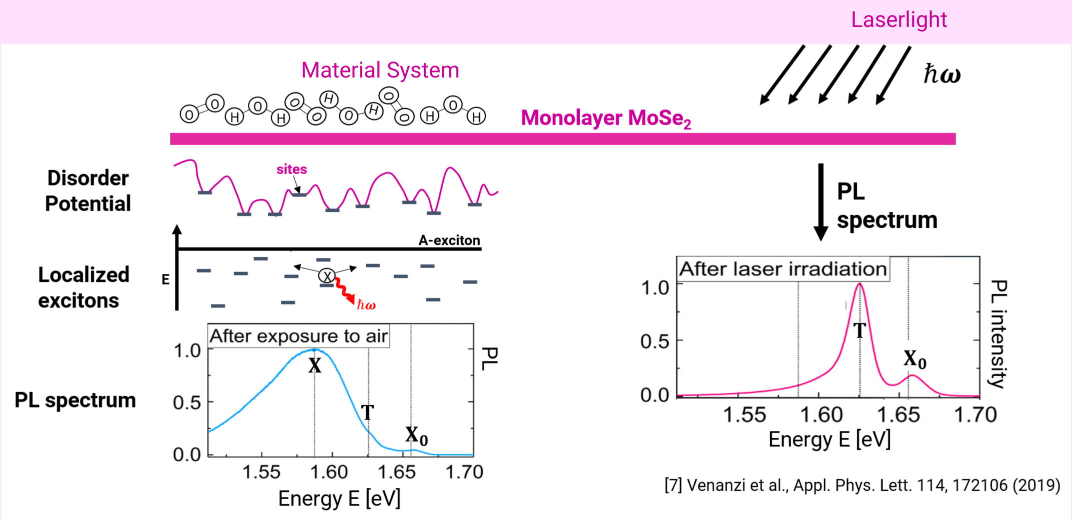
TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

Fakultät für Naturwissenschaften
Institut für Physik
S. Gemming, M. Hentschel, J. Prehl, G. Salvan, A. Thränhardt

Data-driven Physics at Chemnitz University of Technology

Hopping in low-dimensional semiconductors

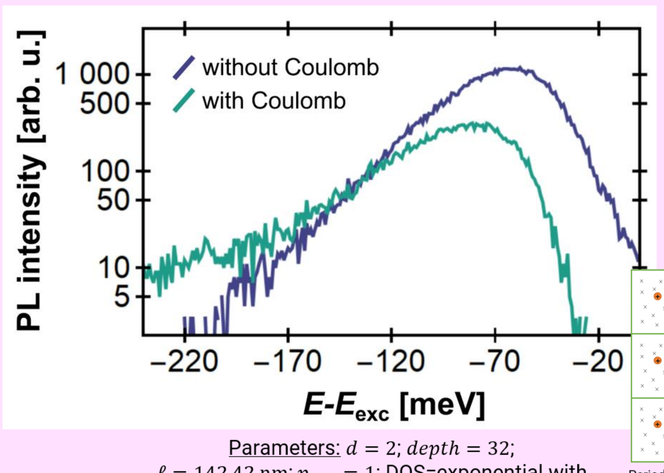
M. Schwuchow, Ch. Wagner, A. Thränhardt



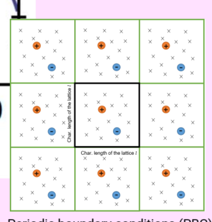
[7] Venanzi et al., Appl. Phys. Lett. 114, 172106 (2019)

Prof. Dr. Angela Thränhardt

- Optical experiments in semi-conductors may be modelled by Monte Carlo hopping
- Nondestructive method of material characterization; here: disorder can be switched on and off
- Here: good fit to experiment only when using temperature-dependent Urbach energy
- Higher densities: Particle-particle interaction required, numerical complexity increases

