



University of Ioannina

Department of Materials Science & Engineering

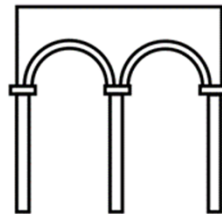
Computational Materials Science Laboratory

Multi-physics and multi-scale modeling of optoelectronic materials and devices

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INSTITUTE OF
MATERIALS SCIENCE
AND COMPUTING

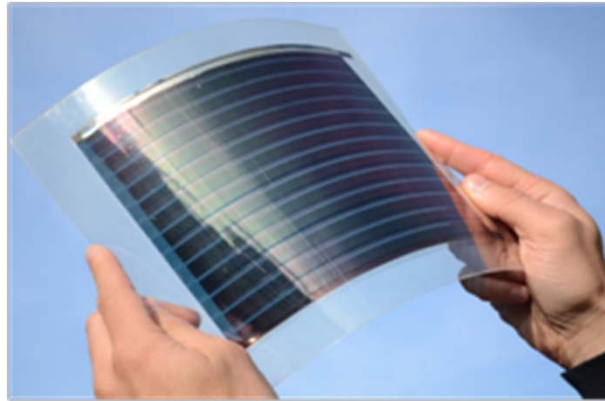
Computation of optoelectronic materials & devices

- **Properties of materials**
 - Optical, electrical, thermal
- **Physical interactions**
 - Optical: absorption, scattering, interference
 - Electrical: carrier excitation, drift-diffusion
 - Thermal: transfer, currents
- **Design and optimization of applications**
 - Photovoltaics, LEDs, photodetectors, sensors, waveguides, modulators

