SOLID21
Research programme 2

Nanoelectronics

Stanislav Kamba

FZU Fyzikální ústav Akademie věd České republiky

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.

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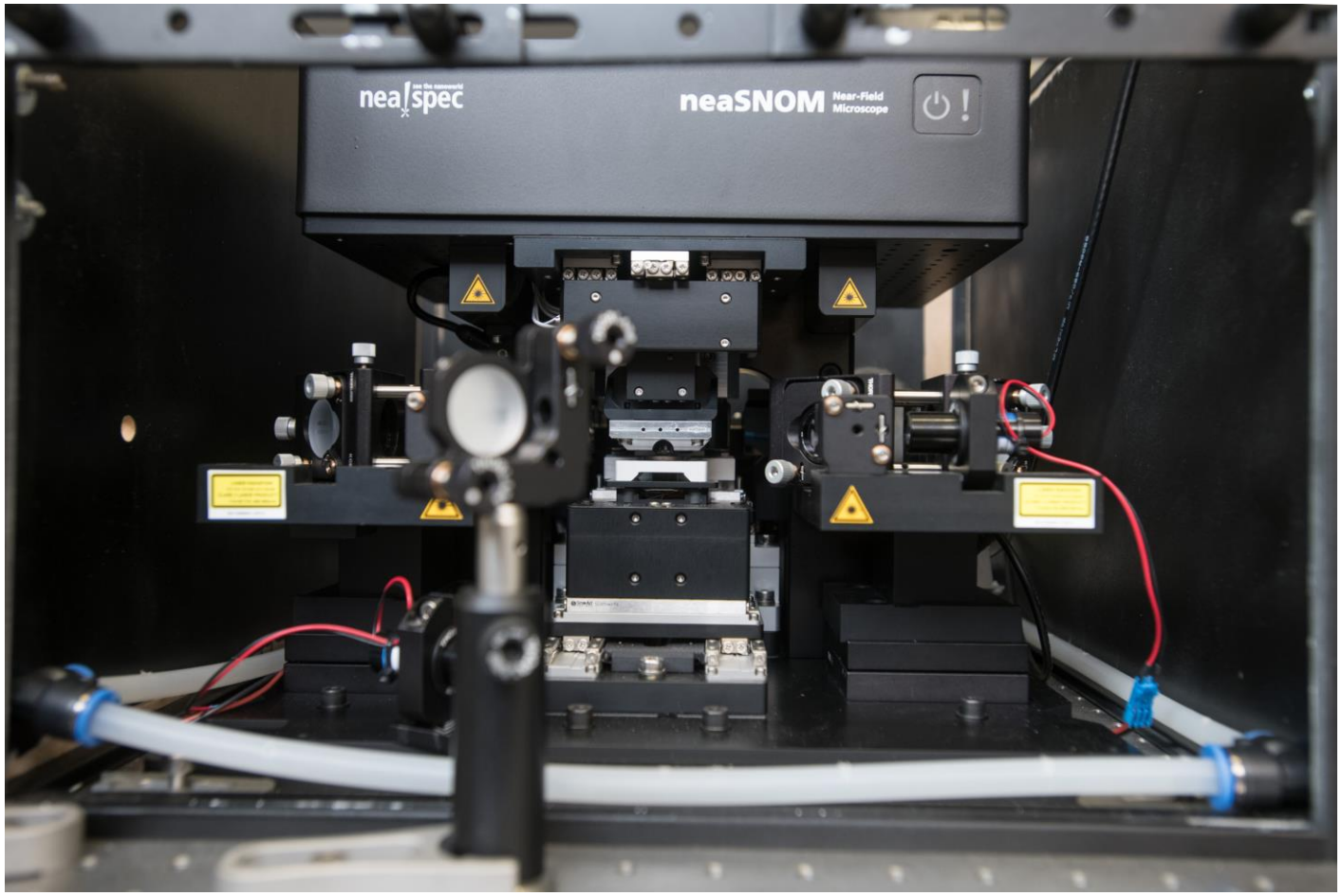
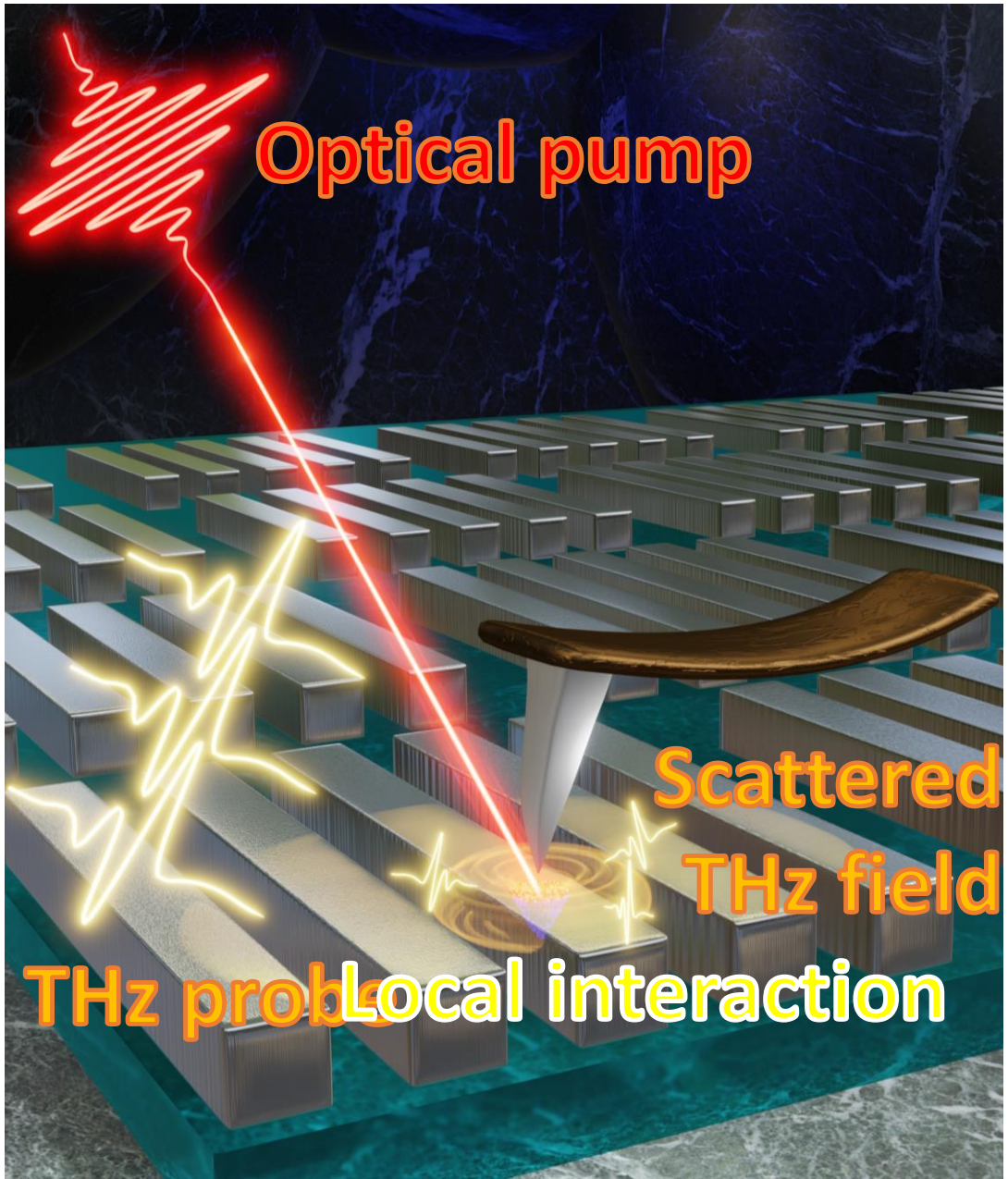
RA1: Nonlinear and local transport phenomena in semiconductor nanostructures

Petr Kužel

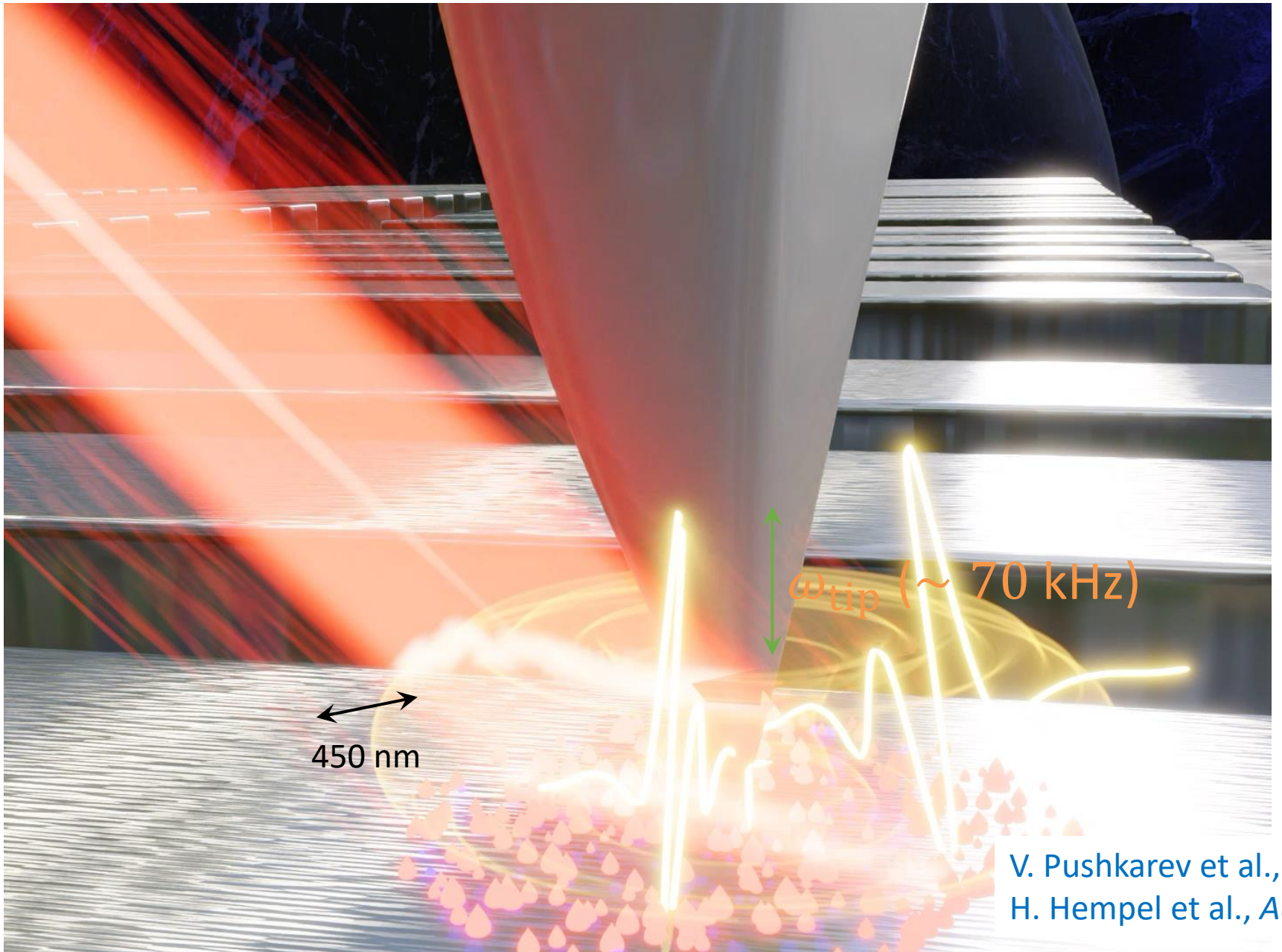
FZU Institute of Physics of the Czech Academy of Sciences

