Executive Progress Reports ISAB SOLID21 for period July 2018-December 2019

Research Programme 2 – Nanoelectronics

Five Research Activities (RA):

RA1. Nonlinear optoelectronic and local transport phenomena in semiconductors and semiconductor nanostructures (P. Kužel)
RA2. Control of single-electron charged states in molecules (P. Jelínek)
RA3. Graphene and 2D materials (J. Červenka)
RA4. Magnetoelectric coupling and spin interactions in multiferroic materials (S. Kamba)
RA5. Magnetic anisotropy and magnetization dynamics in nanostructured strongly correlated magnetic materials (A. Shick)
RA1: Far-field THz measurements

probing local in-plane conductivity of an ensemble over macroscopic area (~ 1mm)

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
RA1: Near-field (SNOM) measurements

- Optical pump (~ 10 μm)
- Probing THz beam (~ 0.5 mm)
- AFM tip in tapping mode (50 nm)
- Scattered THz field is measured (modulated at tapping frequency)

Results
- Time resolution (sub-ps)
- Space resolution (~ 50 nm)
- Measuring of local conductivity in a single nanostructure

M. Eisele et al., Nat. Photon. 8, 841 (2014)

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
**Conductivity: response to the local field**

**Important features:**

- horizontal dash-dot lines: crossover from the classical to the quantum regime
- blue dashed lines: $L_{\text{bal}}$, $L_{\text{diff}}$ are carrier transport distances within one period of radiation in ballistic ($L_{\text{bal}} = v_{\text{therm}} / f$) and diffusion ($L_{\text{diff}} = \sqrt{D / f}$) regimes
- solid magenta line: $E_1 = h f$ is the lowest energy quantum transition
- time resolved microwave conductivity

- THz spectroscopy
- multi-THz spectroscopy

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Conductivity: response to the local field

Peak in $\Delta \sigma$ confined carriers (classical)

H. Němec et al., PRB 79, 115309 (2009)

Drop in $\Delta \sigma$ free carriers Drude

P. Drude, Ann. Phys. 1900

$\tau_{th} = \tau$

$E_1 = k_B T$

$h \nu = E_1$

Si, 300 K

$\Delta \sigma$ featureless (increase) confined carriers (classical or quantum)


Quantum transitions

T. Ostatnický et al., PRB 97, 085426 (2018)

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Towards ordered (or uniform) nanostructures

- Preparation by MBE growth, e-beam lithography
  - GaAs-technology based nanobars, nanoislands

Problem of substrate: should not be photoexcited
(otherwise signal from substrate >> signal from nanostructure)

Optical pump
THz probe

- $d_{\text{GaAs}} = 350$ nm
- $d_{\text{air}} = 250$ nm
- $L = 600$ nm

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Nonlinear response (to local $E$) of GaAs nanobars

(a)

$$a \approx 100 - 500 \text{ nm}$$
$$L \approx 200 - 1000 \text{ nm}$$
GaAs:
$$m = 0.07$$
$$\tau = 100 - 270 \text{ fs}$$

$$\langle v(t) \rangle = E \cdot \text{Re} \sum_{\alpha} \mu^{[\alpha]}(\alpha \omega) \exp(i\alpha \omega t)$$

J. Kuchařík and H. Němec, submitted to PRL
Nonlinear response (to local $E$) of GaAs nanobars

\[ \langle \nu(t) \rangle = E \cdot \text{Re} \sum_{\alpha} \mu^{[\alpha]}(\alpha \omega) \exp(i\alpha \omega t) \]

mobility at 0.5 THz:

\[ |\mu^{(3)}| \]

$|\mu^L|$ vs Potential well width $a$ (nm)

\[ |\mu^L| (\text{cm}^2\text{V}^{-1}\text{s}^{-1}) \]

\[ |\mu^{(3)}| (\text{cm}^4\text{V}^{-3}\text{s}^{-1}) \]

\[ \mu \approx 0 - 1000 \text{ nm} \]
GaAs:
$m = 0.07$
$\tau = 270 \text{ fs}$


The project Solid state physics for the 21st century – SOLID21
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Study of complex azide and nitrene chemistry in UHV on surfaces with precise determination of the final chemical products


RA2: On-surface synthesis of nitride complexes

9-azidophenanthrene on the Ag(111) surface

Study of complex azide and nitrene chemistry in UHV on surfaces with precise determination of the final chemical products.