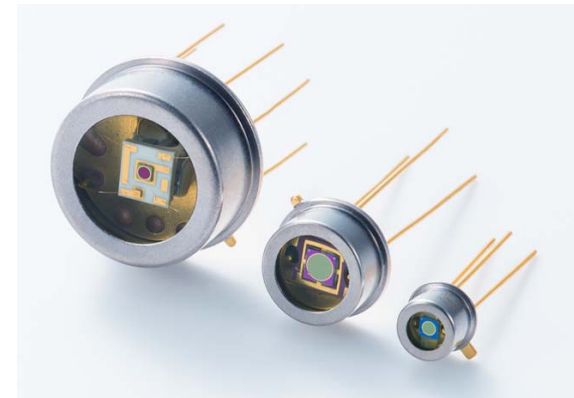


Application – architecture - interactions

organic photovoltaics



graphene optoelectronics



Optical metrology

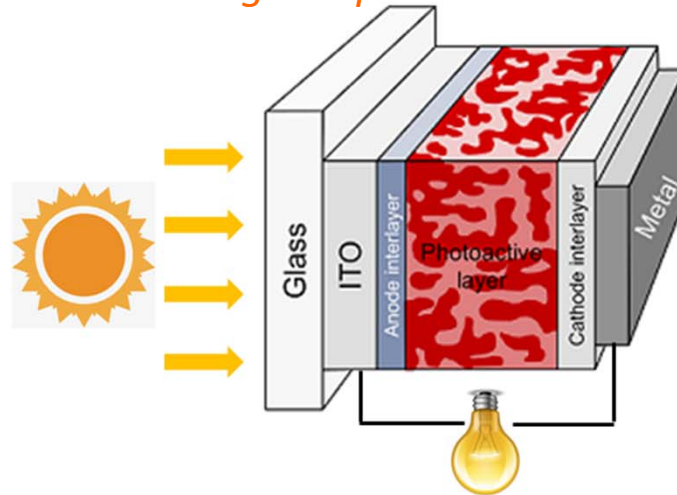


Si/SiN photonics-plasmonics

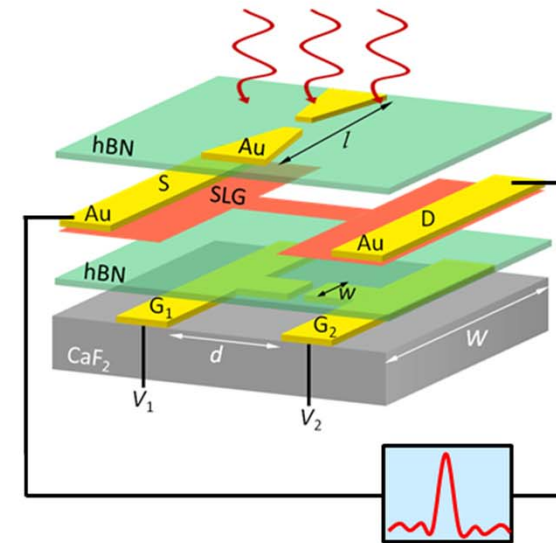


Application – architecture - interactions

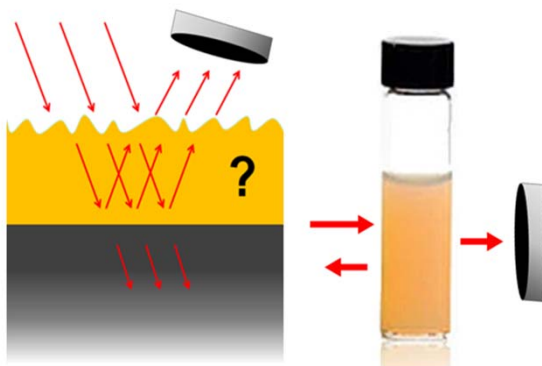
organic photovoltaics



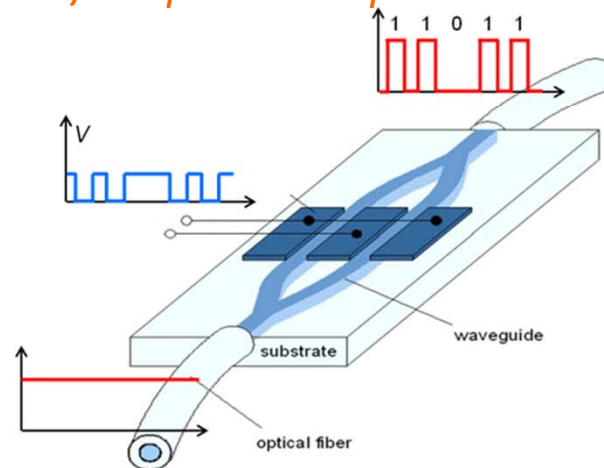
graphene optoelectronics



Optical metrology



Si/SiN photonics-plasmonics



Application – architecture - interactions

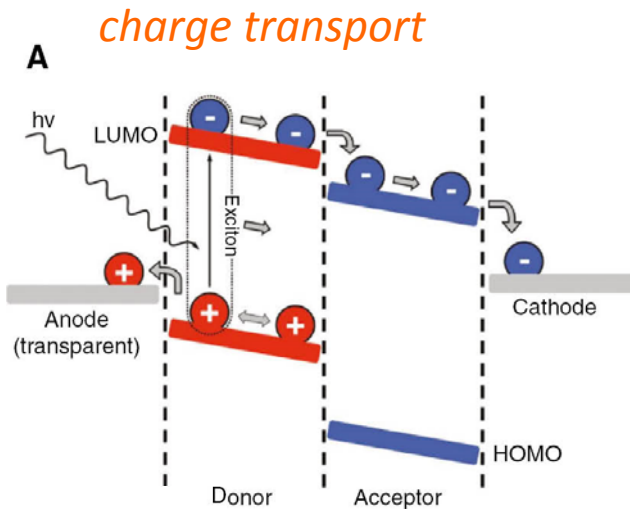
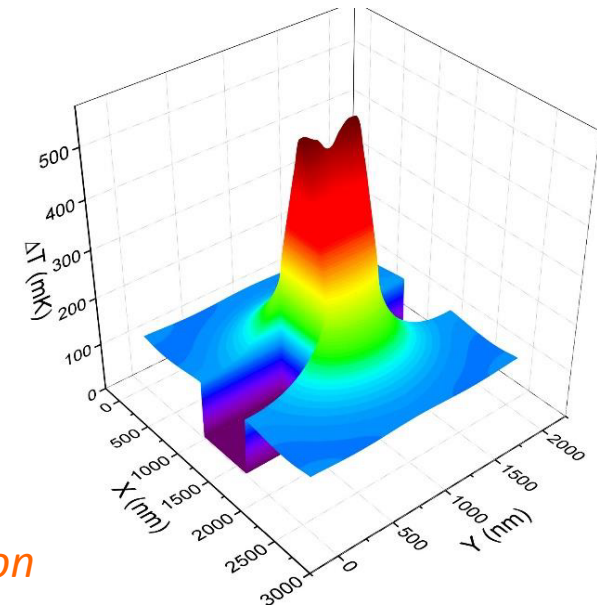


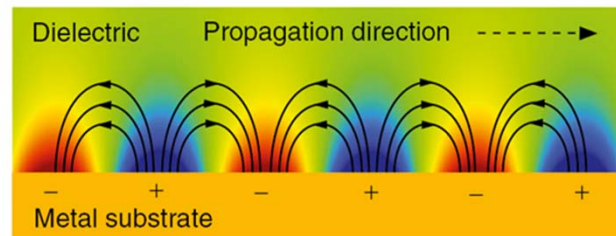
photo-thermo-electric excitations



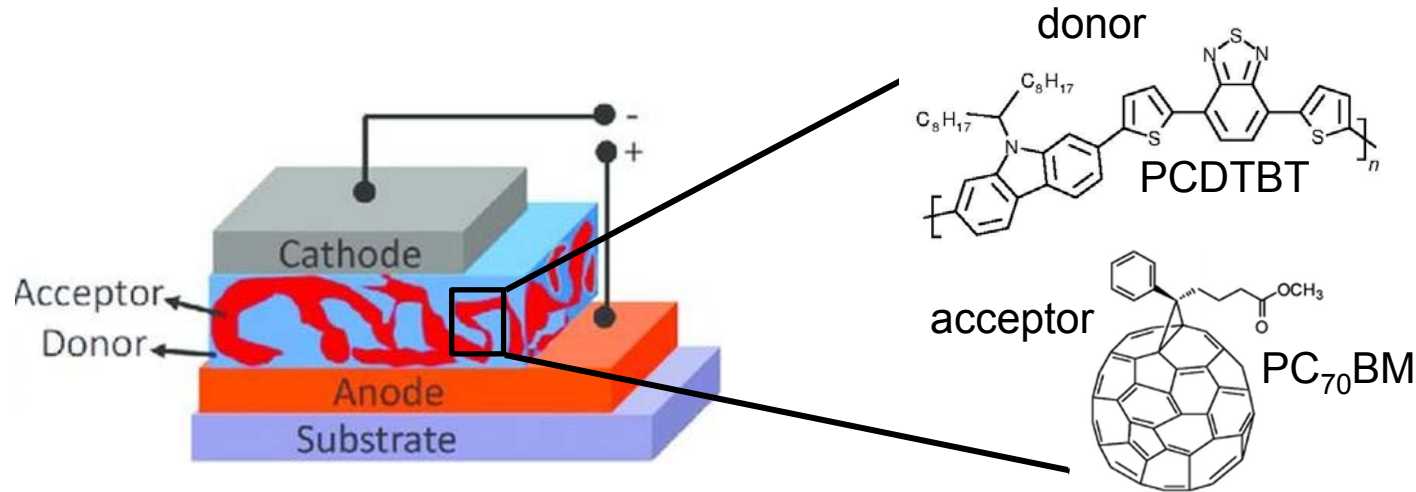
data analysis

```
do{
  reset_minimization(a, thick);
  a->run(1000);
  error = a->get_lower_value();
  if(error < errormin){
    errormin = error;
    store_new_optimal(a);
  }
  thick += dthick;
  noc = a->get_function_counter();
} while(thick < thick_max);
```

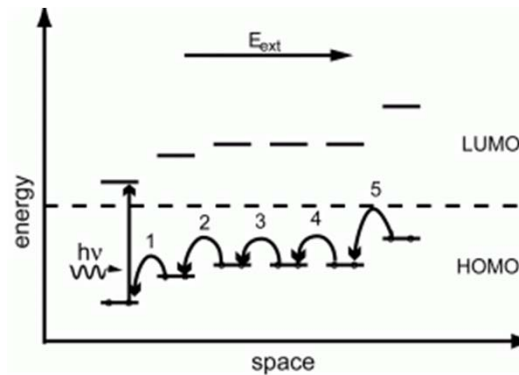
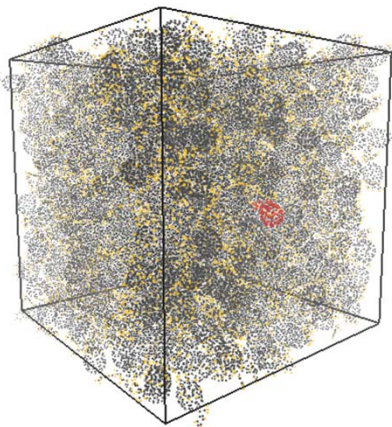
photonic/plasmonic propagation



Transport in organic semiconductors



- Amorphous organic materials → weak intermolecular interactions
 - charge transport proceeds by thermally activated hopping



high temperature limit of Marcus theory

$$\omega_{ij} = \frac{2\pi}{\hbar} \frac{J_{ij}^2}{\sqrt{4\pi k_B T \lambda_{ij}}} \exp \left[-\frac{(\Delta E_{ij} - \lambda_{ij})^2}{4k_B T \lambda_{ij}} \right]$$