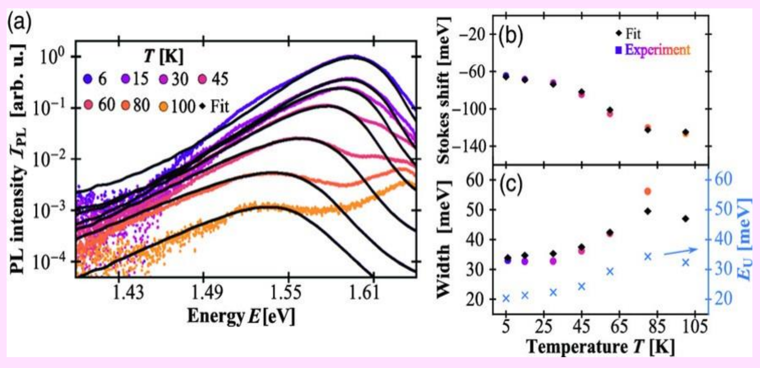


2`000 excitns
20`000 sites
one image set



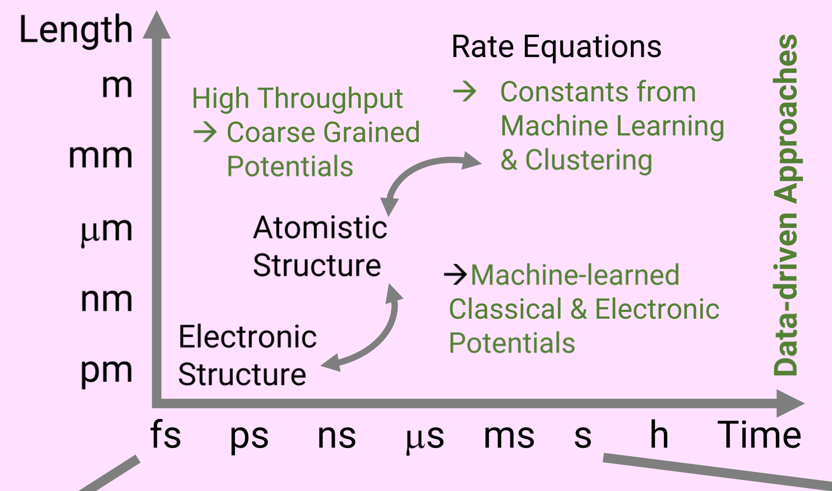
Periodic boundary conditions (PBC)

Parameters: $d = 2$; $depth = 32$; $\ell = 142.42$ nm; $p_{EEA} = 1$; DOS=exponential with $\varepsilon_0 = 0.02$ eV; $\nu_0\tau_0 = 10^3$; $N_0\alpha^2 = 0.5$; $T = 5$ K



Ch. Wagner et al., phys.stat.sol. b*258*, 2100186 (2021).

Quantum Mechanical Processes and Systems

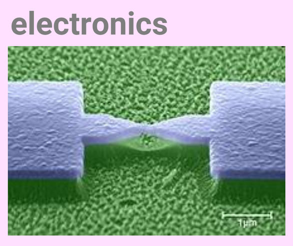


Goals

- ➢ Evaluate quantum effects in classical processes
- ➢ Develop suitable analytical theory & numerical models
- ➢ Implement quantum effects in simulations ex-/implicitly
- ➢ Augment by data-driven approaches
- ➢ Enhance reliability & precision

Prof. Dr. Sibylle Gemming

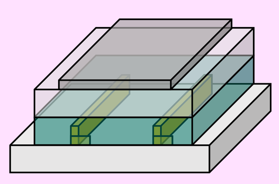
MCBJ / Molecular electronics



0.5 nm x 3 nm

→ DFT-NEGF conductance
→ + Random-walk weighting
→ Single-level model confirmed

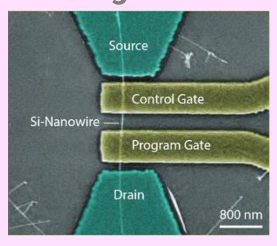
Organic Electronics OFET/OLED



20 nm x 200 nm

→ DFTB-MD structure & electronics
→ + Kinetic MC-type weighting
→ Doping organic films by polar molecules

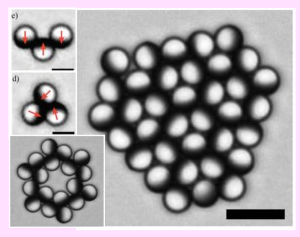
Reconfigurable FET



20 nm x 1500 nm

→ DFT-NEGF conductance
→ + Classical device simulation
→ Switching curve p/n SiNW transistor

