SILPHYDE

(SImuLation PHYsique de Dispositifs Electroniques et optoélectroniques)

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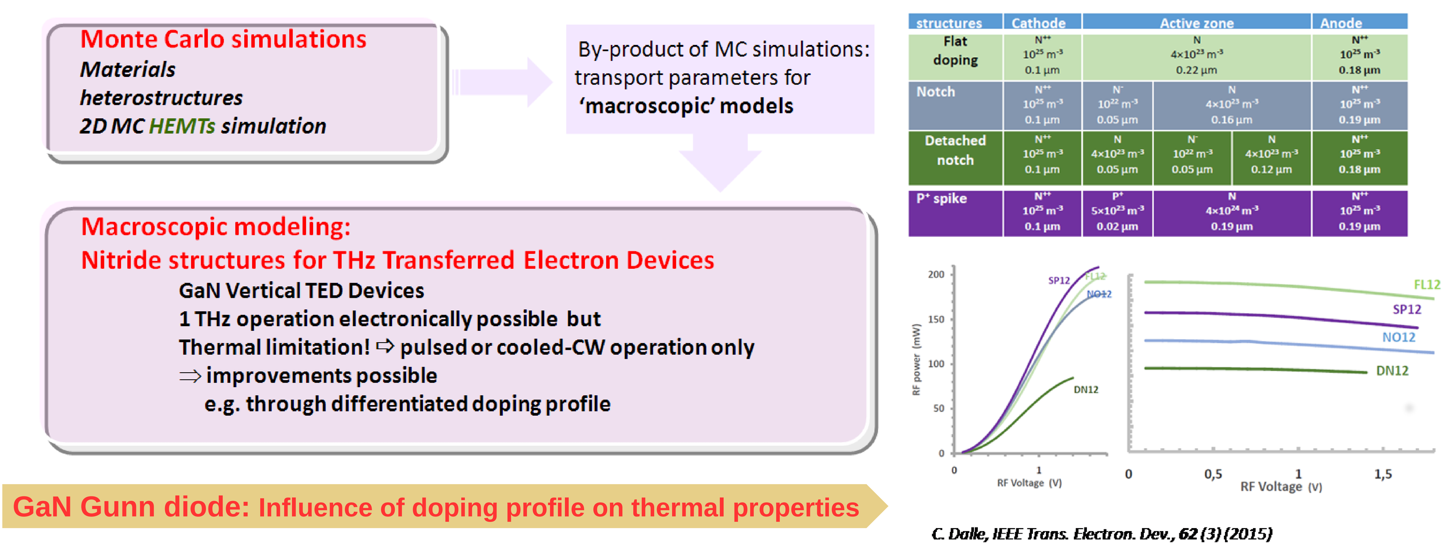
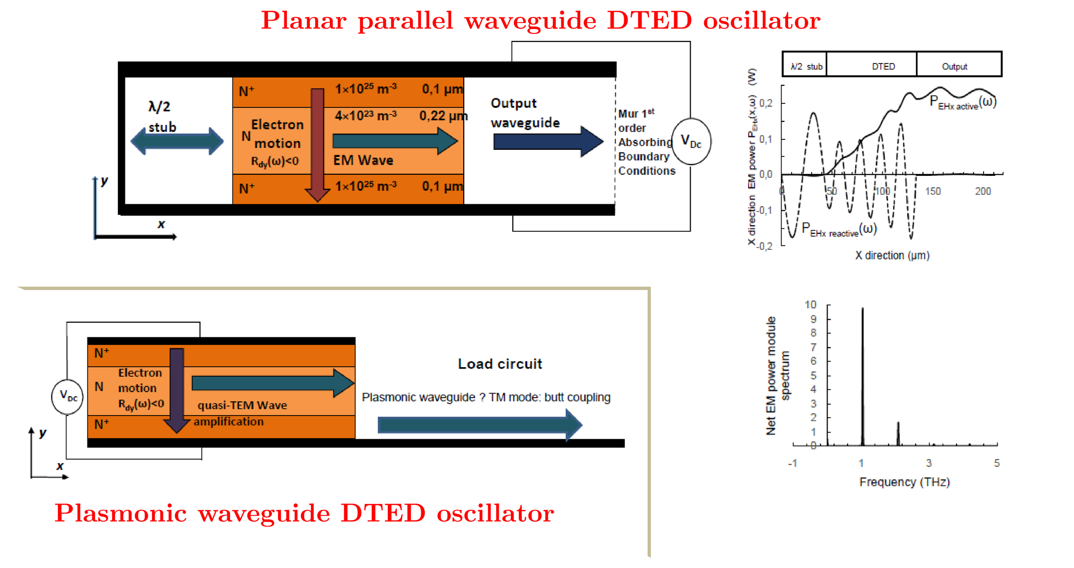
Modeling of electron devices

