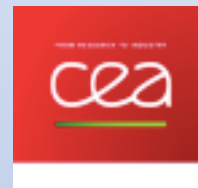


***Dynamics of highly excited electrons in 3D and 2D semiconductors:  
theory and experiments.***

**Jelena Sjakste**

*Laboratoire des Solides Irradiés, CEA/DSM-CNRS-Ecole Polytechnique, France*



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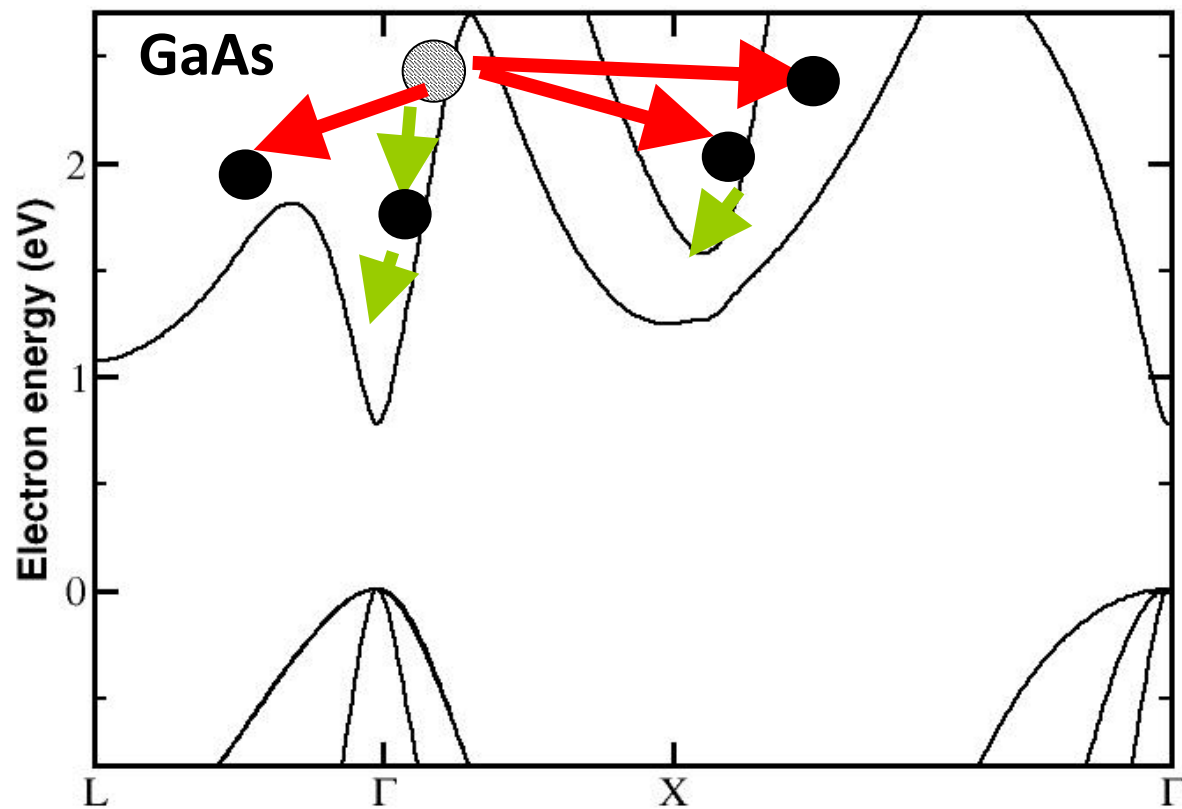
K. Tanimura

# Outline



- *Electron-phonon scattering for highly excited electrons*
- *Electron-phonon coupling from first principles*
- *Highly excited electron relaxation in Si*
- *Photoexcited electron relaxation in InSe*