Colloidal structures



25 000 nm x 25 000 nm

→ MC Potts spins
→ + Coil model for magnetic cap
→ + Dynamic friction
→ Field-reconfiguration of colloidal structure

Methods

- Quantum-mechanical
- Density Functional Theory
- (Post-) Hartree-Fock
- Classical-/Quantum-based
- Molecular Dynamics (MD)
- Kinetic Monte-Carlo (MC)
- Phase Field
- Classical Rate Equations

Projects

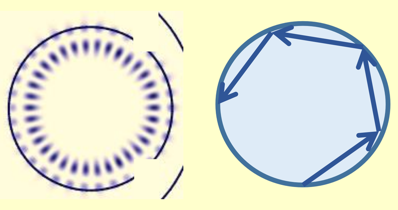
- DFG: INST 270/290-1 FUGB
- DFG: GE 1202/12; EXC 1056
- HGF: ExNet-0028, W3-026
- HGF: IHRS NanoNet

References: Adv. Elect. Mater. (21) 210052; ACS Nano 11 (17) 9989; Sci. Rep. 11 (21) 1; Chem. Mater. 33 (21) 668; ibid. 2635; Nanoscale 10 (18) 17131; JAP 128 (20) 085301; PRR. 2 (20) 023092.

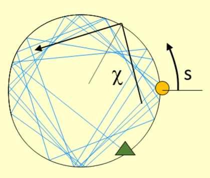
Complex dynamics in mesoscopic systems

Microscopic world	Mesoscopic systems	Macroscopic world
~ sub nm	~ micro meters	~ mm and above
Quantum mechanics	Semiclassics	*Classical mechanics*
Wave description	***Quantum-classical correspondence***	*Particle description*

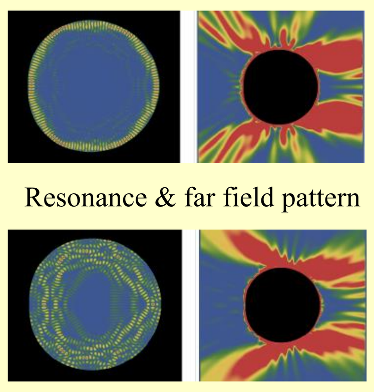
Interference, Coherence — Decoherence



Prof. Dr. Martina Hentschel



Limaçon cavity



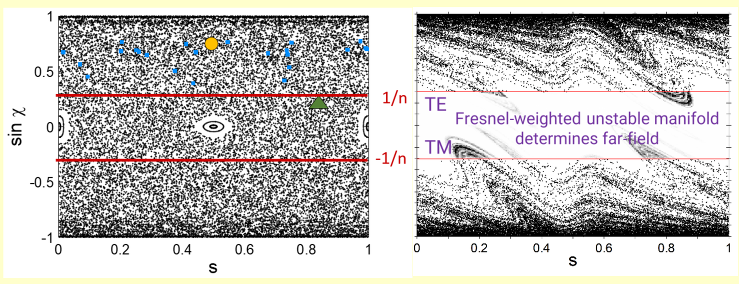
Resonance & far field pattern

Research topics

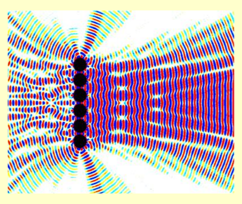
- Optical microlasers/microcavities with directional emission: interplay of geometry – dynamics – application potential
- Coupled, complex systems and array structures, feedback
- Graphene and photonic billiards with sources: perfect (Veselago) lens
- Transport in the mesoscopic regime: Taming light and electrons towards quantum information
- Berry phases in complex (e.g. Möbius) geometries, interference effects as semiclassical corrections