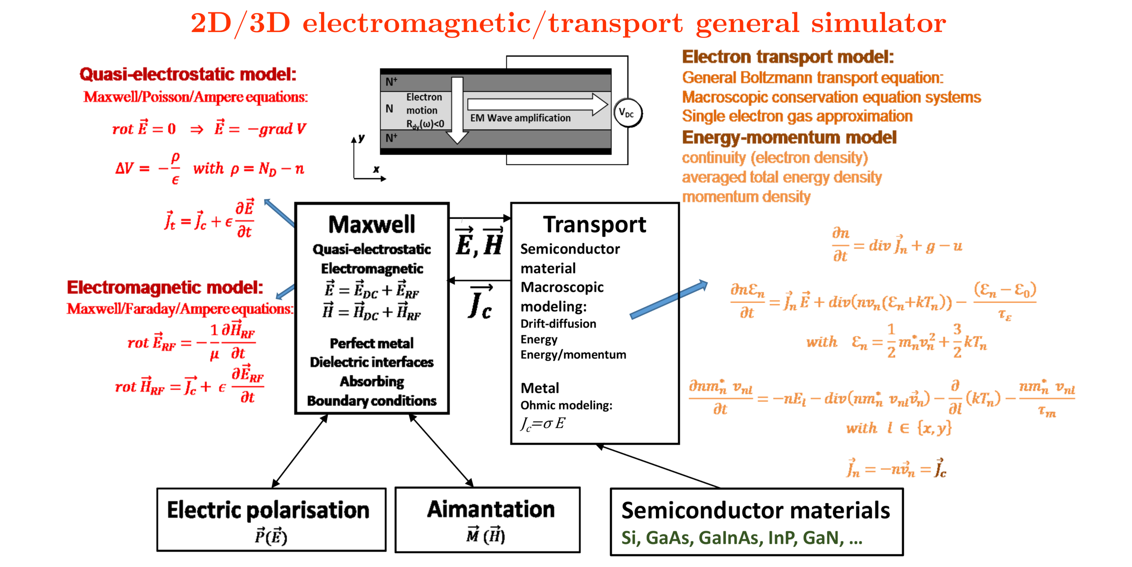
Simulation of GaN-based devices



Simulation of GaN THz oscillators



Prospective : development of SIMAX



Modeling of Quantum Cascade Lasers and related devices

QCLs models in Silphyde group

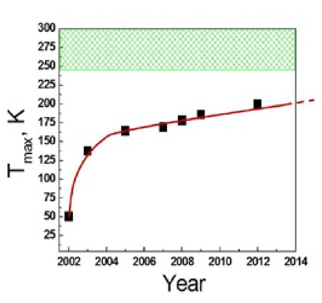
- Monte Carlo (with Warsaw University of Technology)
- **Simplified rate equations** (with Sétif University)