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
Several groups claimed to visualize weak non-covalent (hydrogen, halogen) bonds via appearance of sharp edges in SPM images, see e.g. C₆Br₆ dimer \textit{Zh. Han et al. Science 358,260 (2017)}. However calculated electron density of C₆Br₆ dimer does not show any electron localization in between C₆Br₆ molecules. 

**SPM simulations with a home-built toolkit of the C₆Br₆ dimer**

Theoretical simulations unambiguously demonstrate that sharp edges representing ridges in the potential energy surface, where probe bends laterally.

**The Sharp edges** observed in the experiment are artefact and \textit{cannot be ascribed to real bonds}. 

\textit{A. Gallardo, et al. JPCC 123, 8379 (2019)}

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RA3: Catalyst-induced doping of Si nanowires

FIG. 1. SEM micrographs of SiNWs catalyzed by different metals: (a) Au, (b) In, (c) Sn, (d) Bi, (e) Pb, and (f) Ga.

FIG. 2. HAADF imaging in STEM showing the distribution of metal clusters in (a) In-, (b) Sn-, and (c) Bi-catalyzed SiNWs. The bright contrast areas in the images highlight the catalytic metal atoms due to their higher atomic (Z) number than Si.

FIG. 3. Schematic picture of a SiNW-based electrical device. (a) Schematic image of a SiNW device using an array of SiNWs embedded in a dielectric SU8 epoxy layer which is sandwiched in between a Si substrate (n-type or p-type doped) and a top Al contact. (b) Current-voltage characteristics of Sn-catalyzed SiNWs, In-catalyzed SiNWs, and Ga-catalyzed SiNWs on a p-type doped Si substrate. (c) Arrhenius plot of conductivity of SiNWs (normalized to a single nanowire) grown by different catalytic metals in PECVD. P + Sn and B + Sn denote phosphine- and diborane-doped Sn-catalyzed SiNWs, respectively.

J. Šilhavík et al. APL 114, 132103 (2019)

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
Fabrication of 3D graphene aerogels

1. **Hydrothermal reduction of graphene oxide**
   - Self assembly of reduced graphene oxide
   - Chemical coupling of individual graphene sheets
   - Reduced 3D graphene contains oxygen groups

2. **High-temperature annealing at 1300 °C**
   - Oxygen and defect removal
   - Fabrication of free-standing 3D graphene aerogels

Šilhavík et al., manuscript in preparation

ρ = 22.4 mg/cm$^3$

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
Compression of 3D graphene aerogels

- Elastic regime from $10^3$-10$^6$ Pa
- Electrical resistance changes with mechanical deformation
- Suitable material for electromechanical sensors

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
RA3: 3D graphen superstrings

3D Graphene Superelastic Spring

0 ms  33 ms  66 ms  100 ms  133 ms  166 ms

Fast response < 1 ms

Application: Electromechanical heart rate measurement

Šilhavík et al., manuscript in preparation

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
RA4: Curie-Weiss law and soft phonon behavior in relaxor ferroelectrics

Viehland et al. PRB 46, 8003 (1992)

\[ \chi' \propto \frac{C}{T} \]

\[ T_{\text{T} - \theta} \]

\[ \omega^2_{\text{TO}} = A(T - T_c) \]

\[ \varepsilon_0 \frac{\varepsilon}{\varepsilon_\infty} = \prod_j \frac{\omega^2_{\text{LO}_j}}{\omega^2_{\text{TO}_j}} \]


The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
EMA: Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$ at room temperature

This approach could explain splitting of all three $F_{1u}$ phonons below $T_d$

J. Hlinka et al. PRL 96, 027601 (2006)
Relaxor Pb(Mg$_{1/3}$Ta$_{2/3}$)O$_3$: Dielectric spectra from the Bruggeman-EMA fits

- Dielectric anisotropy is rather pronounced.
- Dielectric contribution of $E$-SM is much higher than $A_1$

D. Nuzhnyy et al. PRB 96, 174113 (2017)
D. Nuzhnyy et al. APL 114, 182901 (2019)

The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
General behavior of relaxor ferroelectrics:

Optical soft phonon is responsible for C-W behavior and induces ferroelectric phase transitions in polar nanoclusters

D. Nuzhnyy et al. PRB 96, 174113 (2017)
D. Nuzhnyy et al. APL 114, 182901 (2019)
Electromagnons in THz spectra of SrMn$_7$O$_{12}$

$T_{OO} = 265$ K
$T_{N1} = 87$ K
$T_{N2} = 63$ K

![Graph showing wavenumber (cm$^{-1}$) vs temperature (K) for SrMn$_7$O$_{12}$](image)

Mode frequencies (cm$^{-1}$)

- $T_{N1} = 87$ K
- $T_{OO} = 265$ K
- $T_{CO} = 404$ K

(a) Rhombohedral incommensurate $R3(001)0$

Plasma frequencies (cm$^{-1}$)

- $\omega_1$
- $\omega_2$
- $\omega_3$
- $\omega_4$

(b) Cubic $Im3$

Temperature (K)
Strained thin films of \((\text{SrTiO}_3)_{n-1}(\text{BaTiO}_3)_1\text{SrO}/\text{DyScO}_3\)
Strained thin films of $(\text{SrTiO}_3)_{n-1}(\text{BaTiO}_3)_1\text{SrO}/\text{DyScO}_3$

\[ FOM = \frac{\Delta k}{k \cdot \tan \delta} \]


The project Solid state physics for the 21st century – SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760 is co-funded by the European Union.
Strained thin films of \((\text{SrTiO}_3)_{n-1}(\text{BaTiO}_3)_1\text{SrO}/\text{DyScO}_3\)

**RA5: Anisotropic unconventional superconductor UTe$_2$**


- *Immm*
  
  (bco, inversion)

**Space group #71**

- **U-chains along a-[100]-axis**

**Superconductivity,**

- $T_c = 1.7K$

- residual $C_V/T$ as $T \to 0$

**Normal carriers (50%) within the SC state!?**

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Normal phase: Curie susceptibility with the local moment $\sim 3 \ \mu_B$

No magnetic order

Non-magnetic DFT+orbital polarization

Ferromagnetic DFT+OP
Metallic and strongly anisotropic

Semi-metallic
13 meV hybridization band gap

Nesting $\sim (0, \pi/b, 0)$
FM becomes unstable

Magnetism of 4f-atoms adsorbed on graphene/metal substrates

RA5: DFT+U+Hubbard-I calculations of Dy@GR/Ir(111)

- Good quantitative agreement with XMCD exp. data
- Positive magnetic anisotropy (MAE) – out-of-plane $M$

<table>
<thead>
<tr>
<th></th>
<th>$\langle M_S \rangle$</th>
<th>$\langle M_L \rangle$</th>
<th>$\langle M_S \rangle + \langle M_D \rangle$</th>
<th>$R_{LS}$</th>
<th>MAE, meV</th>
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<td>”HCP”</td>
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<td>1.28</td>
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<td>”ATOP”</td>
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<td>XMCD Exp.</td>
<td>2.4±0.2</td>
<td>3.9±0.2</td>
<td>3.0±0.2</td>
<td>1.31±0.15</td>
<td>&gt; 0</td>
</tr>
</tbody>
</table>

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Conclusions

1. Two large investments are planned within the project. These are Terahertz Scanning Near-field Optical Microscope (THz-SNOM, 637 kEuro) and equipment for Atomic Layer Deposition (ALD, 522 kEuro). Both apparatus are already ordered and they should be installed till summer.

2. Most of milestones planned for last year and the next term have already been accomplished and the remaining milestones for the next term are well achievable within the planned schedule.

3. We do not expect any potential problem, if the installation of both apparatus is realized in time.

Thank you for your attention!