Methods

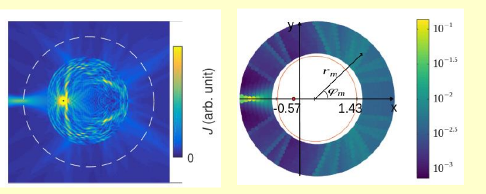
- Simulations in real and phase space space for both classical („ray tracing") and quantum/wave systems (finite-difference time-domain programs)
- Modelling of e.g. Maxwell's equation (e.g. free software package meep)
- Husimi functions as tool to visualize the phase-space temporal dynamics
- Ray-wave correspondence and semiclassical corrections to the ray picture



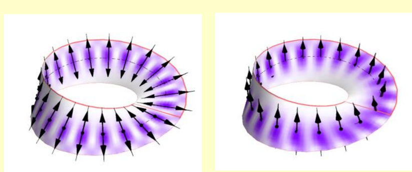
Cavity array: Far-field engineering



Graphene billiards with source: Lensing effect



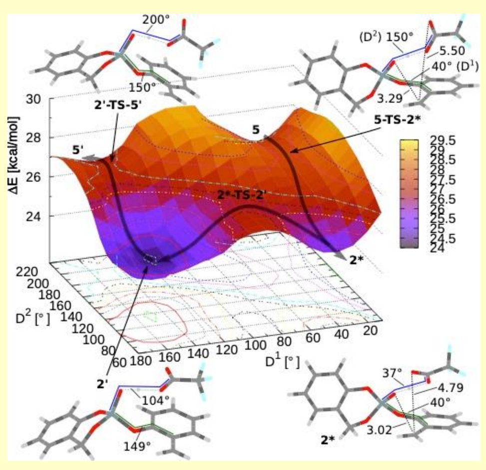
Möbius cavities: Topological effects (Berry phase) even for finite thickness



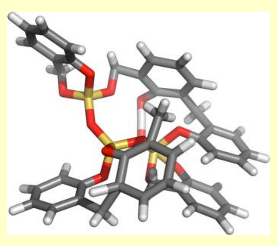
From structure to dynamics

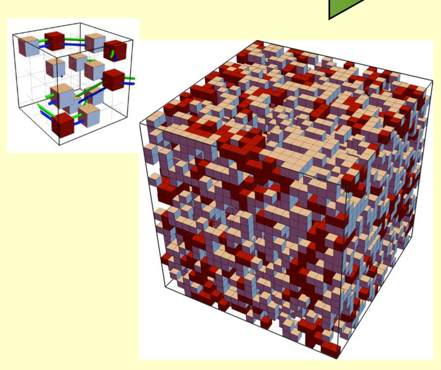
1. Analysis and understanding of **structure formation processes**:
   - Reaction, aggregation and deposition
   - Regard to all relevant length scales
   - Extraction of structure-process-properties

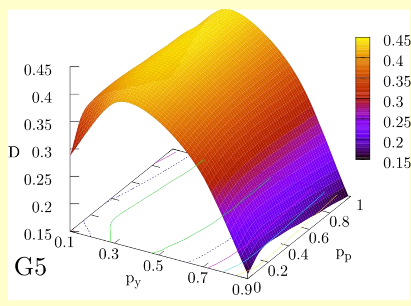
Dr. Janett Prehl



Relevant length scales

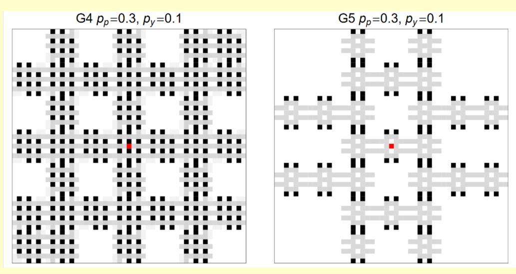






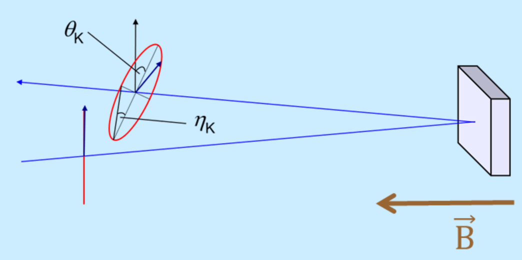
2. Dynamical behaviour of particles within complex media:
   - Numerical approach (random walk approach)
     → Asymptotic behaviours, Interactions, Anisotropy
   - Analytical approach (fractional diffusion equation)

$$\frac{\partial}{\partial t}P(x,t) = D\frac{\partial^\alpha}{\partial x^\alpha}P(x,t) \qquad \begin{array}{c} 1 < \alpha \leq 2 \\ -\infty < x < \infty \\ 0 \leq t < \infty \end{array}$$