Fast, suitable for SPICE-like circuits models

Context : Quest for Room Temperature THz operation

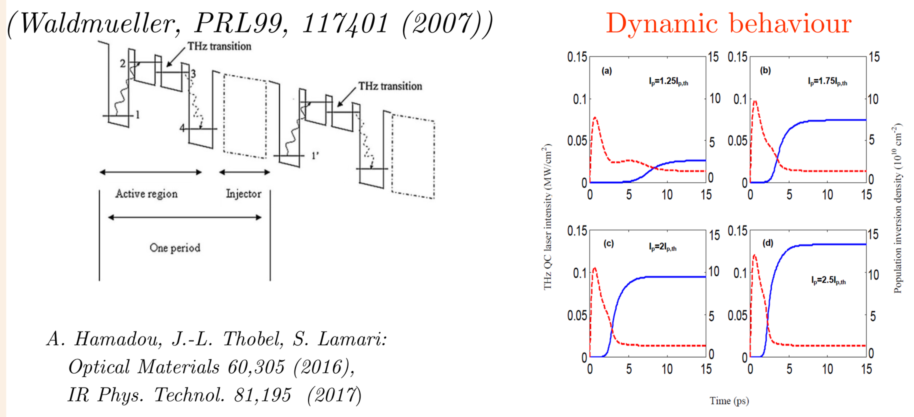
☹ Out of reach for conventional QCL

Solutions : alternative structures derived from QCLs



Optically pumped QCLs

(Waldmueller, PRL99, 117401 (2007))

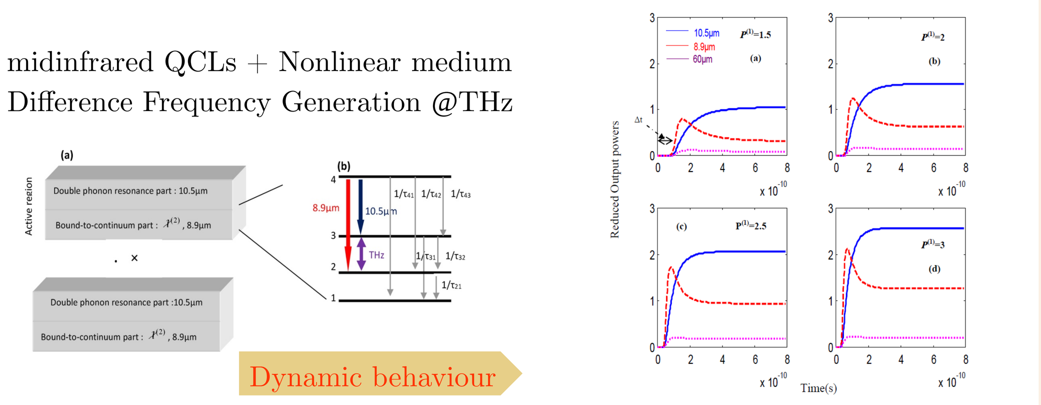


A. Hamadou, J.-L. Thobel, S. Lamari: Optical Materials 60,305 (2016), IR Phys. Technol. 81,195 (2017)

Intracavity DFG QCLs

2 midinfrared QCLs + Nonlinear medium

⇒ Difference Frequency Generation @THz



Hamadou, Thobel, Lamari, Optik 156,596 (2018)

Prospective

- Parametric study
- Thermal effects
- **Improve the model :** e.g. spatial dependencies

Modeling of ferroelectric thin films and nanostructures

Collaboration with Amiens, Rostov on Don, Cambridge University, Argonne National Lab.