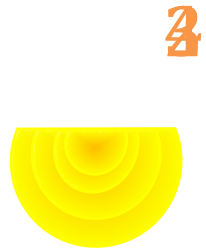
THz SNOM (scanning near-field optical microscope)

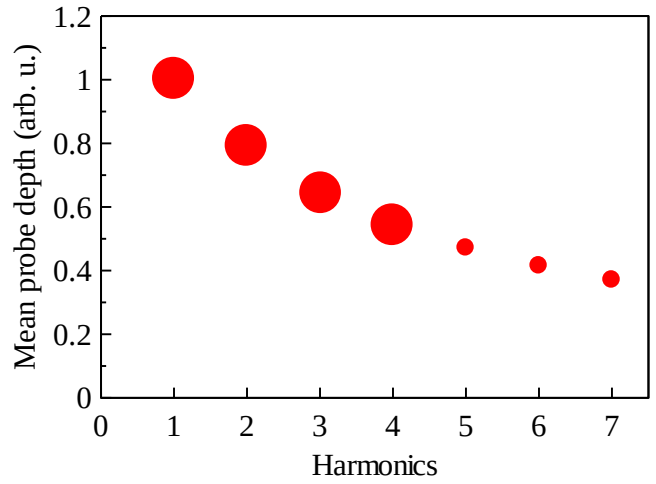




Near-field probing of GaAs nanobars

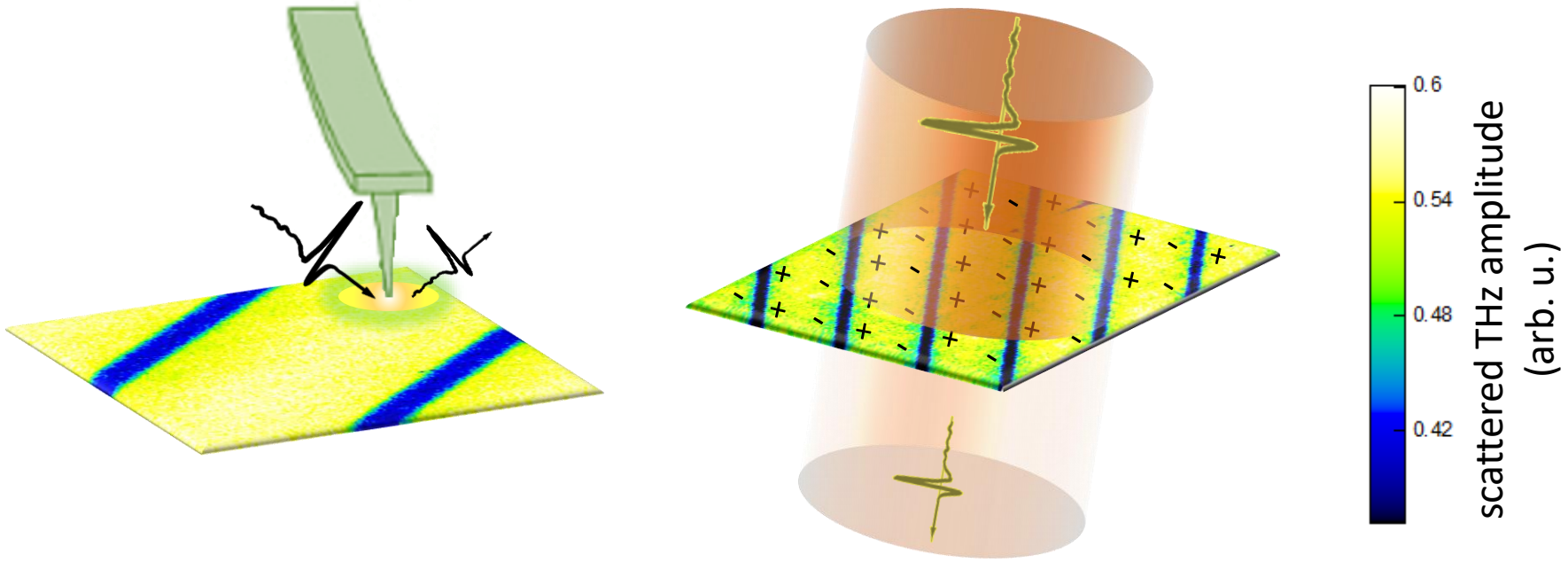






V. Pushkarev et al., *Adv. Funct. Mater.* **32**, 2107403 (2022)
H. Hempel et al., *Adv. Energy Mater.* **12**, 2102776 (2022)

Probing of THz conductivity in graphene nanoribbons



V. C. Paingad et al., *Adv. Funct. Mater*. **31**, 2105763 (2021)
P. Kumar et al., *Nanoscale Adv*. **5**, 2933 (2023)

RA2: Control of single-electron charged states in molecules

Pavel Jelínek, Hector Vázquez

FZU Fyzikální ústav Akademie věd České republiky

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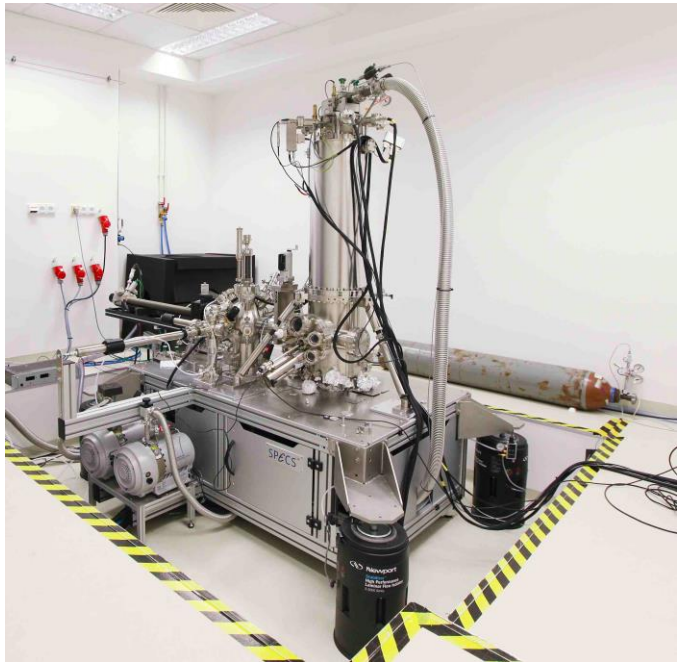
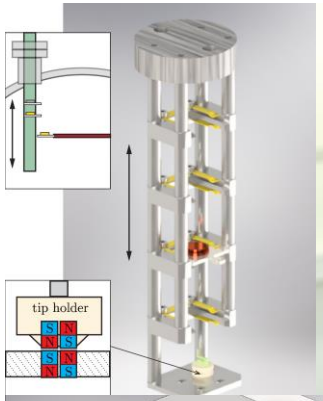
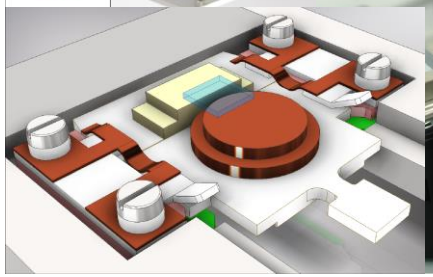
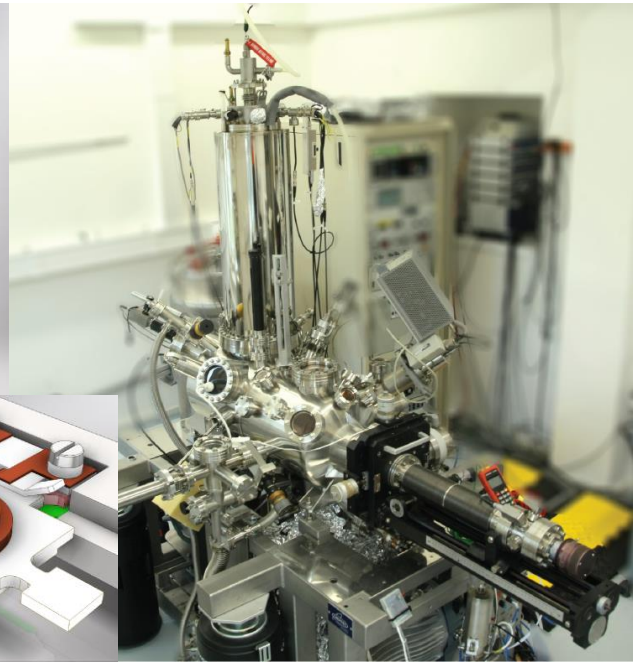
Scanning-probe experimental facilities