Electronic coupling

$$J_{ij} = \langle \psi_i | \hat{H} | \psi_j \rangle$$

Reorganization Energy

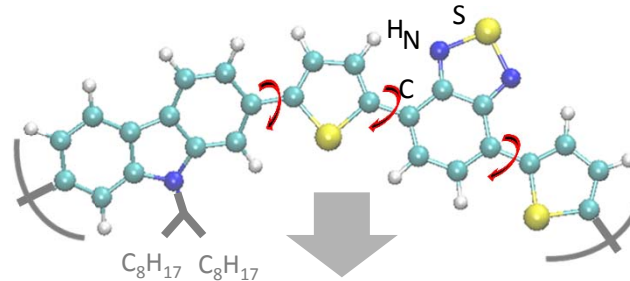
$$\lambda_{ij} = \lambda_{ij}^{int} + \lambda_{ij}^{out}$$

Site Energy Difference

$$\Delta E_{ij}$$

Multiscale modelling overview

- Disordered organic molecules -> large computational cells



Density functional theory:

- molecular deformation, interaction and ionization energies

atomistic
force-fields
parameters



molecular
conformations



charge
transport
parameters



Molecular dynamics:

- conformations
- interaction sites

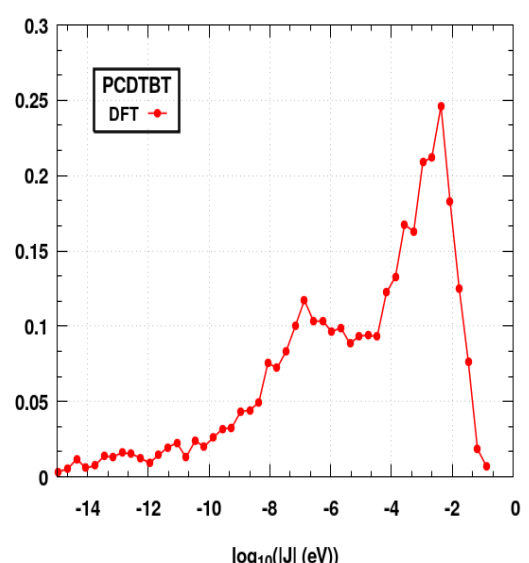
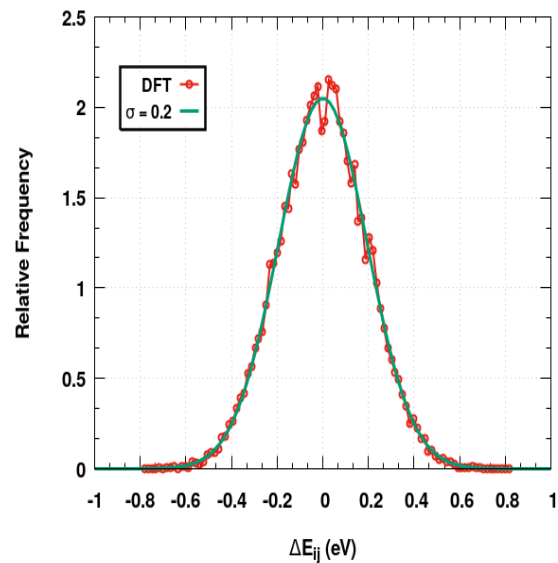
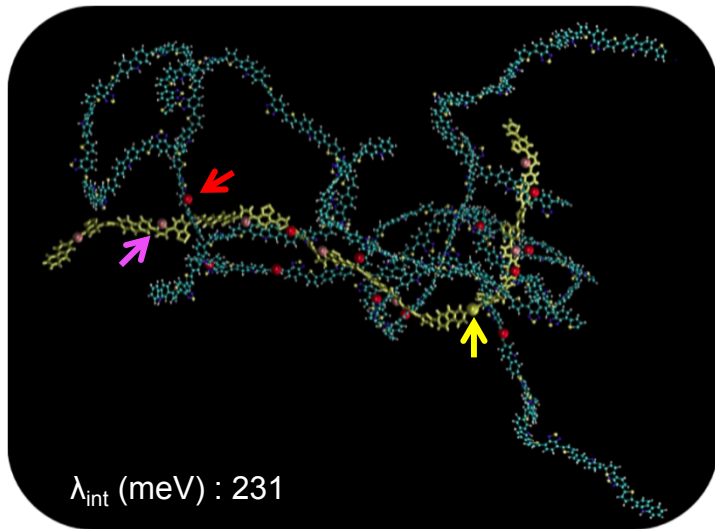
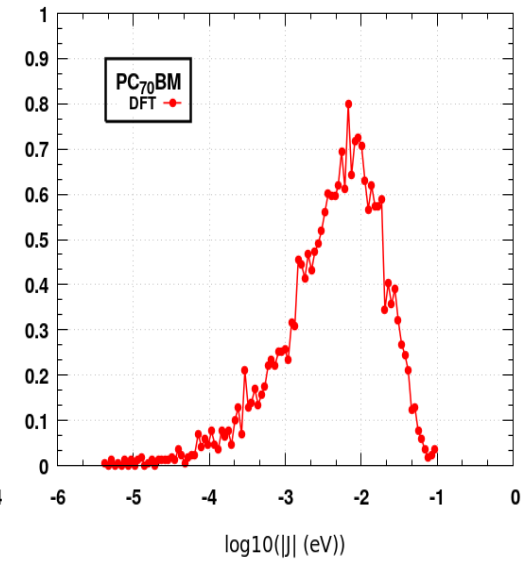
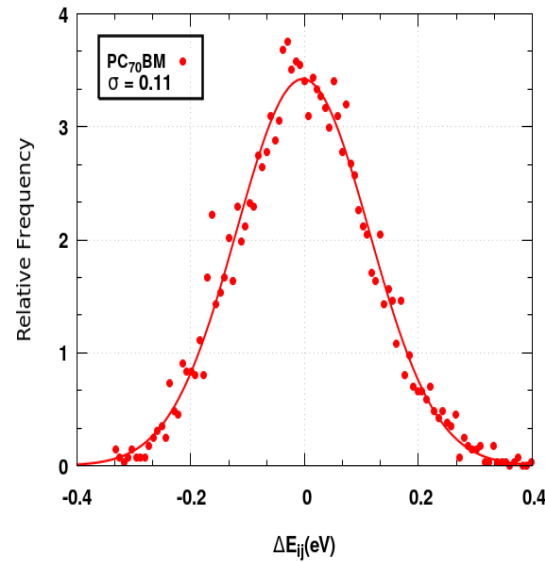
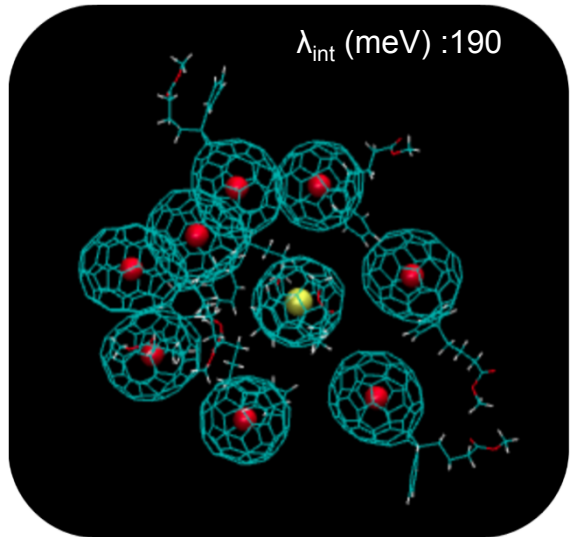
interaction
sites