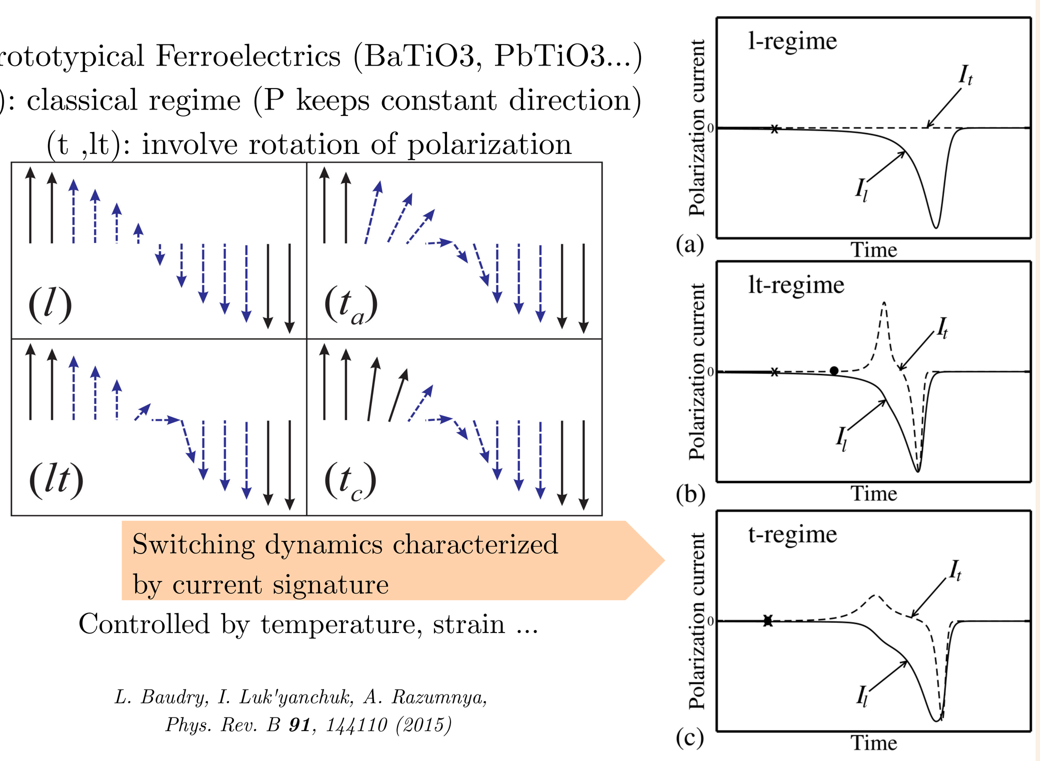
Context: Application to nonvolatile memories (high integration, speed, low consumption)

New switching mechanisms

Prototypical Ferroelectrics (BaTiO3, PbTiO3...)

(l): classical regime (P keeps constant direction)

(t ,lt): involve rotation of polarization



Switching dynamics characterized by current signature

Controlled by temperature, strain ...

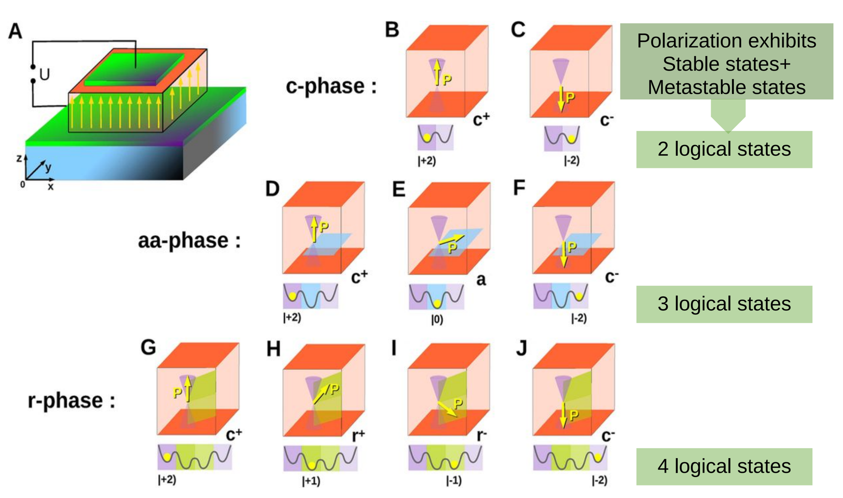
L. Baudry, I. Luk'yanchuk, A. Razumnaya, Phys. Rev. B **91**, 144110 (2015)

Ferroelectric multibit memory cells

- Standard binary logic reaches its limits
- Multivalue logic: higher storage density, less energy loss, relevant for neuromorphic applications

In multiaxial ferroelectric materials (e.g. PbTi03), thin film with misfit strain) :

Multistable polarization states



States protected by symmetry against small random perturbations

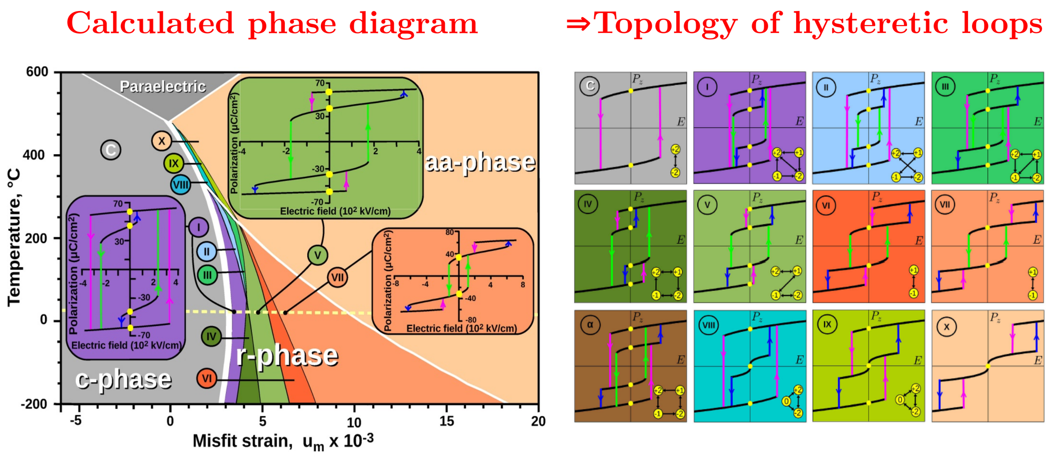
L. Baudry, I. A. Luk'yanchuk, V Vinokur, Scientific Reports. 7, 42196 (2017)

Rich variety of behaviours, controled by strain/temperature

How to access the states ?

Time dependent simulations

Calculated phase diagram ⇒Topology of hysteretic loops



Prospective

Search for new ferroelectric systems for multivalued logic

Consider various materials

- PbZrTiO3 (different compositions)
- Lead-free materials (BaTiO3, BaZrTiO3)
- Heterostructures and superlattices

Study of electrocaloric properties of ferroelectric materials

- Fascinating caloric properties
- High potential candidates for solid state refrigeration devices.
- Role of field-induced phase transition and related mechanisms ?
- Contribution of entropy change during polarization reversal ?

Graphene and 2D materials for electronics, spintronics and valleytronics

Collaboration with Warsaw University of Technology

Context: Strong interest in graphene, wealth of applications, emergence of new 'beyond-graphene' materials

We develop and use Monte Carlo models (Relevant for larger scales than ab-initio model, suitable for future use in device simulators)

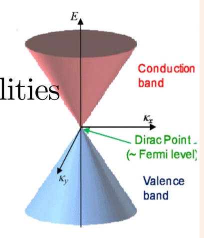
Electron transport

Graphene, Silicene: linear bands

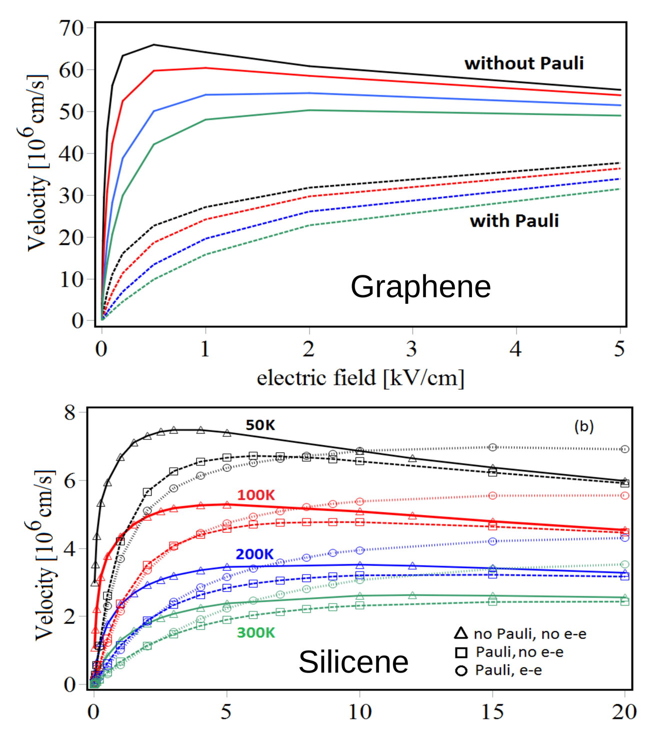
Piecewise analytical scattering probabilities

Special techniques for:

- e-e scattering
- Pauli exclusion



Calculated V-F Characteristics



For silicene experimental data scarce and scattered

P. Borowik, J.-L. Thobel, L. Adamowicz : Semicond. Sci. Technol. **31**, 115004 (2016), Physica Status Solidi (A) Applications and Materials 213(11) (2016)

Spin properties

- Graphene is attractive for spintronics applications
- Retains spin information for a long time

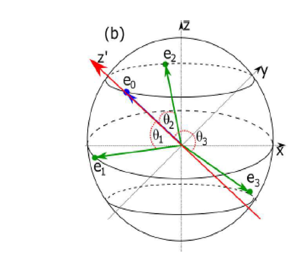
Monte Carlo simulations of spin relaxation in graphene with high electron density

Monitors electrons state including spin vector S

Accounts for:

- coherent evolution (precession)
- incoherent (random spin flips)

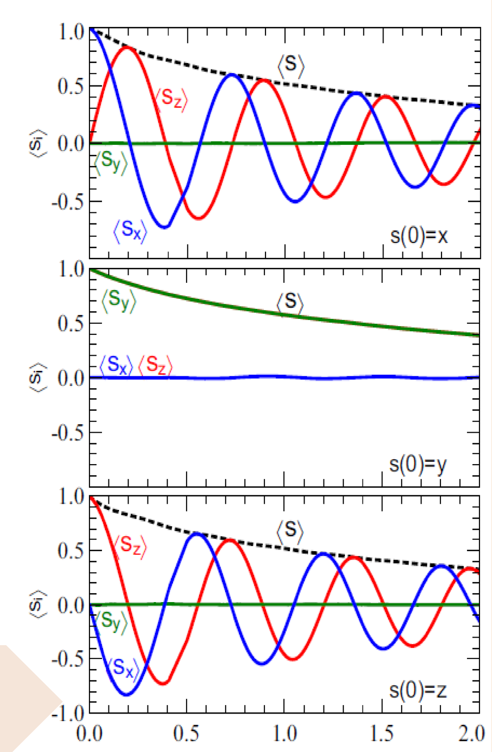
⇒ Special technique for Pauli Principe



$$f(\mathbf{k}) = \frac{1}{N_{max}^{1}} \sum_i \frac{1}{2}(1 + \mathbf{s}_0 \cdot \mathbf{s}_i)$$

avec $\mathbf{s}_0 \cdot \mathbf{s}_i = \cos(\theta_i)$

P. Borowik, J.-L. Thobel and L. Adamowicz, Journ. Appl. Phys. 122, 045704 (2017)



Oscillations due to spin precession

Relaxation time in nanoseconds,

(depends on chosen parameters)