Data Modelling in Magneto-Optics

Measurement of the polarization state of the light delivers information on the magnetization and electronic states of the



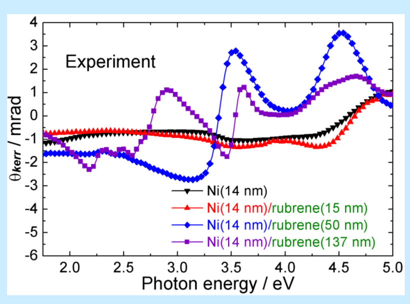
dielectric tensor

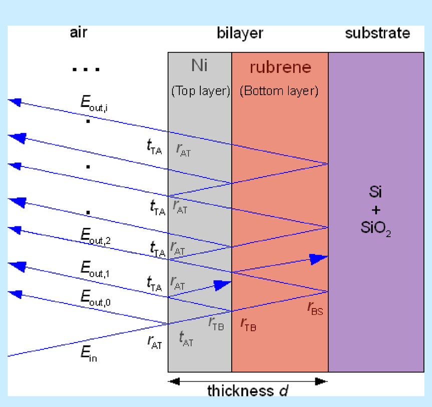
$$\begin{pmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix} \Rightarrow \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

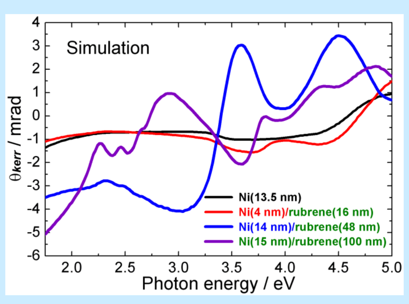
uniaxial case — medium exposed to an external magnetic field $\vec{B}$

Prof. Dr. Georgeta Salvan

Interference effects caused by multiple reflections need to be considered when interpreting the magneto-optical spectra → numerical simulations with optical layered models are required.





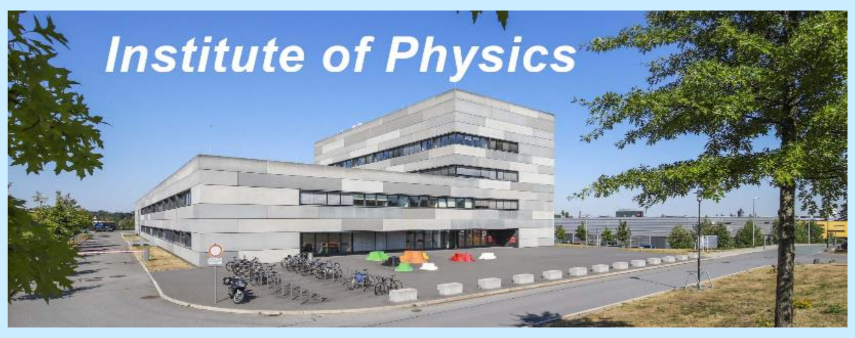


In the exemplary organic/ferromagnetic heterostructure shown here:

- Bilayer spectra can be simulated with the optical constants of the constituent materials → chemically sharp interfaces

→Ni acts as a capping layer, preventing oxidation of the organic layer

W. Li, …. G. Salvan, J. Am. Chem. Soc. ***132*** *(2010) 5687.*
M. Fronk, …, G. Salvan, Phys. Rev. B ***79*** *(2009) 235305*
A. Sharma…, G. Salvan, Phys. Rev. B 101 (2020) 054438.



Due to the close connection between chemistry and physics, we focus on the four research areas: Complex Materials, From Molecules to Functional Materials, Natural Science Modeling and Simulation, and Sensors and Cognition. These strategic priorities are currently being addressed by the following research areas at the Institute of Physics.