Kinetic Monte Carlo:

- charge trajectories
- mobility evaluation

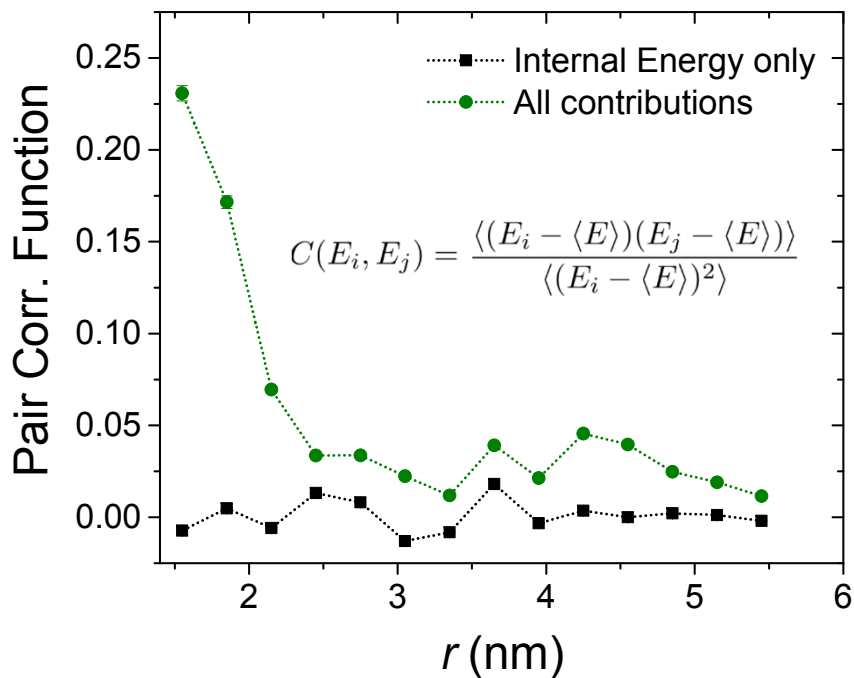
mobility

Transport parameters for PC₇₀BM and PCDTBT

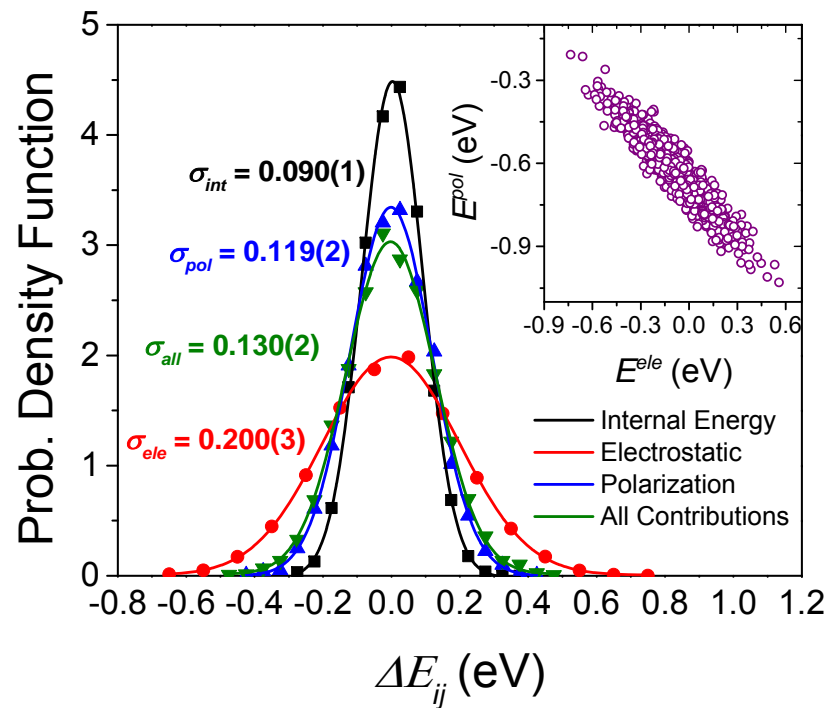


Electrostatic phenomena in organic semiconductors

Correlated Energetic Landscape



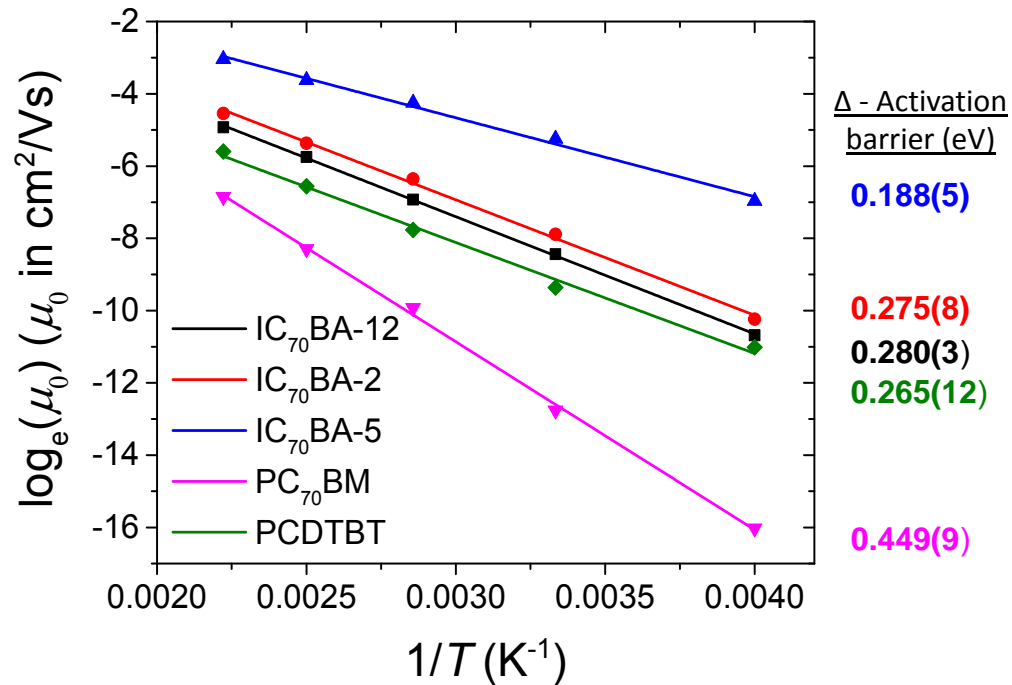
Anticorrelations of Electrostatic and Polarization energy