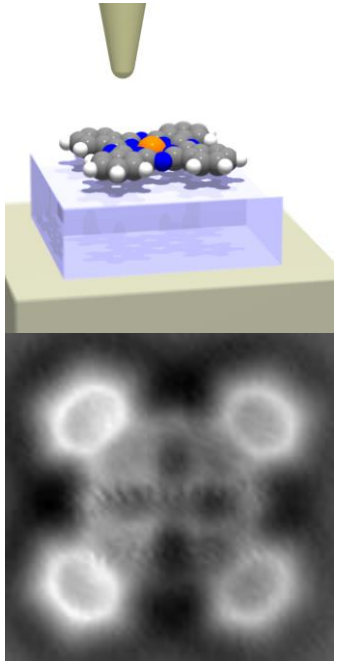
Nanosurf lab (P. Jelínek) https://nanosurf.fzu.cz
Customized LT-SPM, LEED, PES: high-resolution imaging (STM / AFM / IETS) and surface characterization











Collaboration with experimental groups

To achieve a full understanding of molecular junctions, we combine our DFT-based simulations with collaborations with experimental groups.

Cooperation with experimental groups. In the past 3 years, we have collaborated with the following experimental partners from abroad:

Tokyo Inst. of Technology
JAPAN

Forschungszentrum Jülich
GERMANY

Columbia University
USA

Boston University
USA

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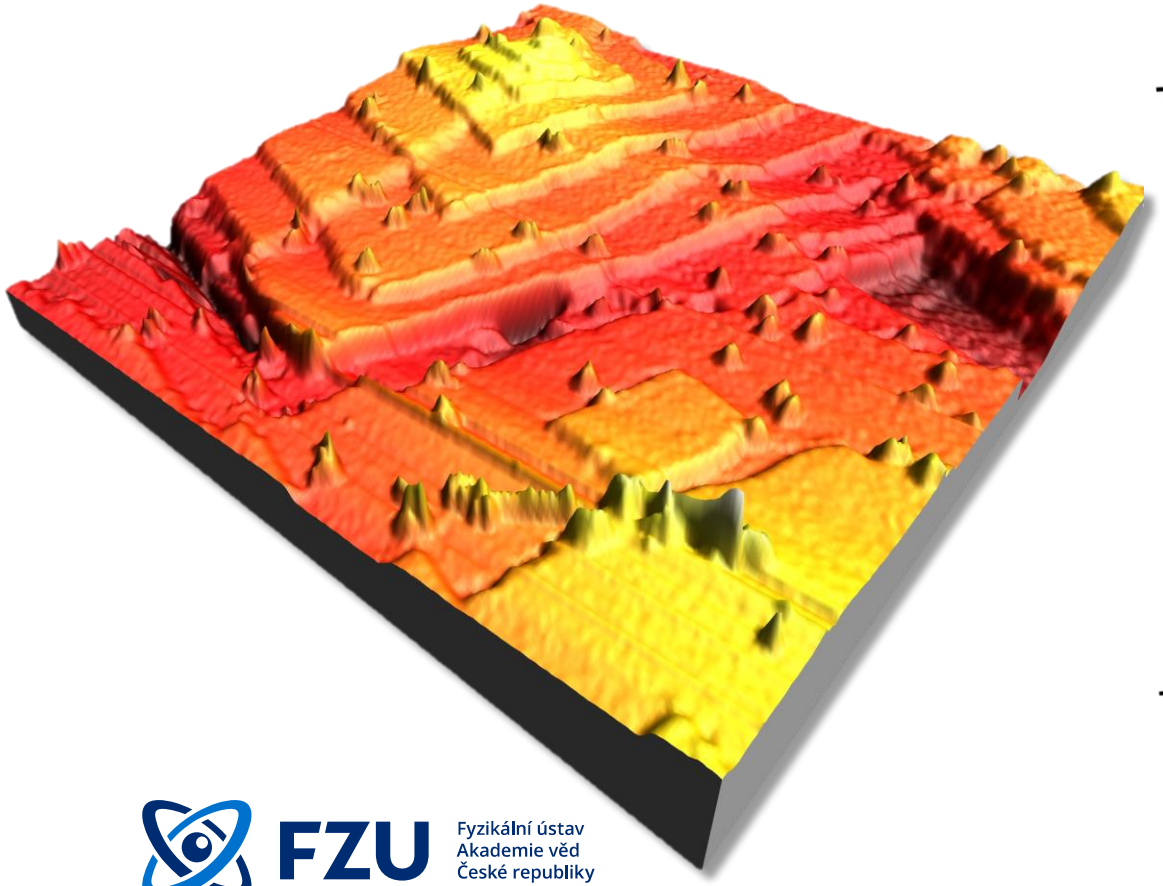
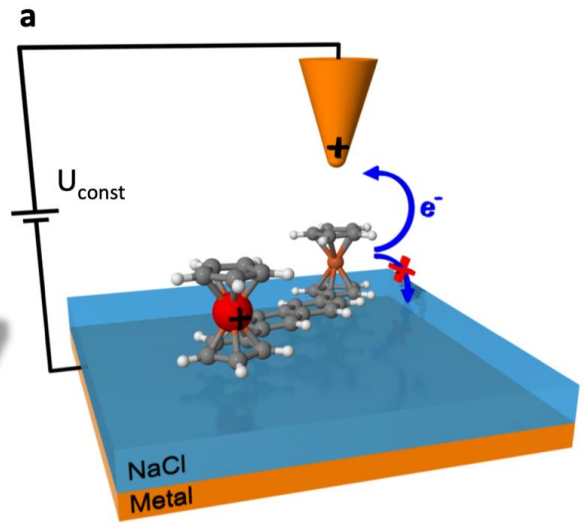
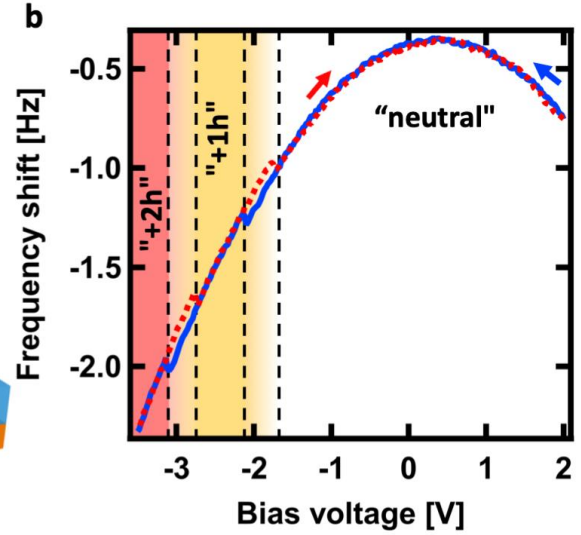
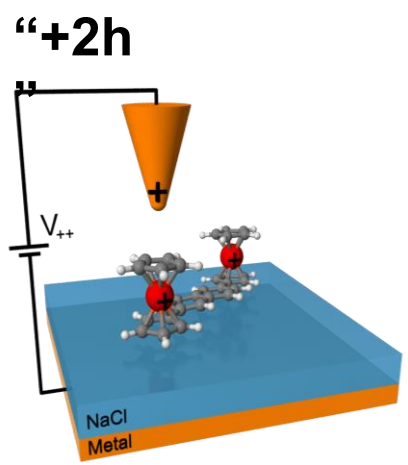
Formation of single electron charge states

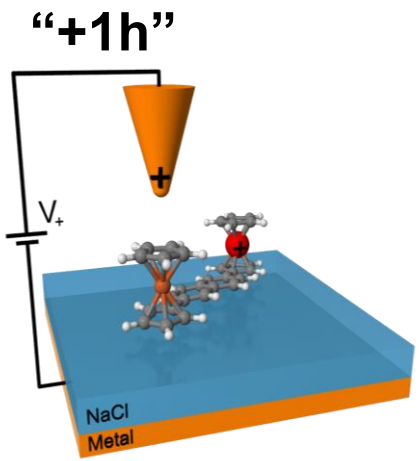
Control deposition of bis-ferrocene molecules on an insulating substrate under UHV conditions and formation of single electron charge states by controlled application of external bias on SPM probe

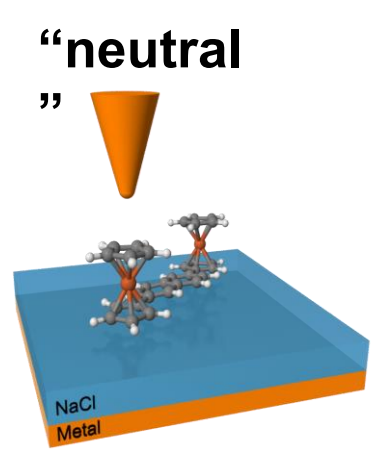












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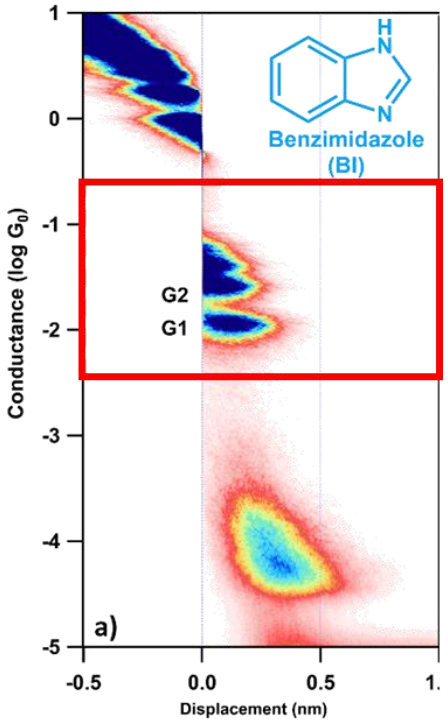
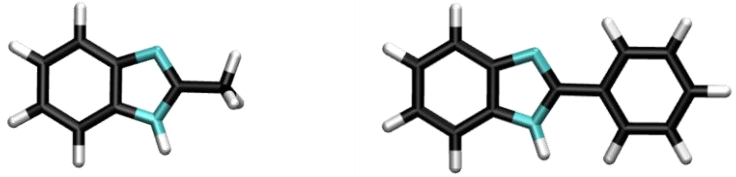
J. Berger et al Nat. Comm. 11, 1337 (2020)

