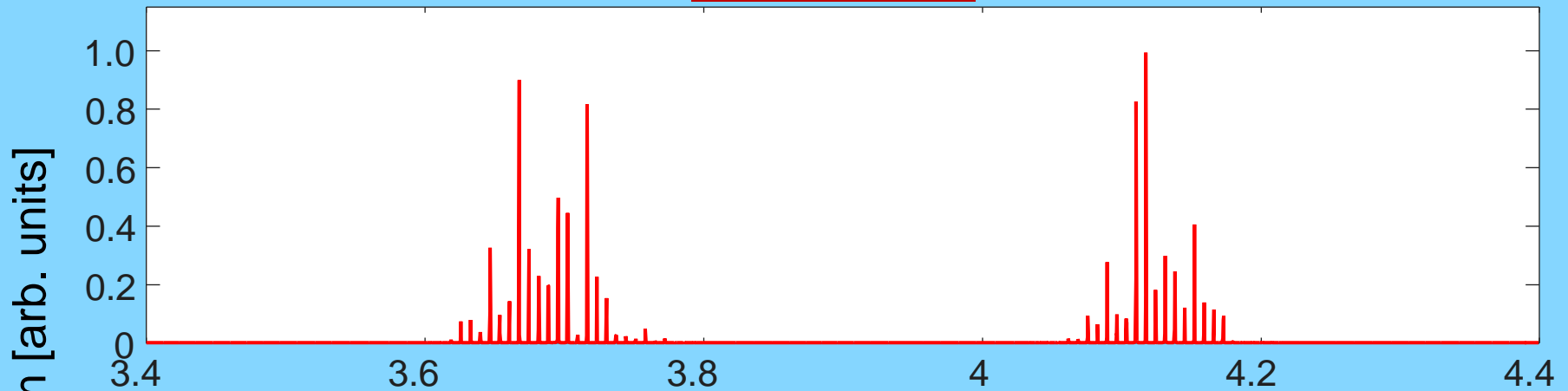
## Discrete optical spectrum $\triangleq$ frequency comb



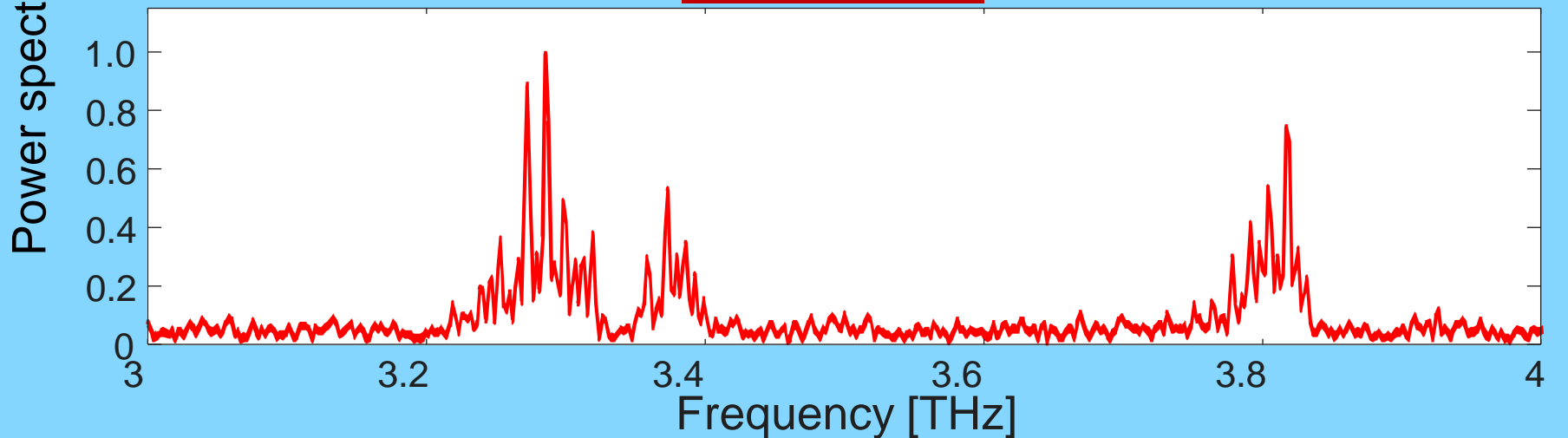
- Compact QCL-based frequency combs in mid-infrared/THz range
- Precision spectroscopy, molecular fingerprint detection (strong rotational-vibrational bands of many molecules at these frequencies)
- Modeling based on Maxwell-Bloch/EMC approach