Mobility dependence on temperature and field

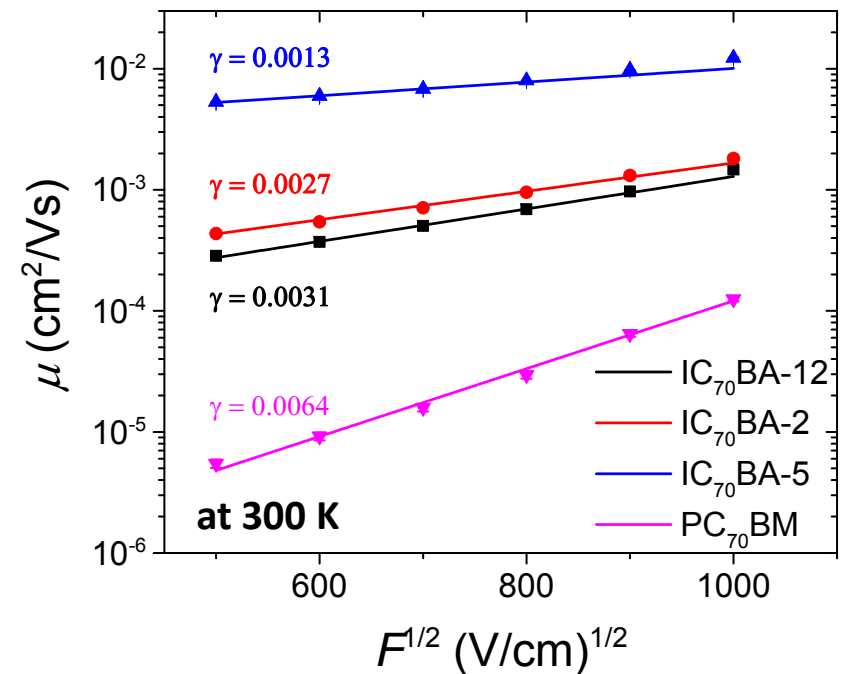
Arrhenius-like law fitted

$$\mu_0(T) = \mu_\infty \exp(-\Delta/k_B T)$$



Poole-Frenkel field dependence

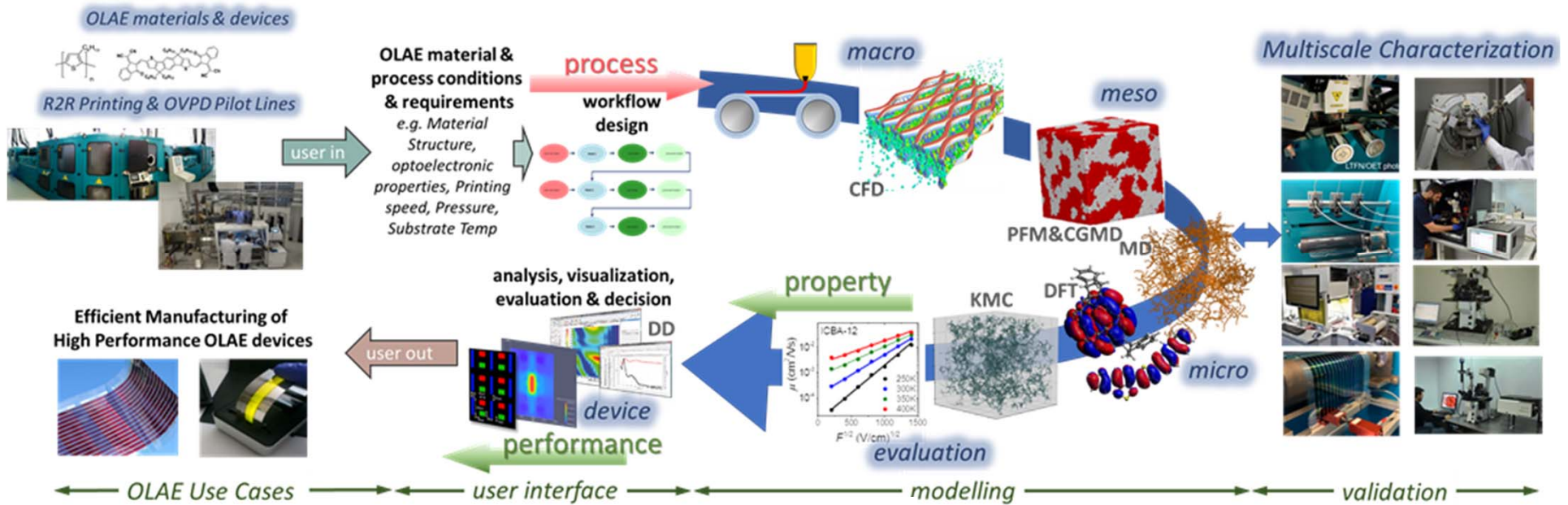
$$\mu(F) = \mu_0(300) \exp(\gamma\sqrt{F})$$