Relaxation phenomena

Powerful tool to reveal physical mechanisms

'Hot electrons': at the heart of many devices operation

Monte Carlo simulations of relaxation in spin-polarized graphene

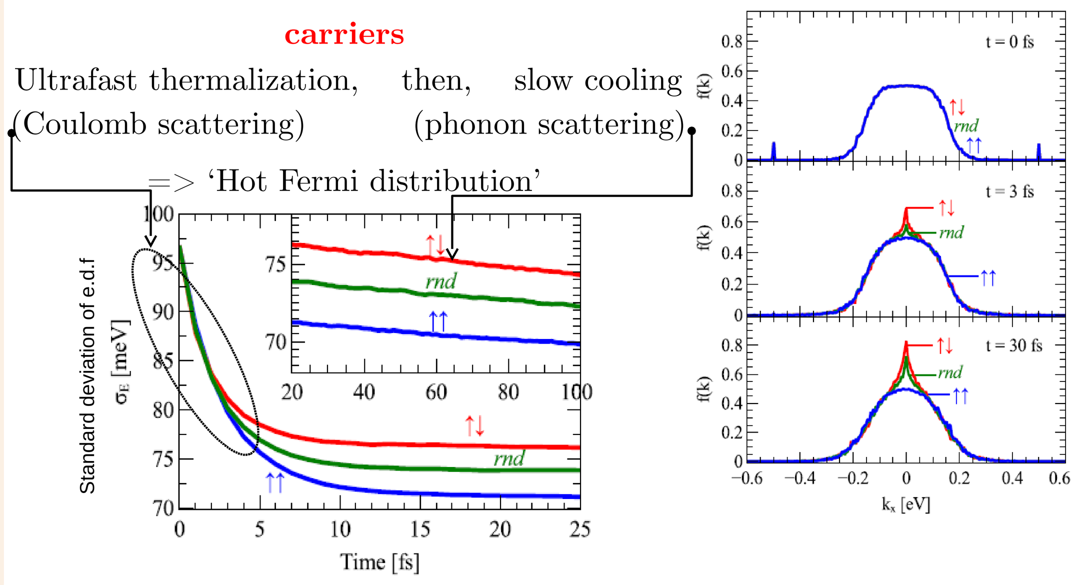
(Assume the material initially populated with a definite spin polarization)

Time evolution of distribution of excited carriers

Ultrafast thermalization, then, slow cooling

(Coulomb scattering) (phonon scattering)

=> 'Hot Fermi distribution'



Depending on spin polarizations of bckgd/exc. carriers, accessible states are in different regions of Brillouin zone

⇨ alters relaxation dynamics

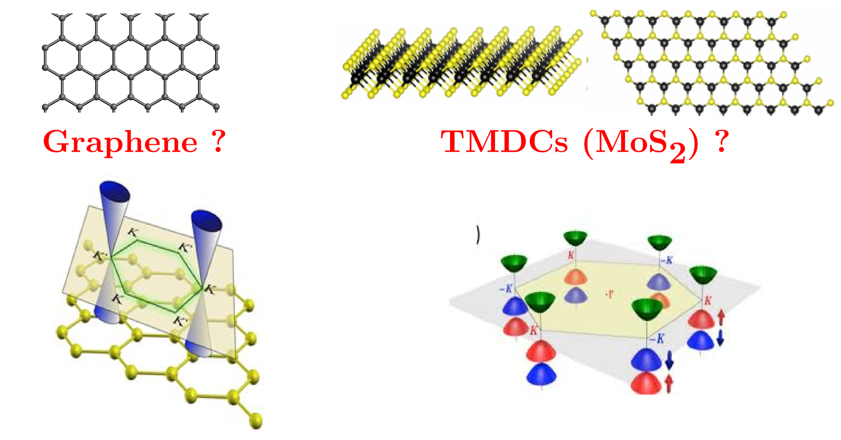
P. Borowik, J.-L. Thobel, L. Adamowicz : Semicond. Sci. Technol. **32**, 125006 (2017), Applied Physics A, **124**(2) (2018)

Prospective: valleytronics

Idea: 2 valleys (K,K') non-equivalent, energetically degenerate

Valley index can be used to carry information like spin in Spintronics

What materials ?



Due to symmetry: long valley life time.

No inversion symmetry. Easy to act on valley (optically...)

+ Variety of materials and possible associations (Van der Waals heterostructures)

Whatever the materials, Valley dynamics still poorly known.

Goal: Develop Monte Carlo models for studying valley dynamics in systems of interest and, at longer term, devices.

First step: valley relaxation in graphene with defects/impurities.

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