# ELECTRON-PHONON SCATTERING: GENERAL PICTURE

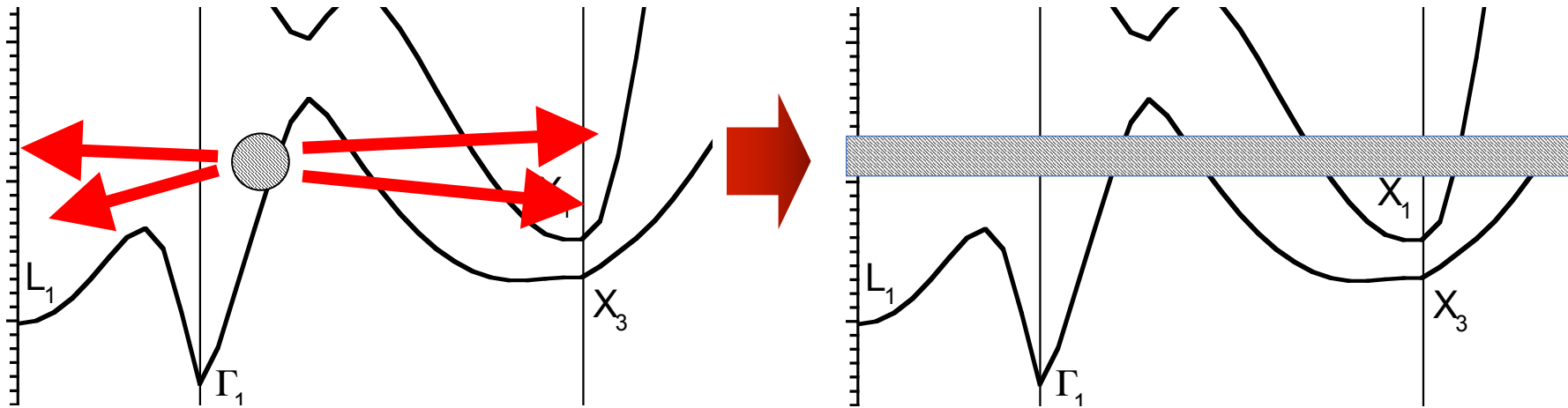


Intervalley scattering

Intravalley scattering

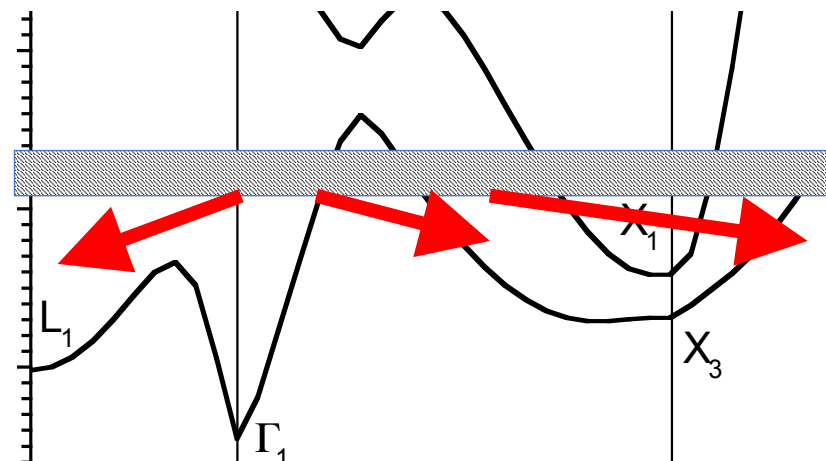
# ELECTRON-PHONON SCATTERING: HIGHLY EXCITED ELECTRONS

## FORMATION OF HOT-ELECTRON ENSEMBLE (HEE)



some fs -  
some tens of fs

## ENERGY RELAXATION OF HOT-ELECTRON ENSEMBLE




10 times  
slower  
than formation  
of HEE

Tanimura et al, PRB 93 (2016) 161203 (R).

Sjakste et al, J. Phys: Cond. Mat. **30**, 353001 (2018).

# Outline

- *Electron-phonon scattering for highly excited electrons*
-  - *Electron-phonon coupling from first principles*
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# ELECTRON-PHONON COUPLING: DFPT

$$\langle \Psi_{n,k} | \Delta W_q^\lambda | \Psi_{n',k+q} \rangle$$

DFPT: Baroni et al, Rev. Mod. Phys. 2001

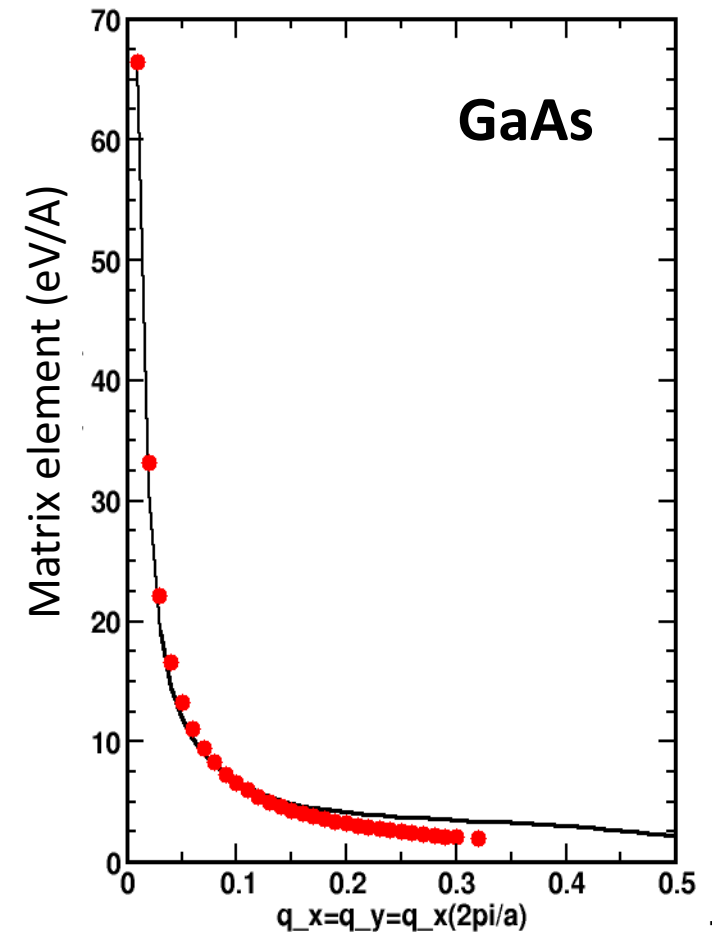


FRÖHLICH INTERACTION

$$\frac{4\pi e}{\epsilon_\infty q^2} q_\mu \sum_\alpha Z_{\mu\lambda}(\alpha) e_\lambda(\alpha \hat{q})$$

Vogl, PRB 13 (1976).

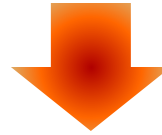
J. Sjakste et al, Annual Review of Heat Transfer, Begell House, Vol. 17 (2014).



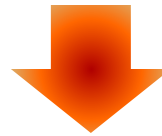
# INTERPOLATION FOR POLAR MATERIALS

Reciprocal space  
Bloch functions  
Initial grid

$$\langle \Psi_{n,k} | \Delta W_q^\lambda | \Psi_{n',k+q} \rangle - \text{Non-local part if polar}$$



**Real space**  
**Maximally localized Wannier functions**  
**Interpolation on dense grid**



Reciprocal space  
Bloch functions  
Dense grid


$$\langle \Psi_{n,k} | \Delta W_q^\lambda | \Psi_{n',k+q} \rangle + \text{Non-local part if polar}$$

*J. Sjakste, N. Vast, M. Calandra, F. Mauri, PRB 92 (2015) 054307*

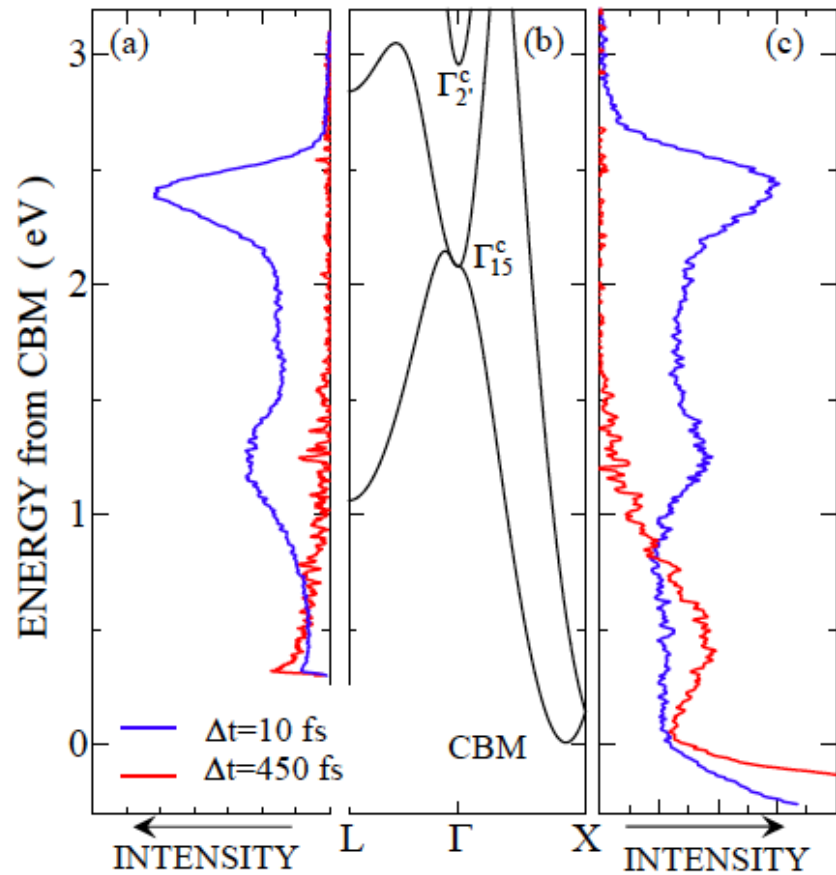
*C. Verdi, F. Giustino, PRL 115 (2015) 176401*



# Outline

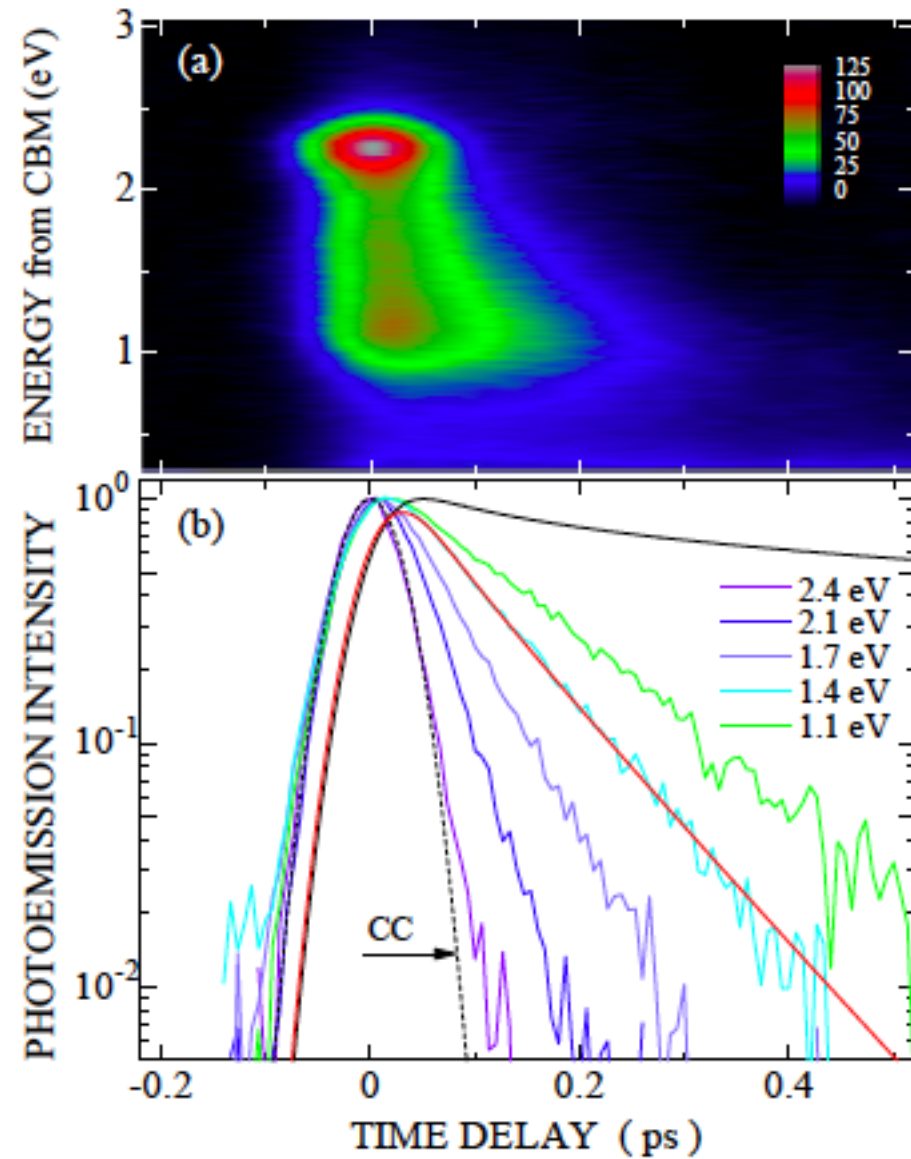
- *Electron-phonon scattering for highly excited electrons*
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# HIGHLY EXCITED ELECTRONS IN SILICON: 2PPE



Tanimura *et al*, PRB (2019), accepted.

Ichibayashi *et al*, Phys. Rev. B 84, 235210 (2011).

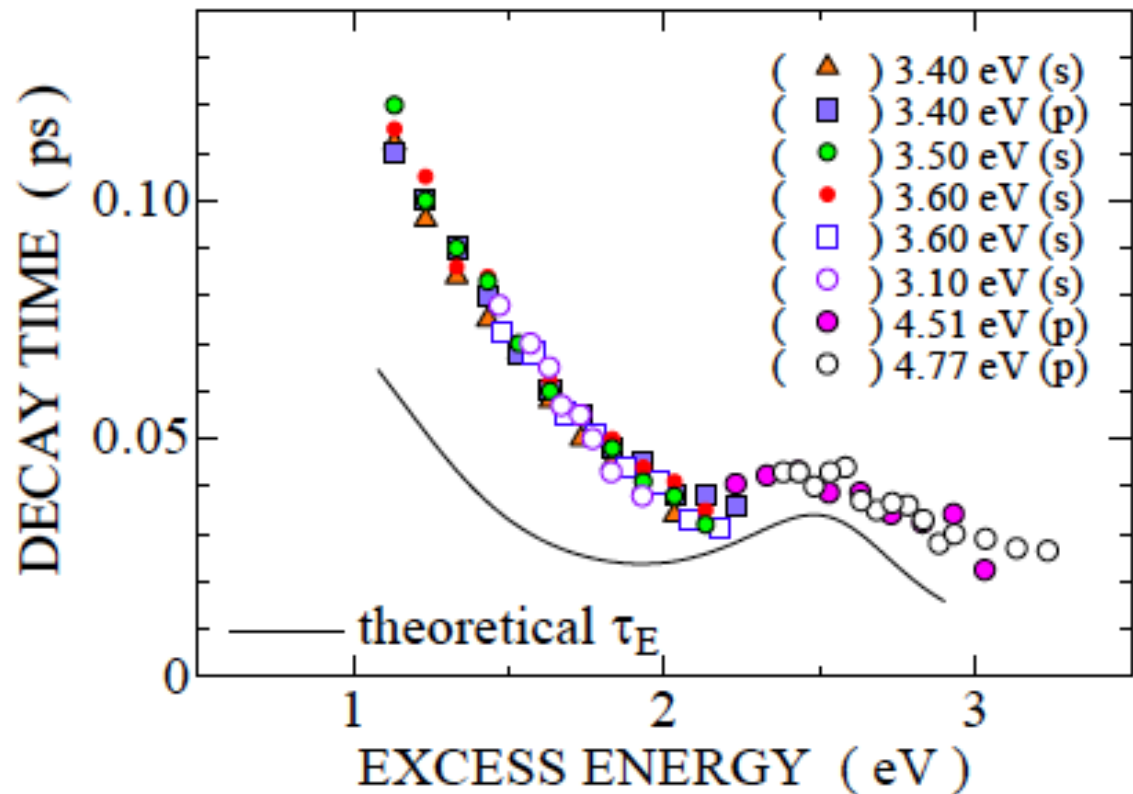


# HIGHLY EXCITED ELECTRONS IN SILICON: INTERPRETATION PROBLEM

Previous work: contradiction theory/ab initio data:

*Measured relaxation times 10 times longer than calculated ones*

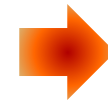
Ichibayashi *et al*, Phys. Rev. B 84, 235210 (2011).