K. Kaklamanis et al., in preparation

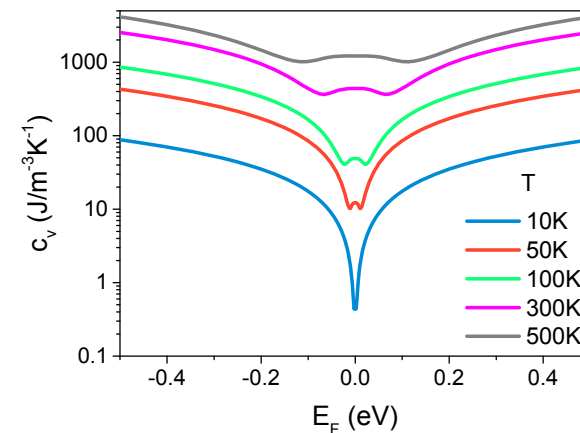
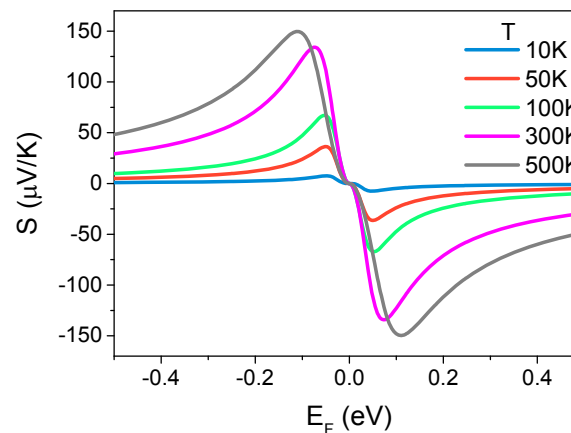
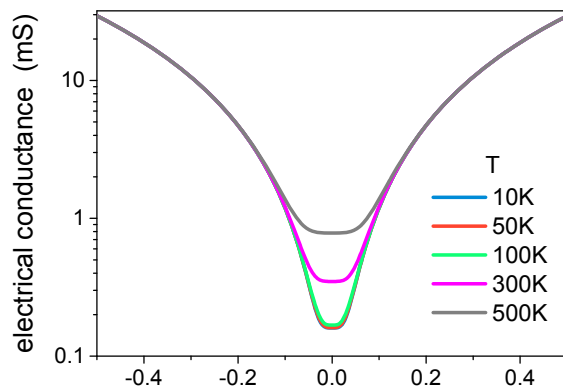
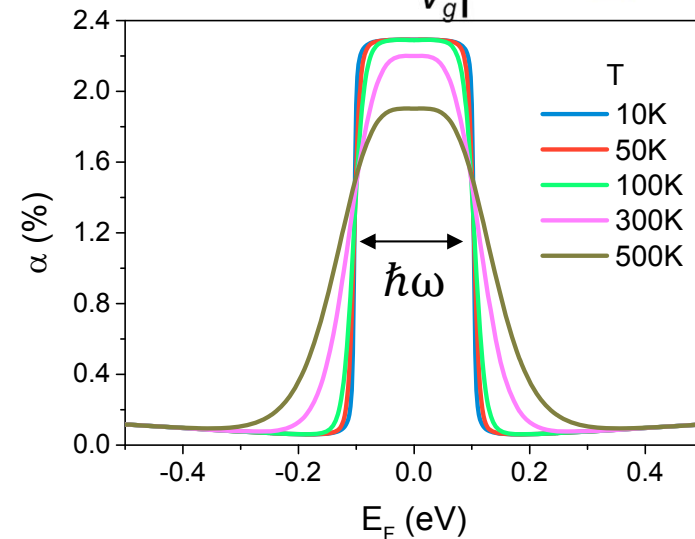
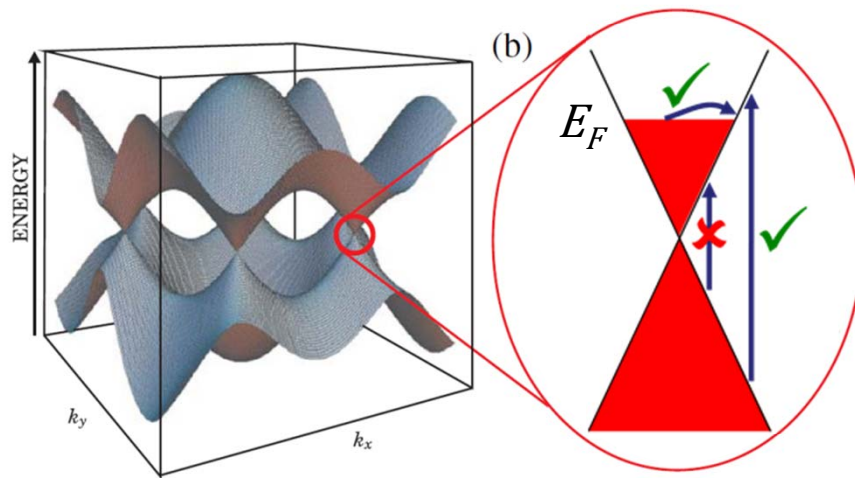
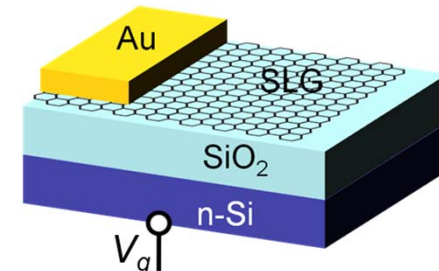
New EU project “MUSICODE” (2021-2024)