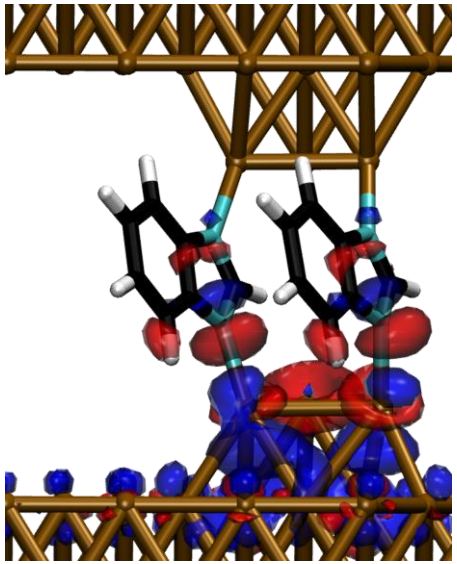
Nanoelectronics: π–stacked benzimidazole circuits



Distance-conductance 2D histograms from experiment show G2 peak (dimer) and G1 peak (monomer), with **G2 = 2.3 × G1** for benzimidazole

- Energetically most favorable geometry has benzimidazole molecules bonded in parallel
- Intermolecular attraction > 20 k_BT
- π-π interaction stabilizes dimer structure
- Intermolecular cooperative interactions harnessed in other, new, benzimidazole derivatives:





Current-carrying states in the benzimidazole dimer junction

Work shows new ways of **engineering molecular circuits by tuning π-π intermolecular interactions**

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X. Pan, **E. Montes**, B. Lawson, **W.Y. Rojas**, **H. Vázquez*** and M. Kamenetska*, Nano Lett. (under review)

RA3: Graphene and 2D materials

Martin Šilhavík, Zahid Ali Zafar, Prabhat Kumar, Abdul Wahab, and Jiří Červenka

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ALD laboratory

Atomic layer deposition (ALD)

- growth of atomically thin films
- oxides (Al_2O_3, HfO_2, ZnO, TiO_2, SiO_2)
- nitrides (Si_3N_4)

Prize: 13.3 MCZK ≈ 0.53 M€

The laboratory has been in operation since February 2021.

Activity 3 - Graphene and 2D materials

Activity leader: Jiří Červenka

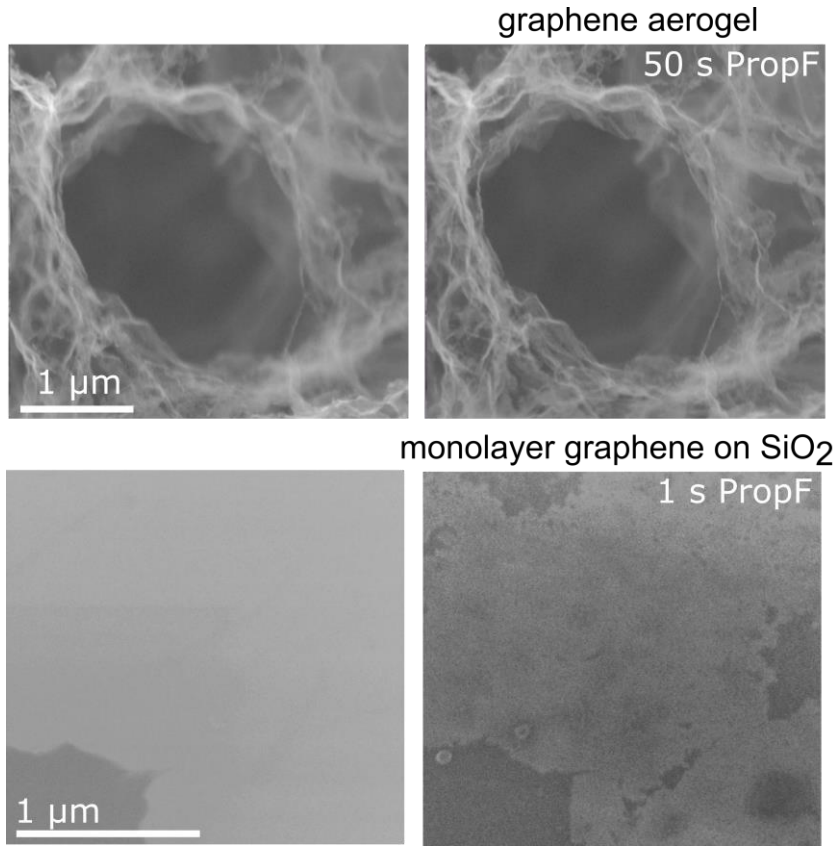
We investigate physical properties of 3D porous structures made of 2D materials

- Graphene aerogels
- MXenes and TMDs

Applications

- Electromechanical sensors
- THz applications
- Batteries and supercapacitors

Fire resistance of 2D and 3D graphene to propane flame (1200 °C)



M. Šilhavík et al., ACS Nano 16, 11, 19403-19411 (2022).

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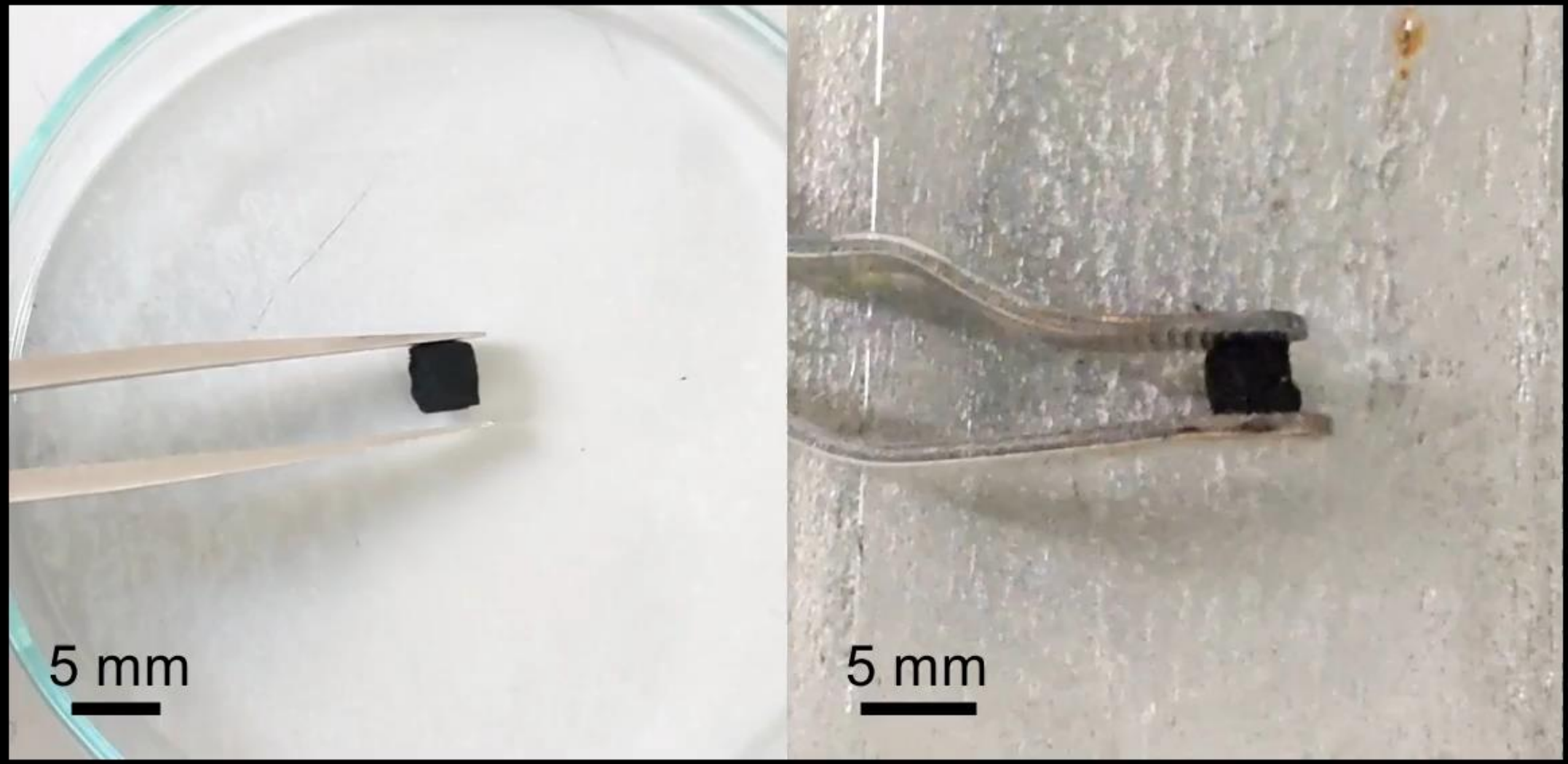
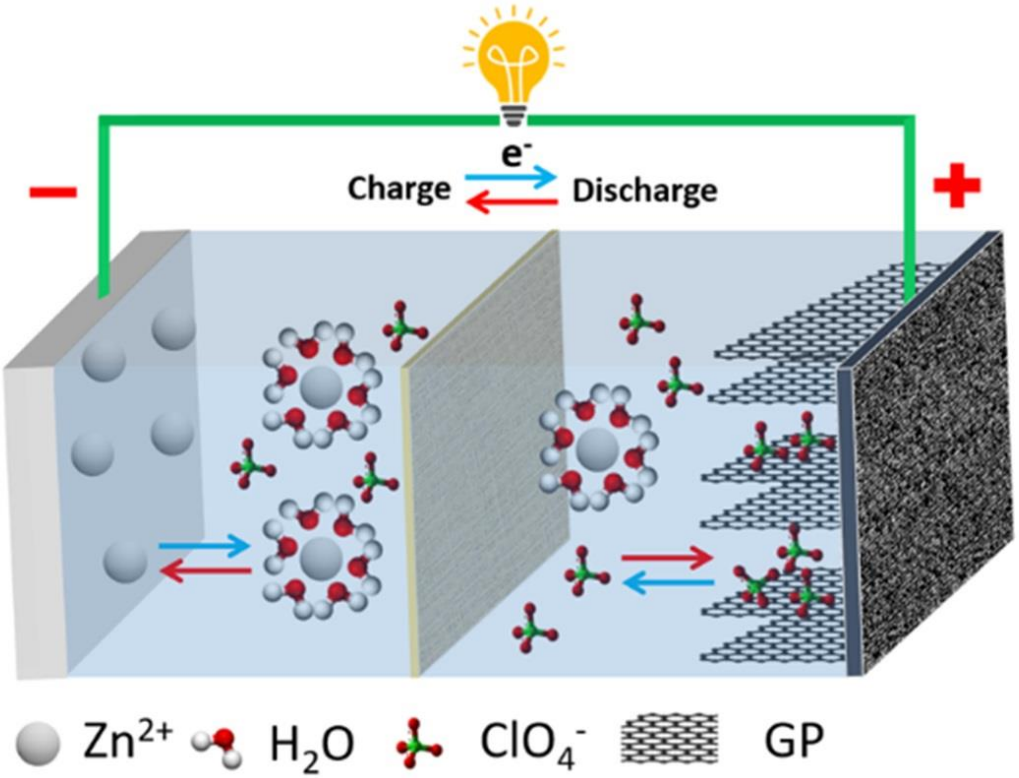
Superelasticity of graphene aerogels at high and low temperatures



High-voltage aqueous batteries

Zinc-graphite dual-ion battery based on zinc perchlorate water-in-salt electrolyte



[2] Zafar *et al.*, J. Mat. Chem. A 10, 2064-2074 (2022)
[3] Zafar *et al.*, Patents LU101731 and EP3896762

RA4: Magnetoelectric coupling and spin interactions in multiferroic materials

Stanislav Kamba

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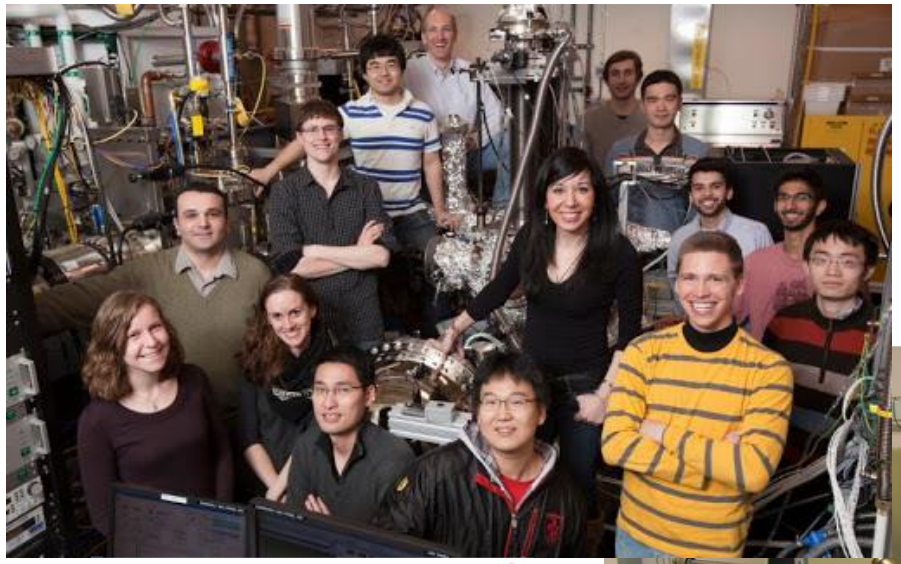
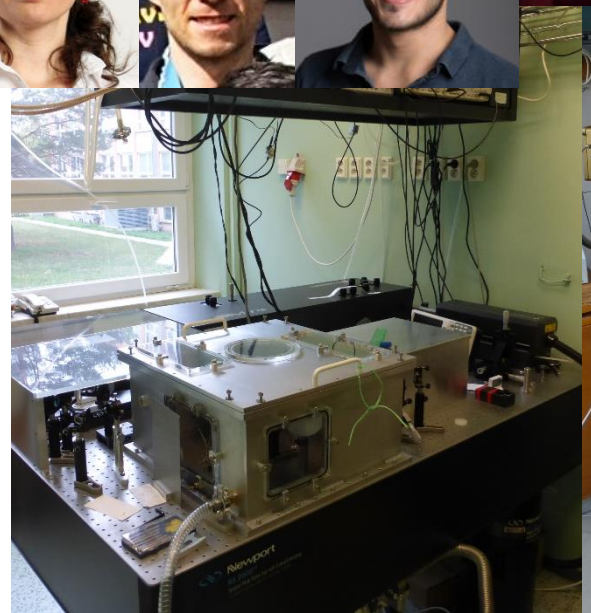
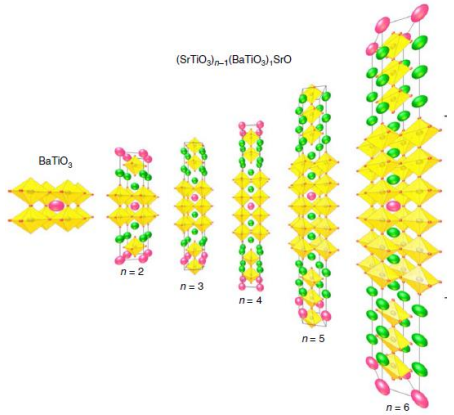
FZU Institute of Physics of the Czech Academy of Sciences

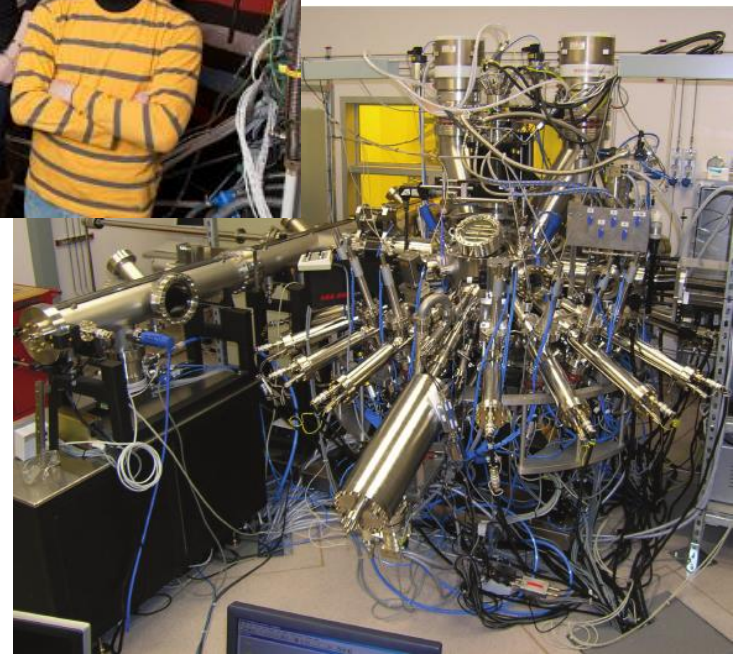
CORNELL UNIVERSITY FOUNDED A.D. 1865

Strengthening collaboration of S. Kamba with the group of D. Schlom from Cornell University, **14 joint articles in the last 12 years, 5 of them in Nature Research journals**

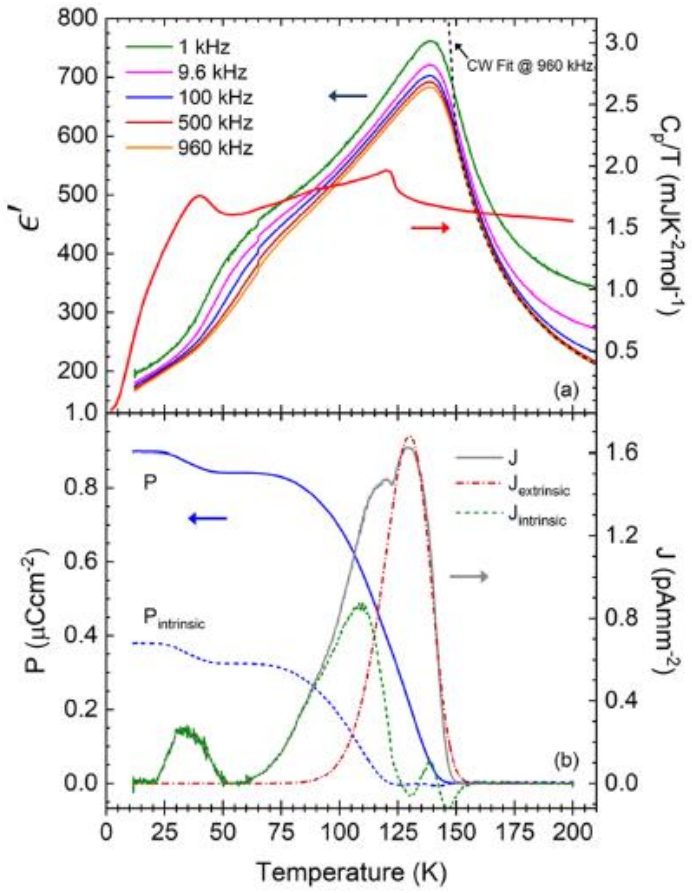


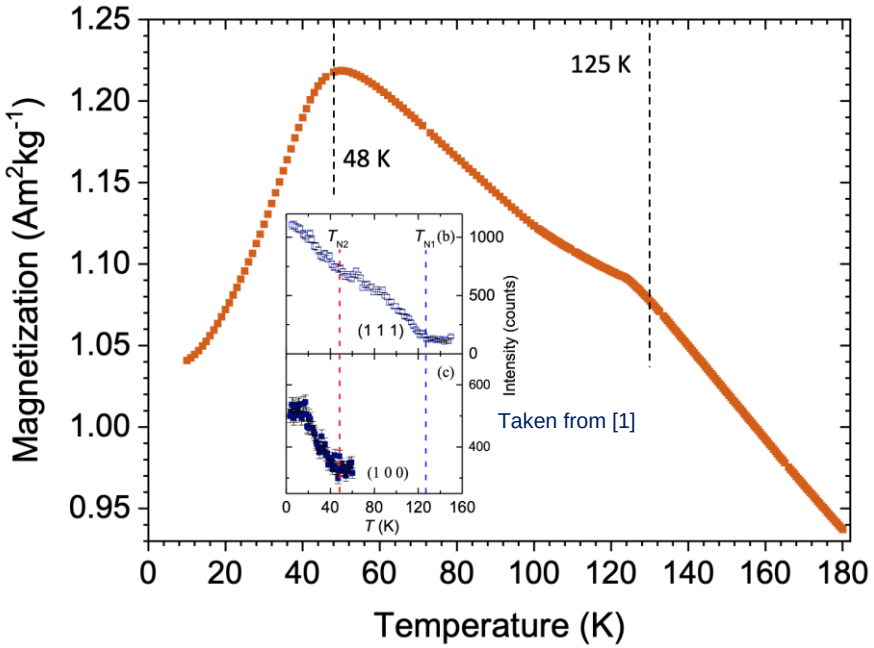


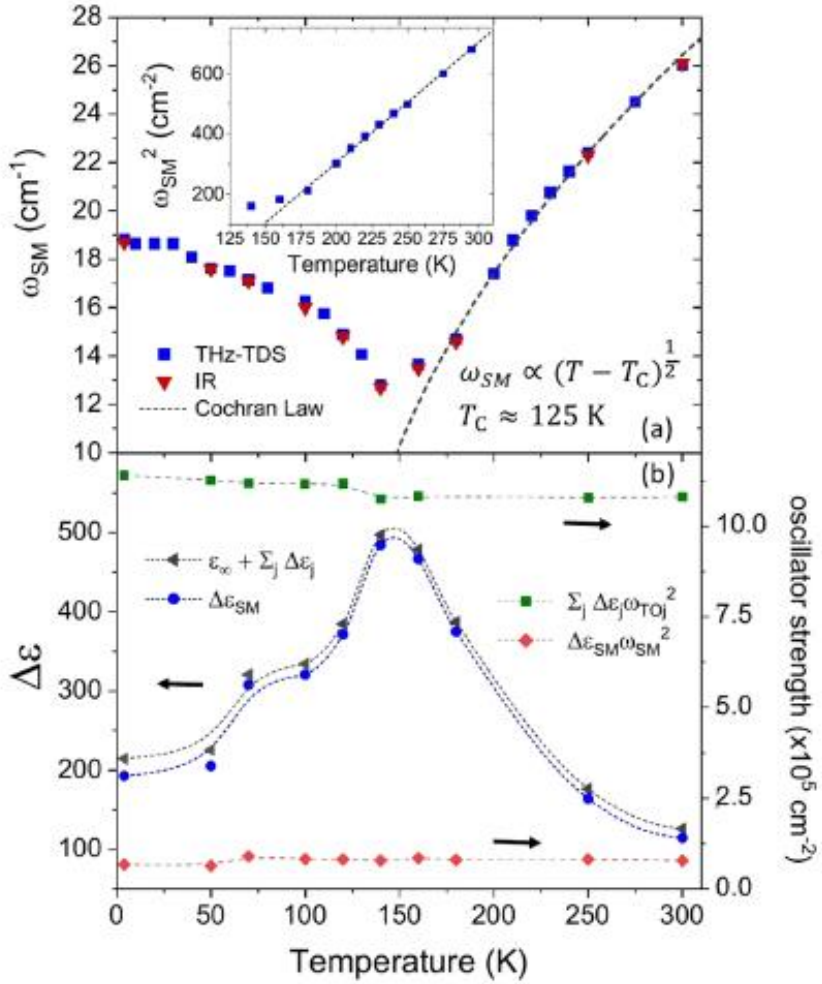




$BiMn_3Cr_4O_{12}$: AFM order induced by ferroelectric phase transition







Two AFM phase transitions (G-type):
Cr^{3+} at 125 K and Mn^{3+} at 48 K.

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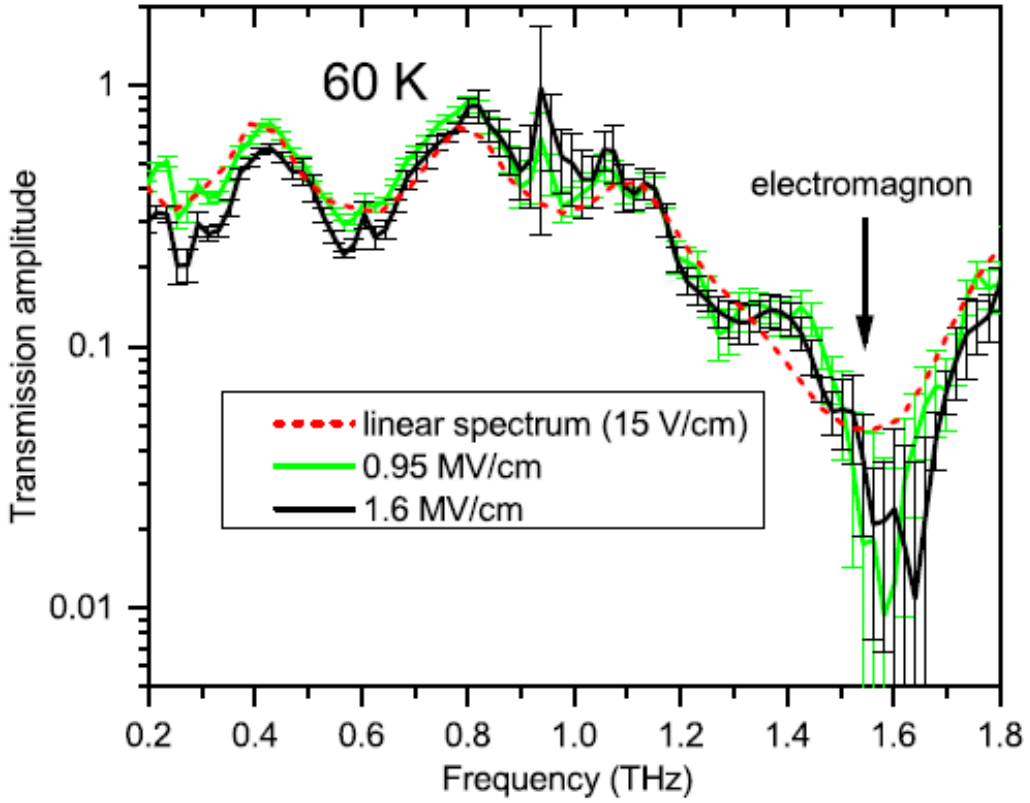
Zhou et al., Adv. Mater. **29**, 1703435 (2017)
A. Maia et al., J. Eur. Ceram. Soc. **43**, 2479 (2023)

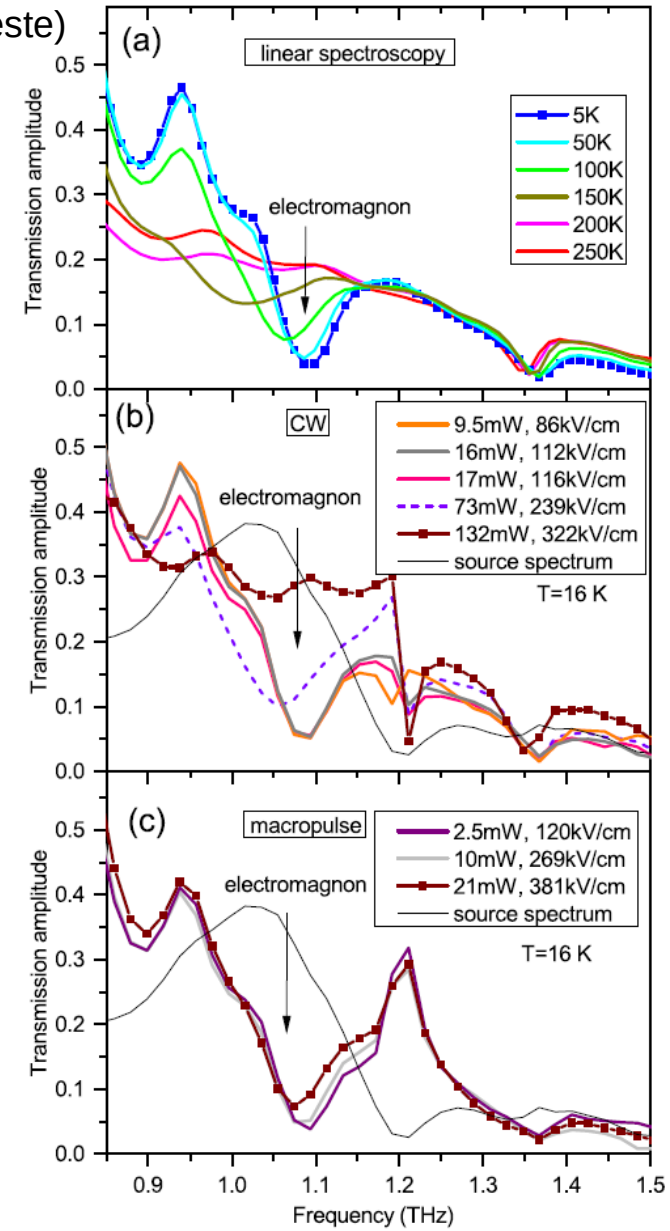
Nonlinear THz absorption by electromagnons in multiferroic Y- and Z-type hexaferrites

Experiments with free-electron lasers at TELBE (HZDR) and TeraFERMI (Trieste)

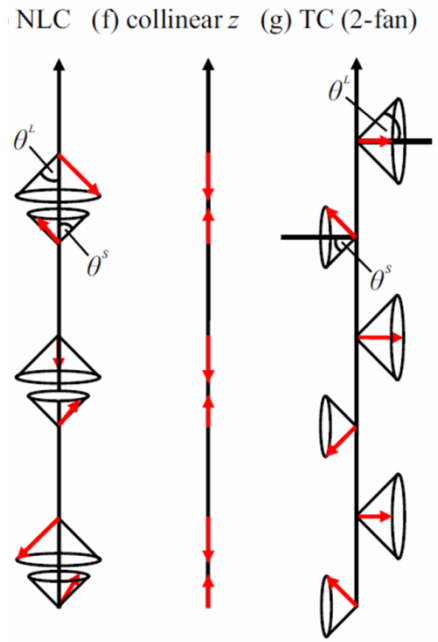
Y-type hexaferrite $BaSrCoZnFe_{11}AlO_{22}$



J. Vít et al., J. Phys. Soc. Jpn. **91**, 104703 (2022)



Z-type hexaferrite $(Ba_xSr_{1-x})_3Co_2Fe_{24}AlO_{41}$



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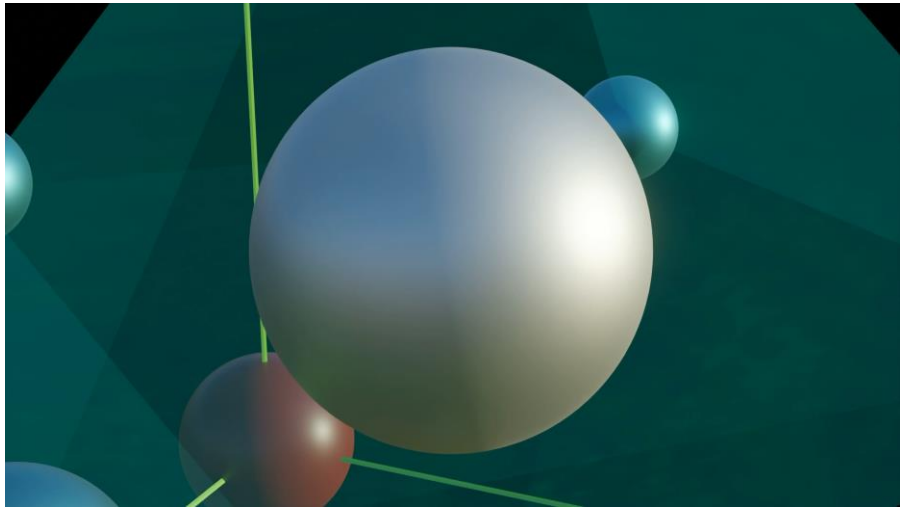
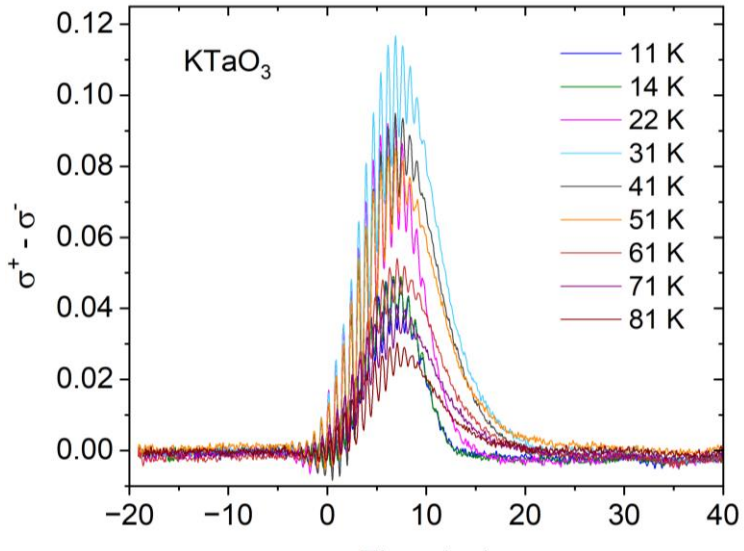
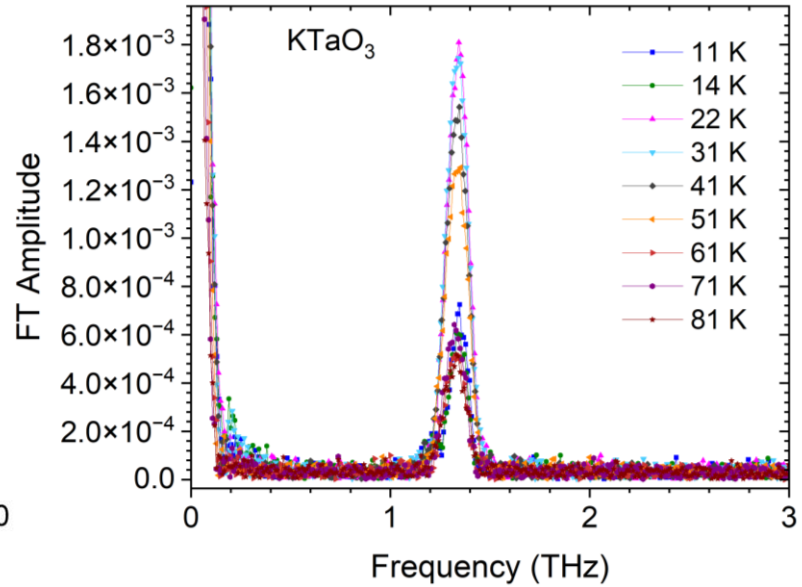
THz-field-induced magnetization and polarization in diamagnetik $KTaO_3$



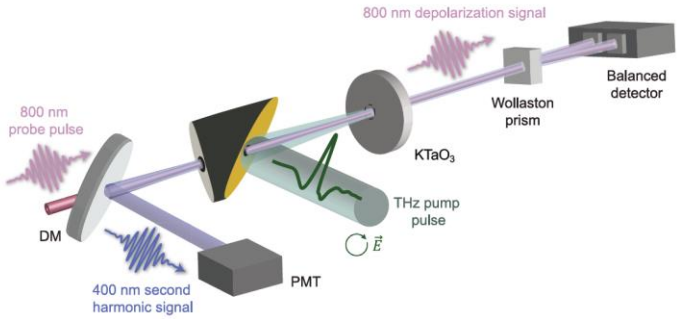


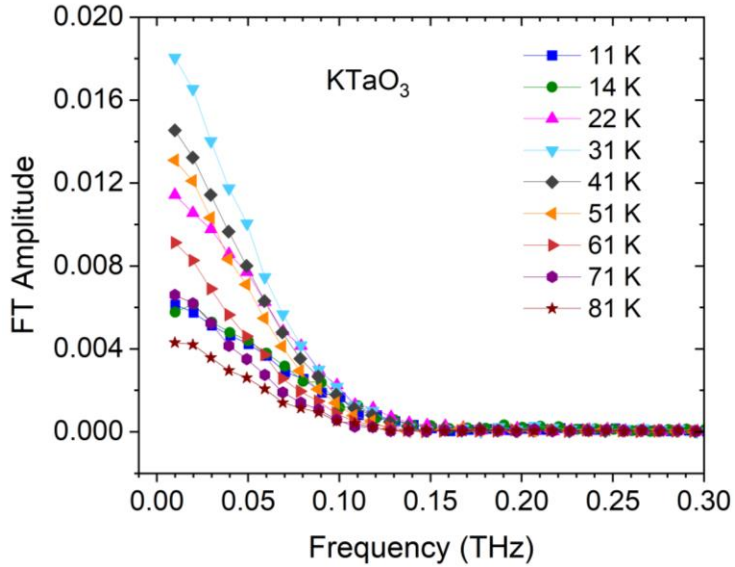


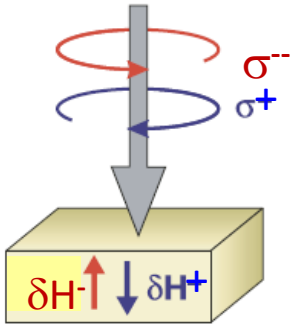
$$\boldsymbol{M}(t) \sim \left[\frac{\omega_+}{2}\sin(\omega_- t + \varphi) - \frac{\omega_-}{2}\sin(\omega_+ t + \varphi)\right] \boldsymbol{A}_1 \boldsymbol{A}_2 z$$

$\omega_- = \omega_1 - \omega_2 = 0$

$\omega_+ = \omega_1 + \omega_2 = 2\omega_{SM}$







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RA5: Magnetic anisotropy and magnetization dynamics in nanostructured strongly correlated magnetic materials and 2D materials

Alexander Shick et al.

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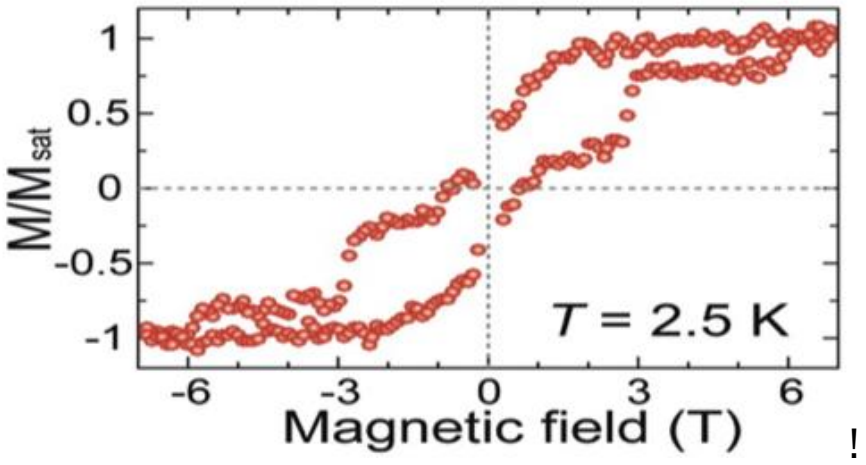
Search for ultra-high density data storage media ~100 Tbit/in^2

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



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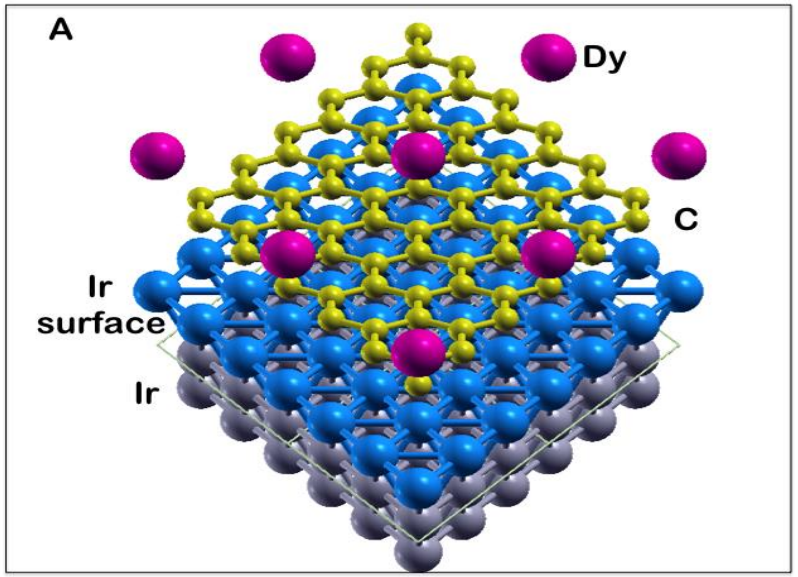
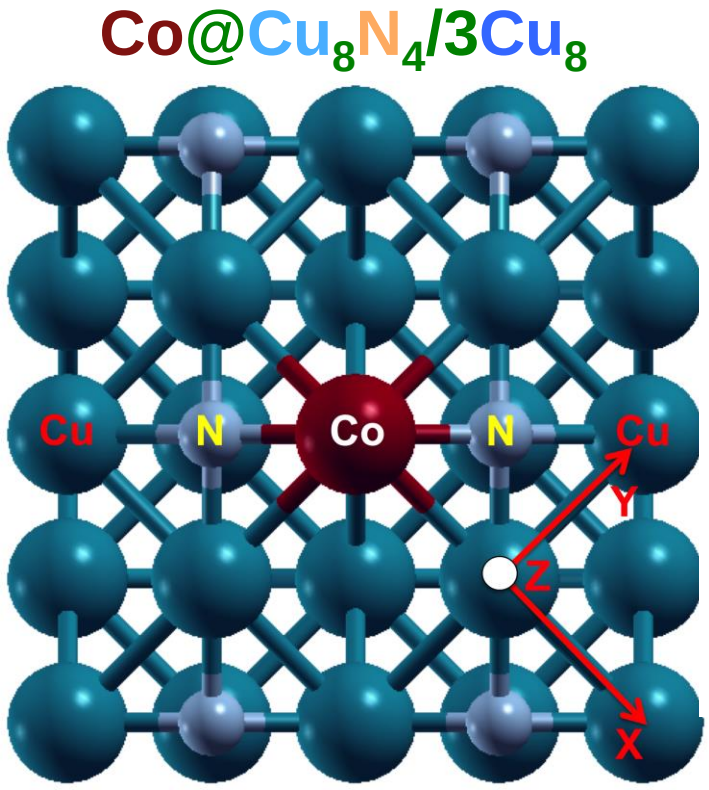


- **Good quantitative agreement with XMCD experimental data**
- **Positive magnetic anisotropy energy (MAE) – out-of-plane *M***

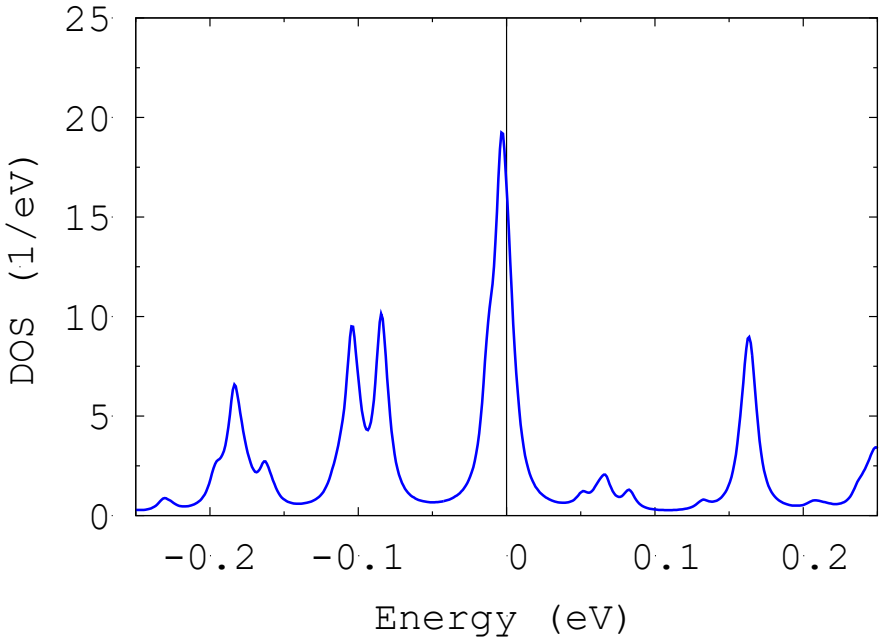
A. B. Shick, J. Kolorenč, A. Yu. Denisov, and D. S. Shapiro, Phys. Rev. B 102, 064402 (2020)

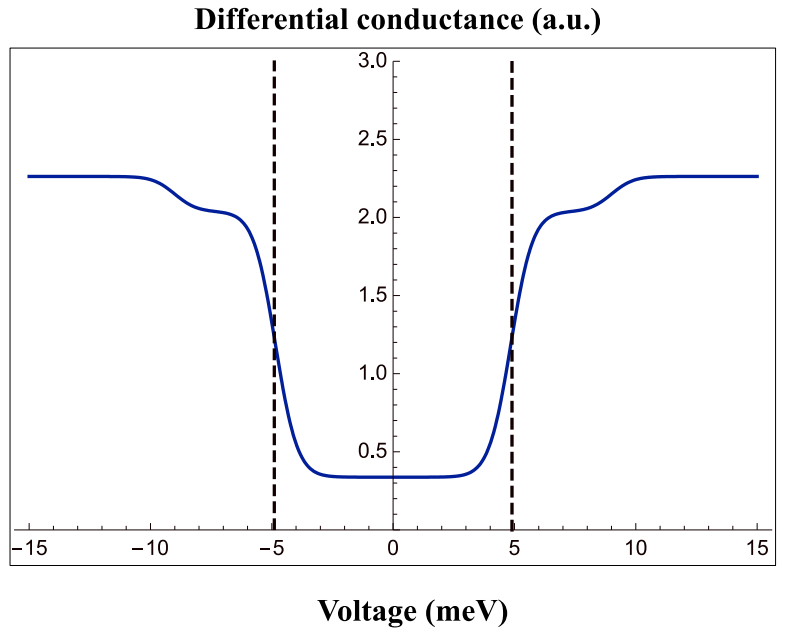
Spin – orbit coupling and Kondo resonance in Co-adatom on Cu_2N/Cu(100) surface

M. Tchaplianka, A. B. Shick and A. I. Lichtenstein, New Journal of Physics 23, 103037 (2021)
A.B. Shick, M. Tchaplianka, and A. I. Lichtenstein, PRB 106, 245115 (2022)



- DFT + Exact Diagonalization of AIM (DFT+ED)





Singlet Ground state + Kondo resonance in DOS
+Steps in differential conductance in agreement with STM/ISTS experiments

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Benefits of Project Solid21 for our Research Teams:

- Two new devices (ALD, THz-SNOM) were acquired which are crucial for the development of our research, i.e. for the preparation of thin films and investigation of charge carrier transport in semiconducting nanostructures.
- New experimental equipment enabled us to strengthen scientific cooperation within the Institute and with foreign countries (EU, USA, Japan etc).
- A total 12 PhD students from Charles University and Czech Technical University were involved in this RP, four of them have already defended their dissertations, the others should finish this year or next year.
- Three international patents on high-voltage water batteries and highly thermally insulating graphene aerogel, one granted, two filed.

Ensuring long-term sustainability and top-quality research in FZU

- Active participation in the submitted project OP JAK TERAFIT for research on altermagnets (submitted by T. Jungwirth).
- Two Marie Skłodowska-Curie grants.
- Support of the Ministry of Education, Youth and Sport of the Czech Republic (CzechNanoLab Research Infrastructure, e-Infrastruktura CZ, MGML).
- A number of our team members are involved in the EU COFUND project.
- A number of ongoing projects at the Czech Science Foundation.
- Many new grants submitted to the Czech Science Foundation.
- Cooperation with industry - e.g. Noliac (piezoceramics) and T-Ceram.

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Thank you for your attention!