This work: HEE idea

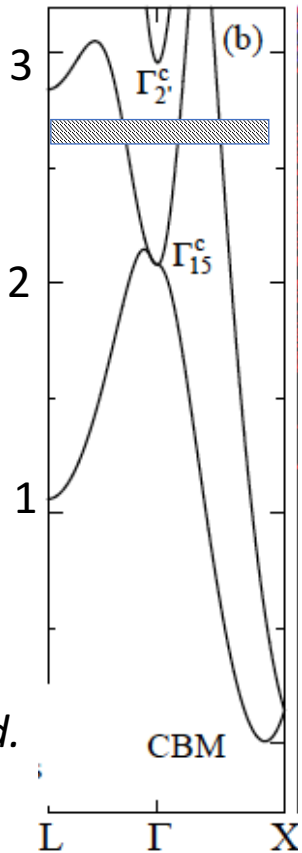


Initial relaxation:  
*too fast to be measured*



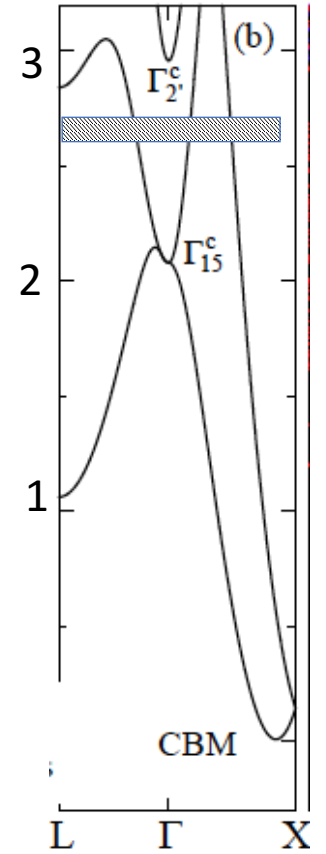
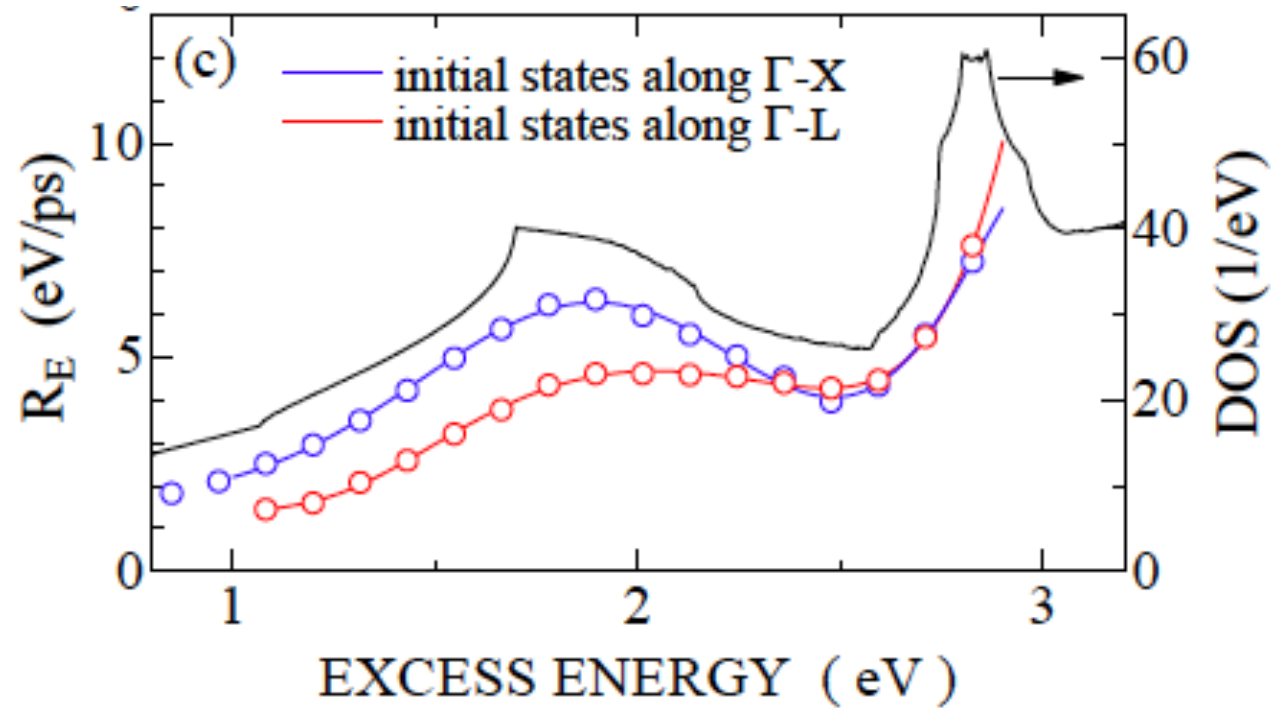
Measured relaxation times:  
*energy relaxation*

Tanimura *et al*, PRB (2019), accepted.



# HIGHLY EXCITED ELECTRONS IN SILICON: ENERGY RELAXATION

$$dE / \tau_E = \Gamma_{em} \omega_{em} - \Gamma_{abs} \omega_{abs}$$



Energy relaxation:  
**Determined by DOS of final electronic states**

Tanimura et al, PRB (2019), accepted.

# Outline

- *Electron-phonon scattering for highly excited electrons*
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# Photoexcited electron relaxation in InSe

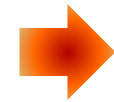
Luca PERFETTI  
Zhesheng CHEN  
Zailan ZHANG  
Raphael CABOUAT  
Jelena SJAKSTE  
Cristine GIORGETTI  
Valerie VENIARD  
Abdelkarim Ouerghi  
Hugo Henck



Evangelos PAPALAZAROU  
Marino MARSI



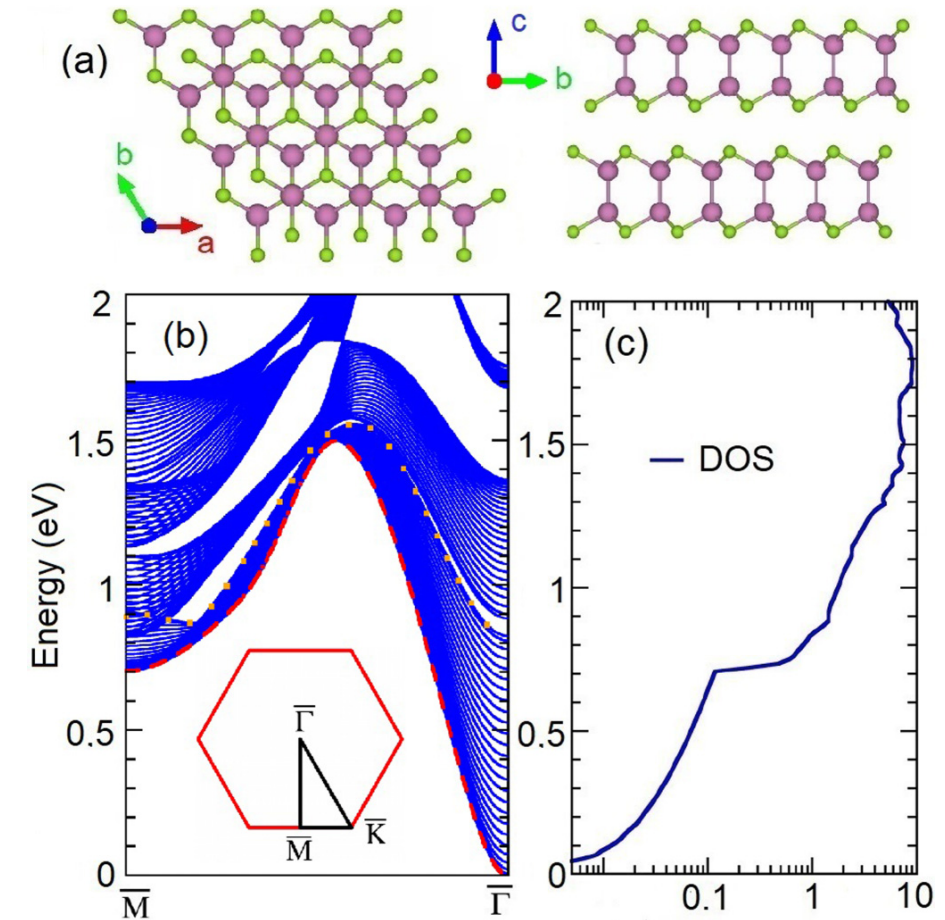
Layered material



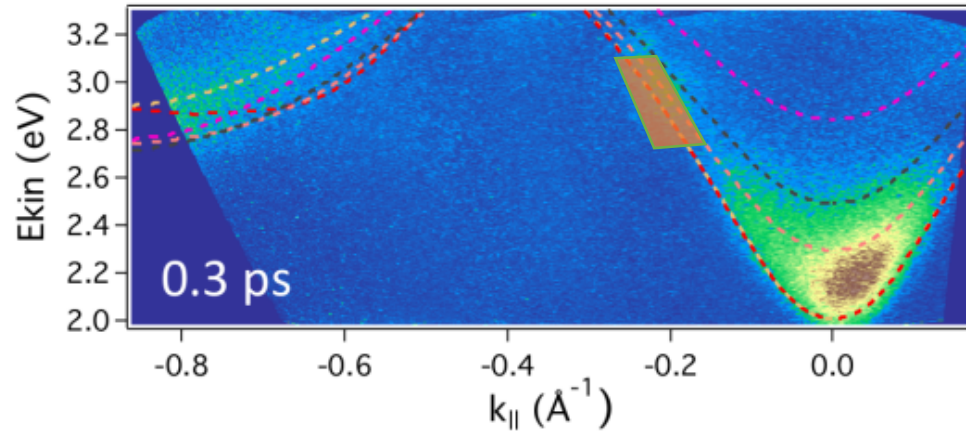
Very narrow  $\Gamma$  valley



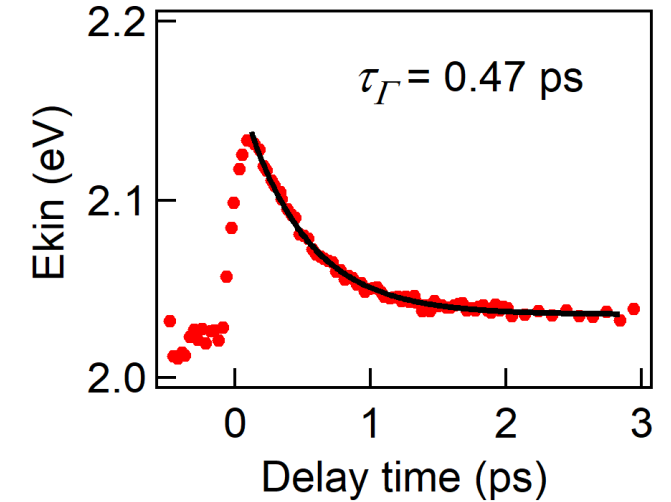
Large M valley



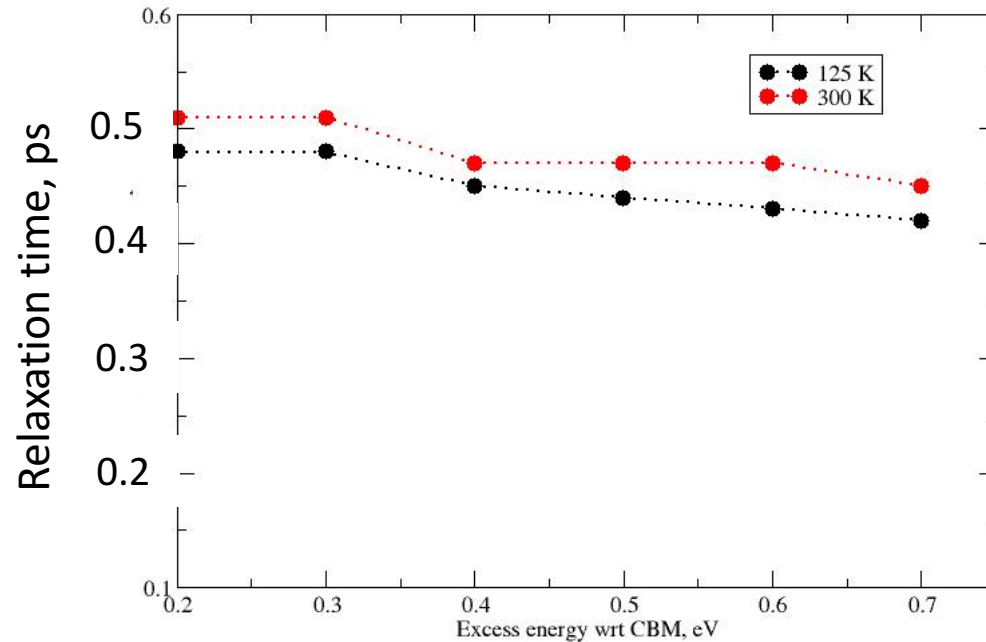
# InSe: energy relaxation in $\Gamma$ valley



Experiment



Theory: energy relaxation due to Fröhlich coupling

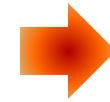
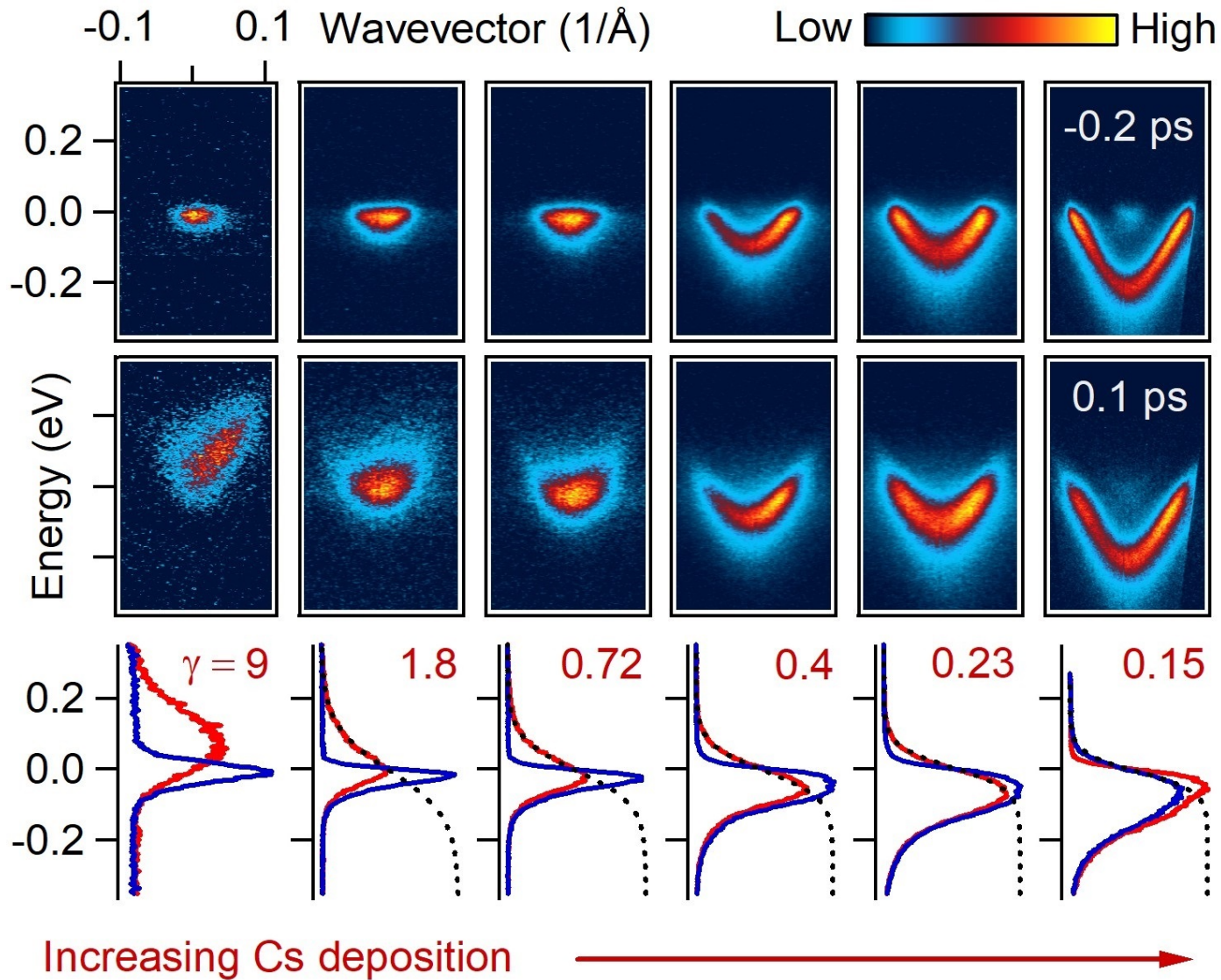


$$\frac{4\pi e}{\epsilon_{\infty} q^2} q_{\mu} \sum_{\alpha} Z_{\mu\lambda}(\alpha) e_{\lambda}(\alpha \hat{q})$$



Good agreement  
between theory and  
experiment.

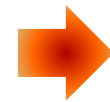
# Energy relaxation in doped InSe



Electron gas: 2D or 3D ?



Photoexcited electrons:  
effect on relaxation ?

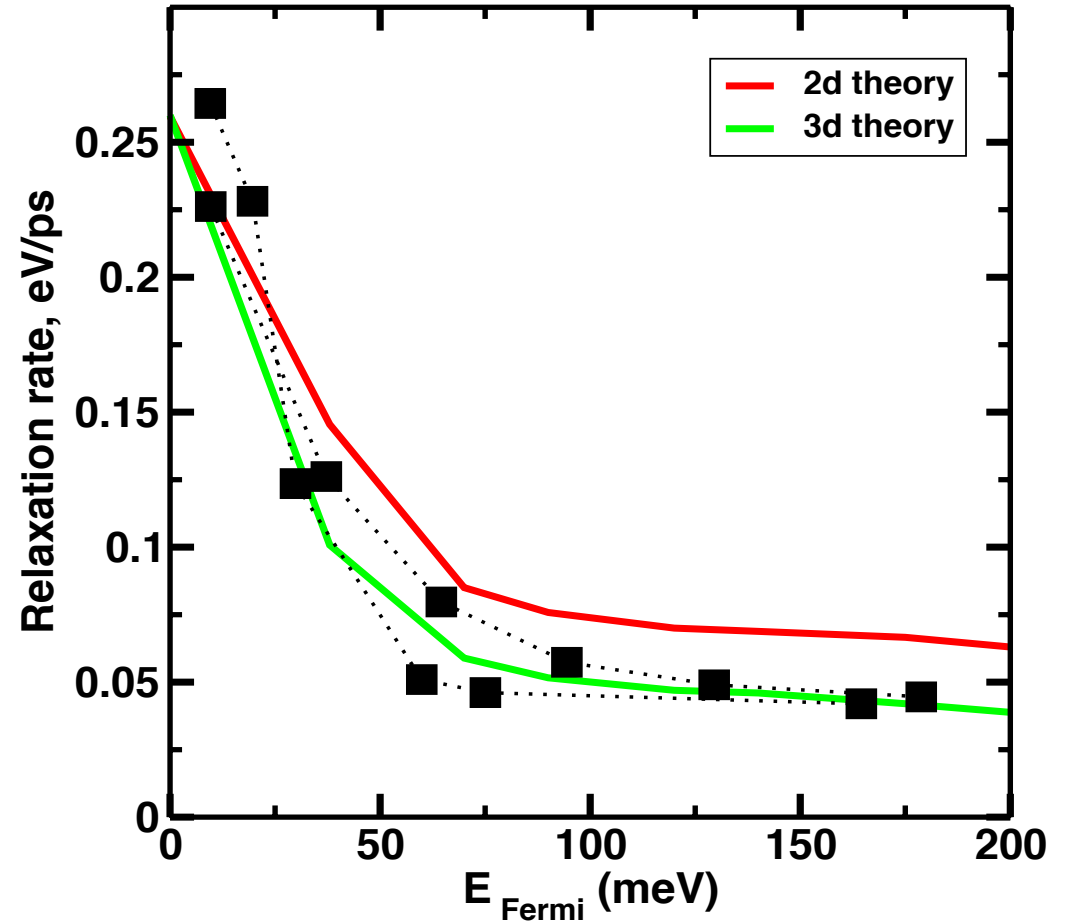
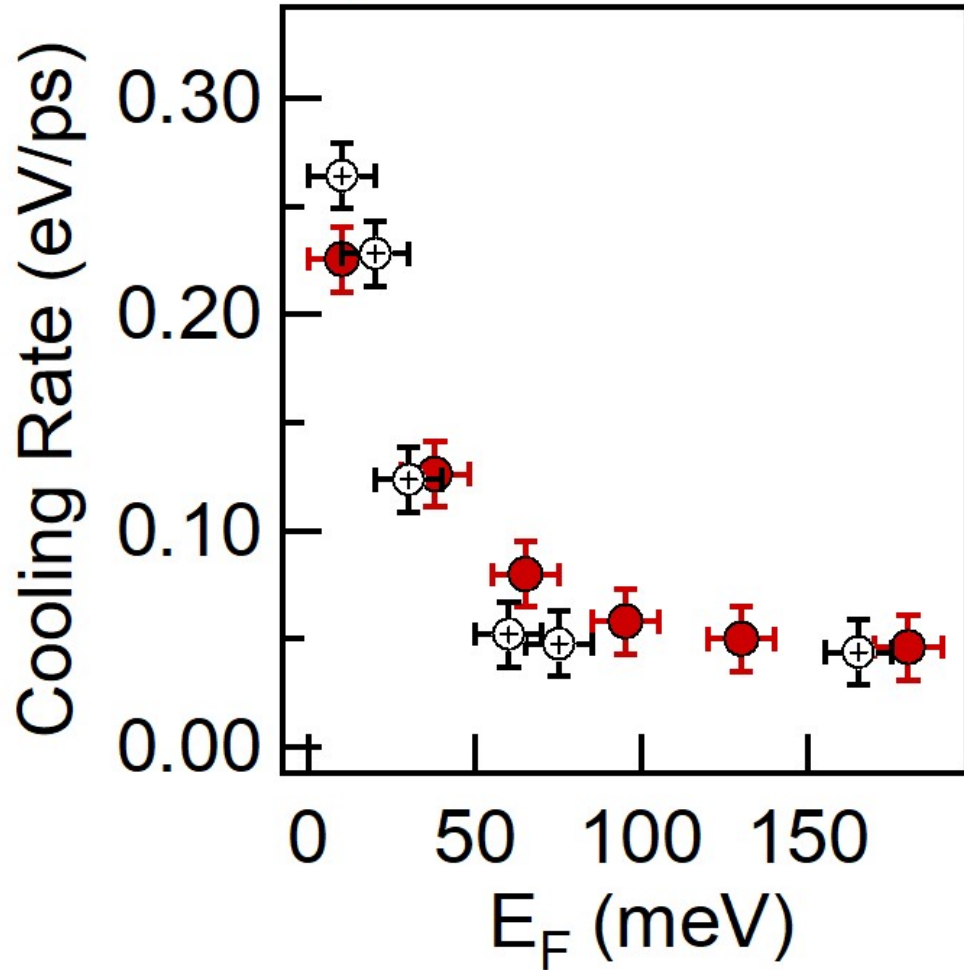


Highly excited or  
hot electrons ?

$$\gamma = T_e / E_F$$



# Energy relaxation in doped InSe



Doping: screening of Fröhlich interaction



From non-thermal to thermal distribution

# Conclusion

*Dynamics of relaxation of highly excited (or « hot »?) electrons in Si and in InSe*

- ➔ *The concept of hot electron ensemble allowed us to interpret the relaxation times of highly excited electrons in silicon.*
- ➔ *In Si, energy relaxation is determined by the DOS of the final electronic states*
- ➔ *In InSe, at excess energies below 0.7 eV, energy relaxation is determined by Fröhlich coupling.*
- ➔ *Doped InSe:*
  - ➔ *screening of Fröhlich coupling*
  - ➔ *non-thermal/thermal distributions.*

***Thank you for your attention!***