- Create an Open Innovation Platform for Materials Modelling



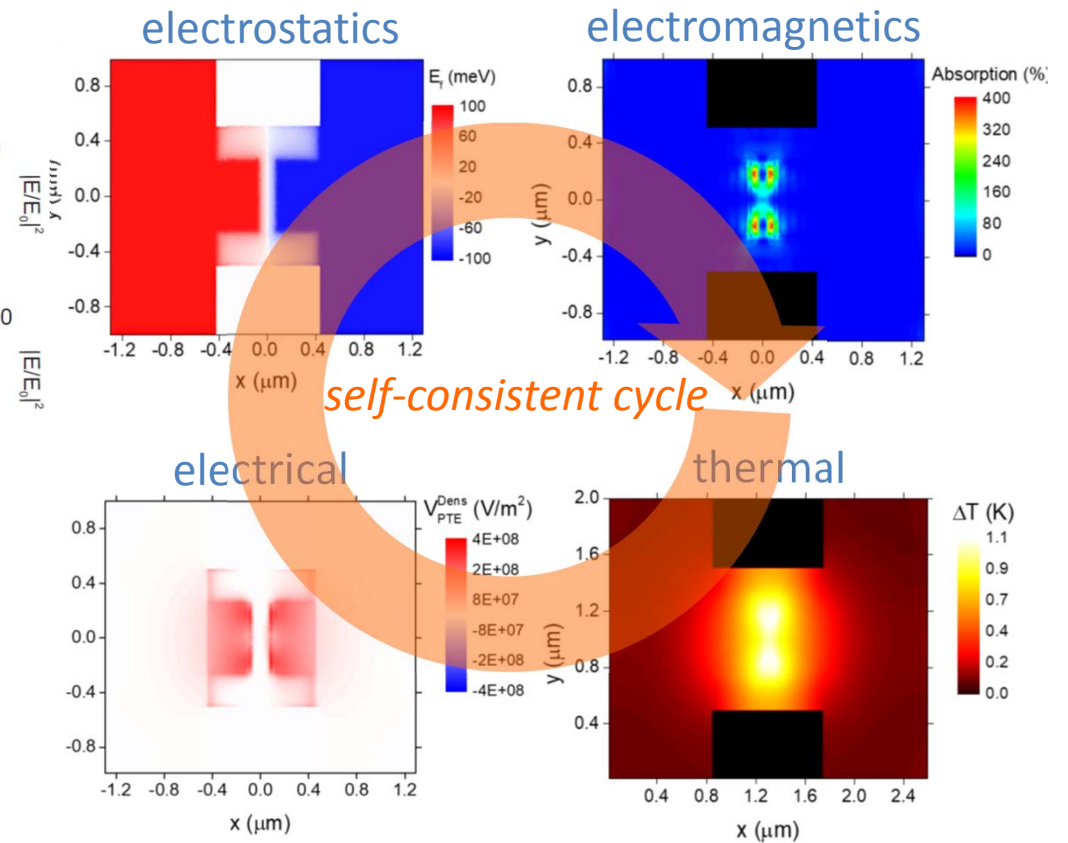
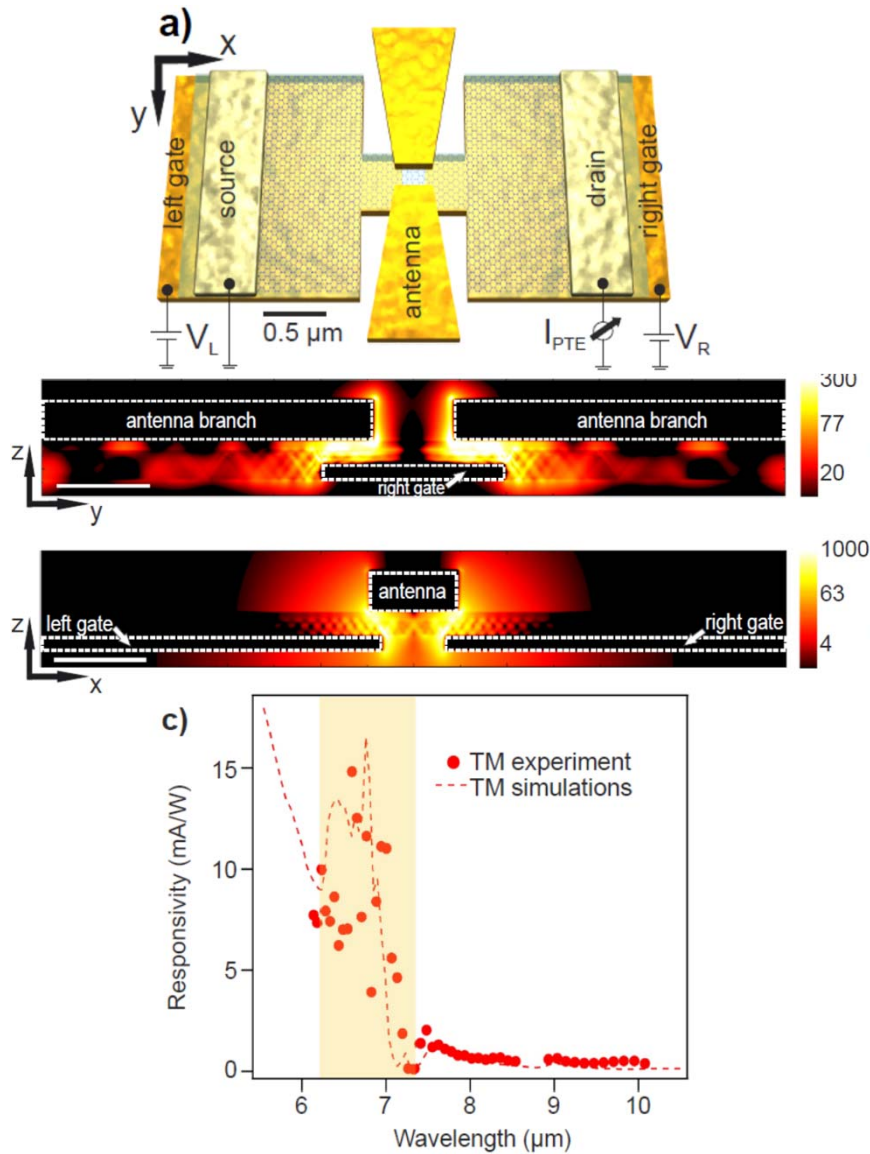
Graphene optoelectronics

- Strongly-coupled photo-thermo-electric effects
- Ambipolar effect → gate-tunable response



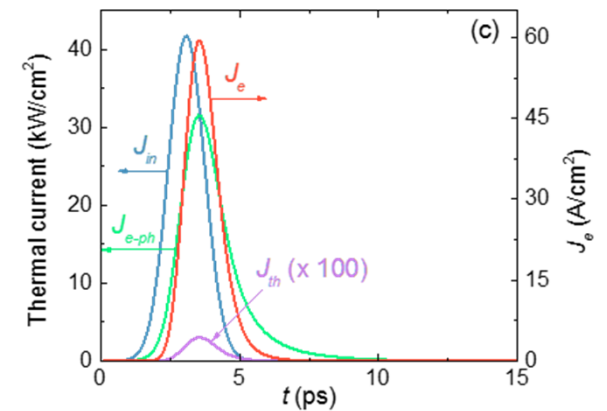
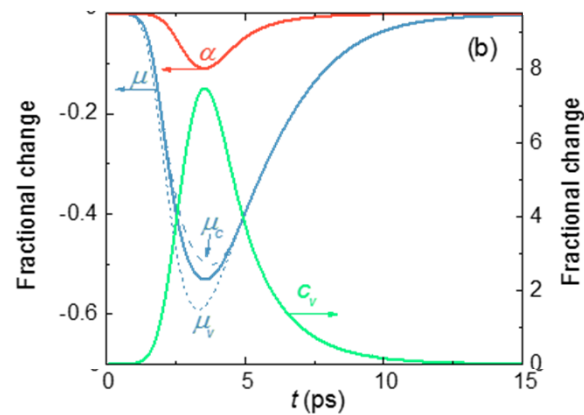
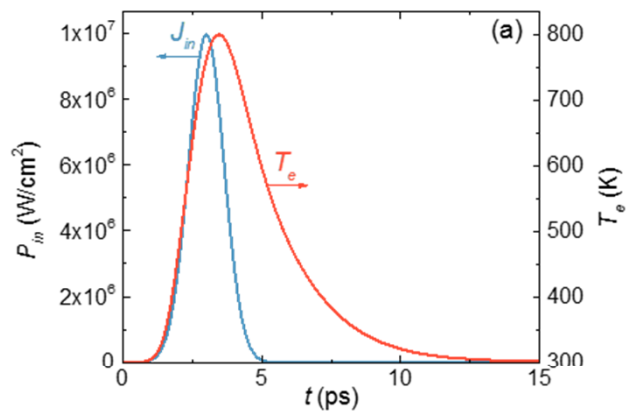
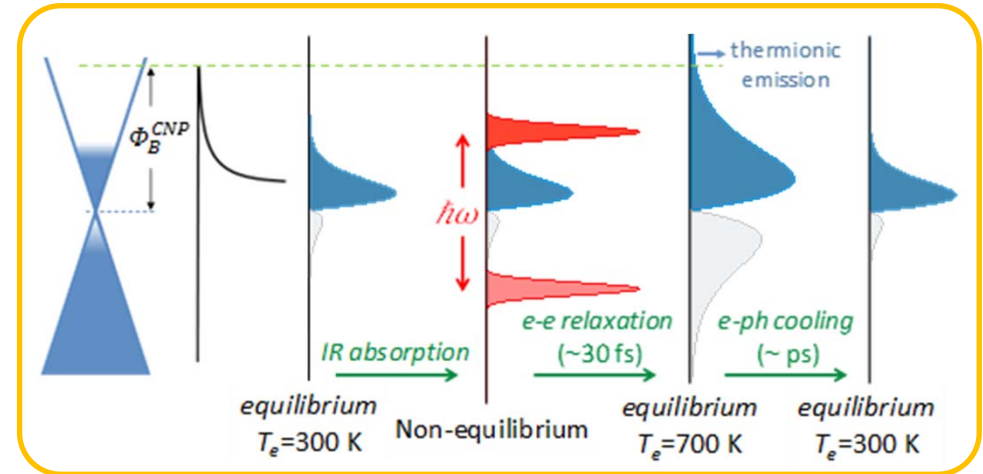
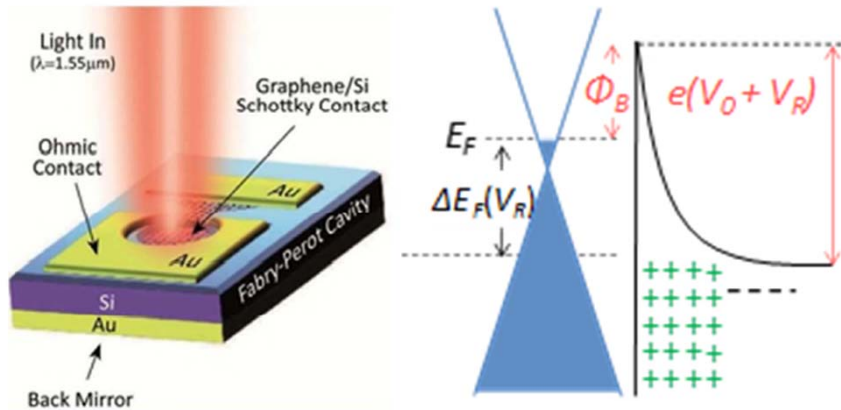
Example: plasmonic IR graphene photodetector