# Terahertz Frequency Comb

## Simulation



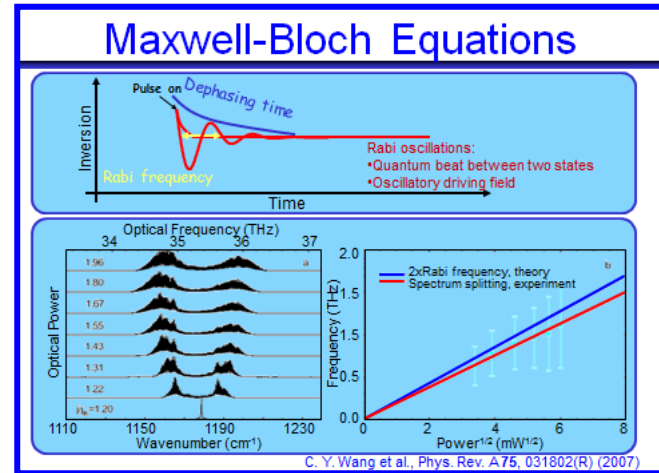
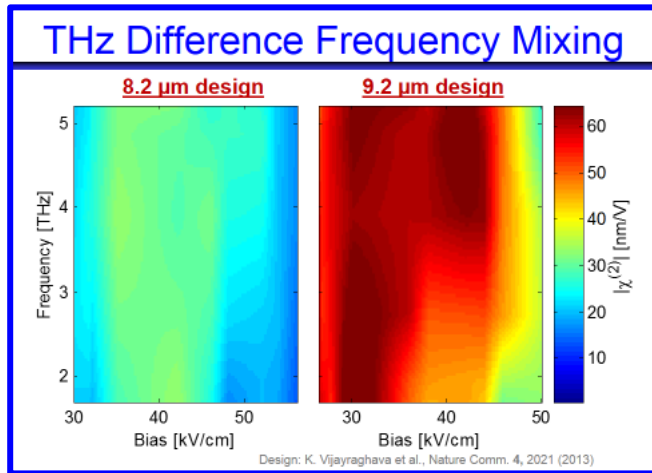
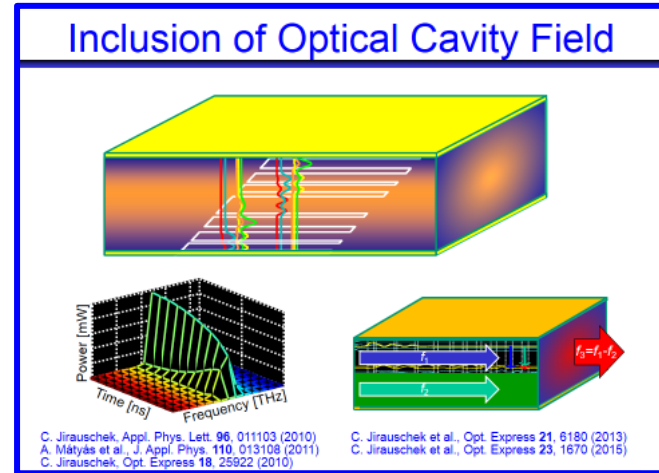
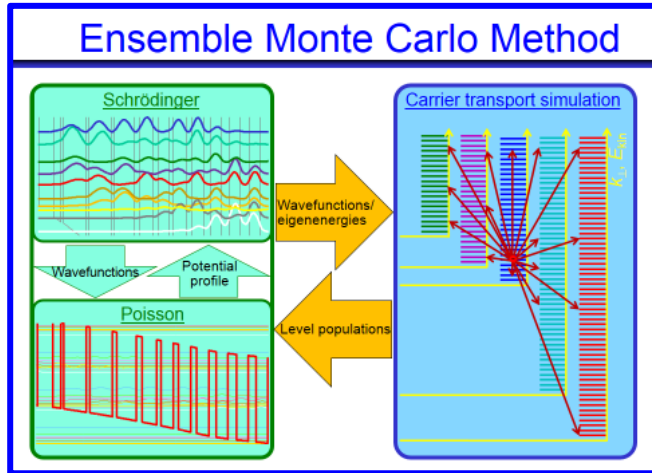
## Experiment



Design: D. Burghoff et al., Nature Photon. **8**, 462 (2014)



# Conclusion



C. Jirauschek and T. Kubis, Appl. Phys. Rev. 1, 011307 (2014)



# Acknowledgment

## Group members

Alpar Matyas  
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