- Accurate simulations of full device functionality



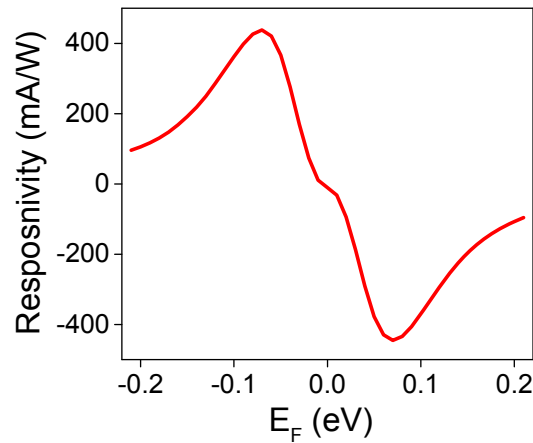
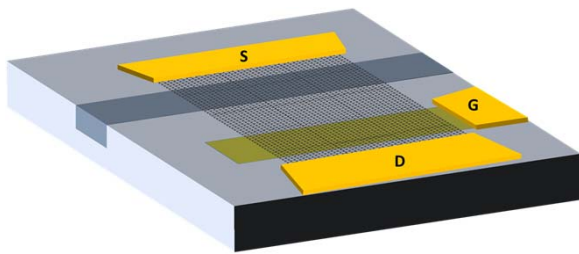
Reverse-biased G/nSi Schottky MIR photodetector

- Time-domain simulation of hot-electron dynamics

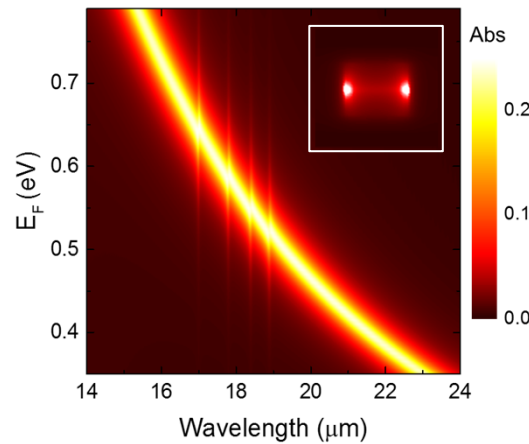
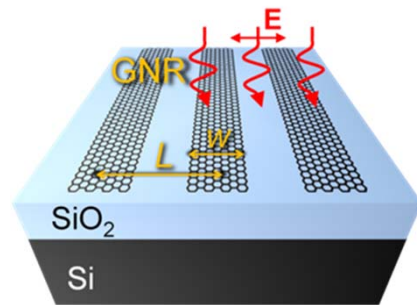


Other graphene devices of interest

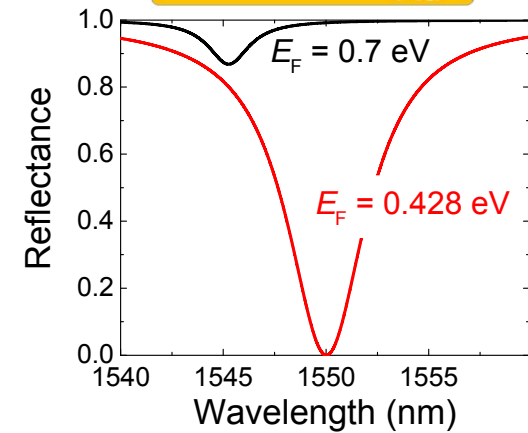
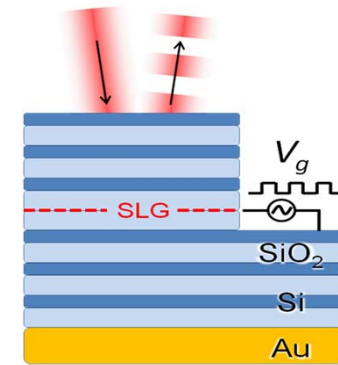
Integrated unbiased graphene photothermoelectric detector
(Vangelidis *et al.*, *in preparation*)



Chemical sensing by graphene nanoribbon plasmons
(Doukas *et al.*, *in preparation*)



Free-space graphene modulator
(Doukas *et al.*, *APL* 113, 011102 (2018))



Acknowledgements

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- Konstantinos Kordos
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- Charalampos Trapalis



Close collaborators:

