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)

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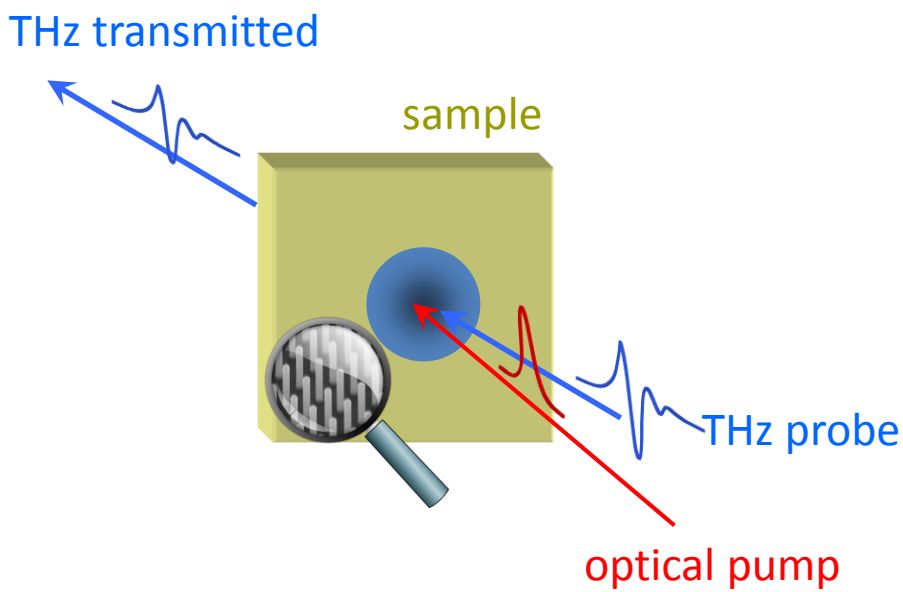
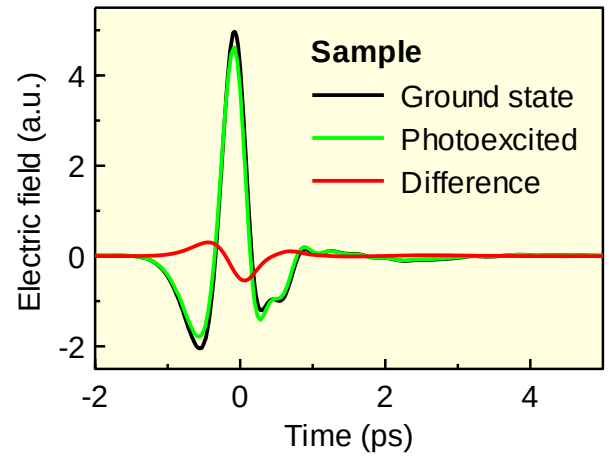
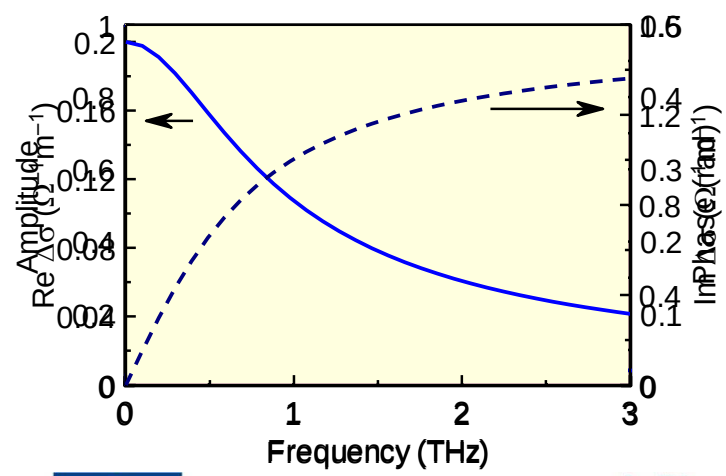
RA1: Far-field THz measurements





transient conductivity: $\Delta\sigma \propto \frac{\Delta E_t}{E_t}$



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

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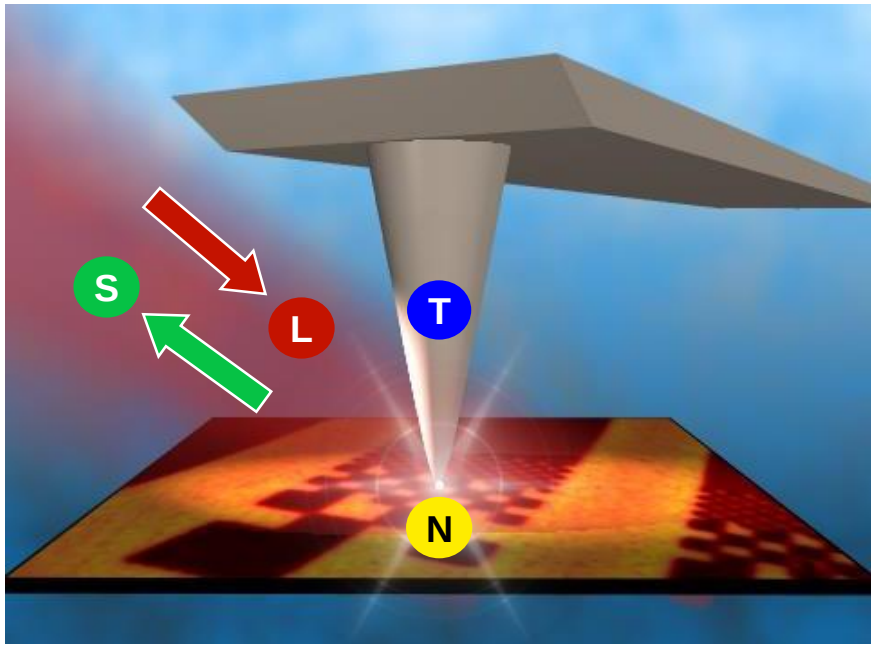
RA1: Near-field (SNOM) measurements

- 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)

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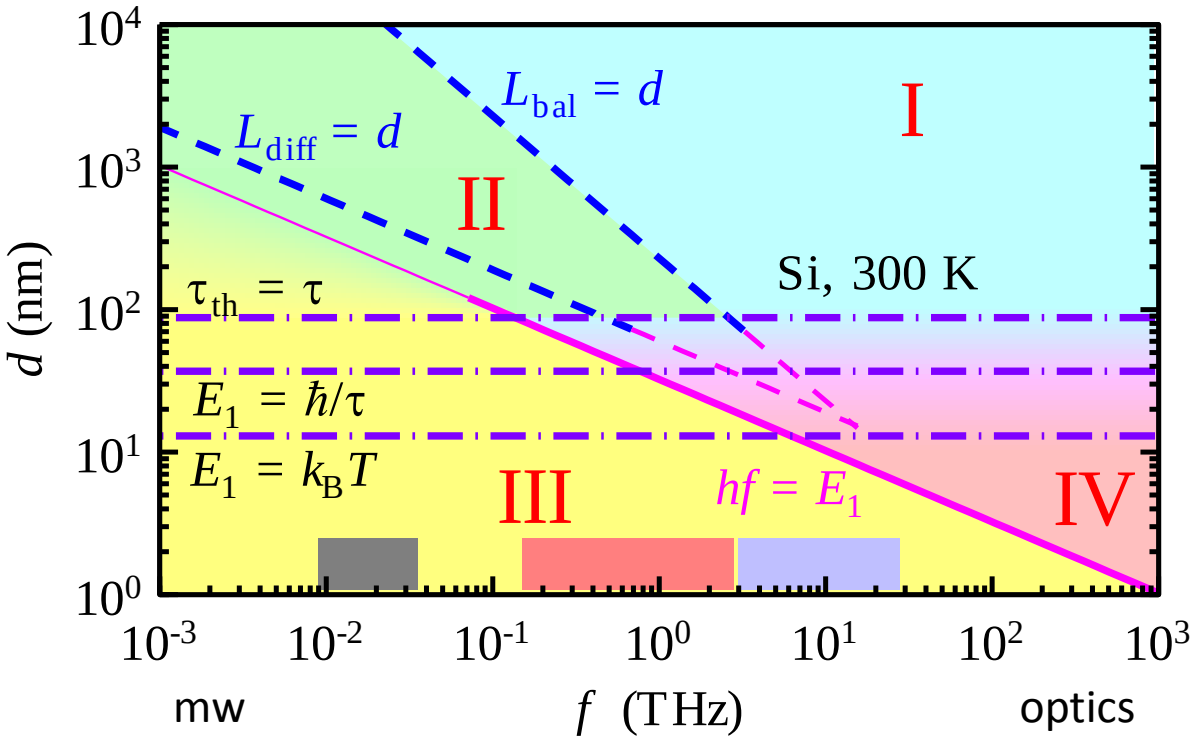
Conductivity: response to the local field



Important features:

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

P. Kužel and H. Němec, Adv. Opt. Mater. **7**, 365301 (2019)

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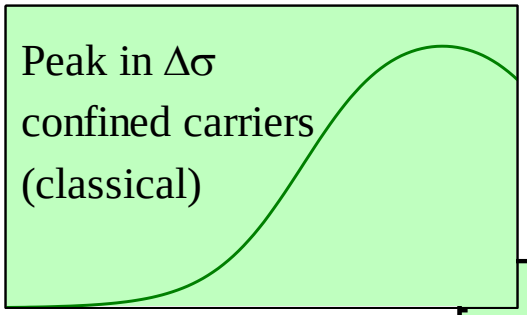
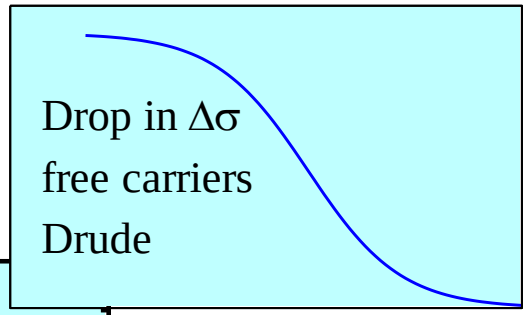
Conductivity: response to the local field

Peak in Δσ
confined carriers
(classical)

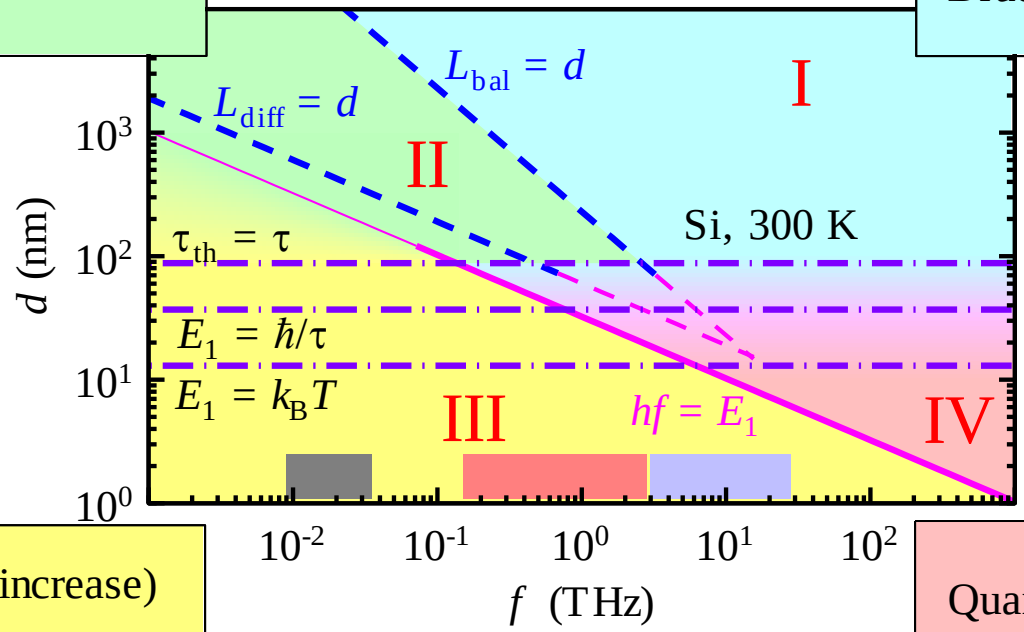


H. Němec et al.,
PRB 79, 115309 (2009)

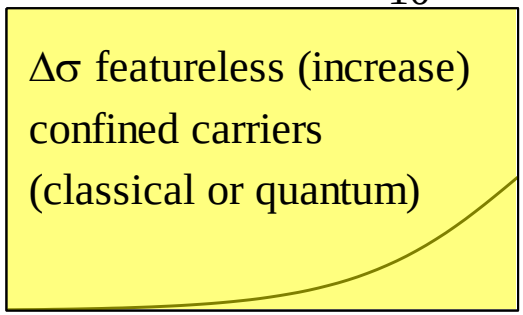
Drop in Δσ
free carriers
Drude



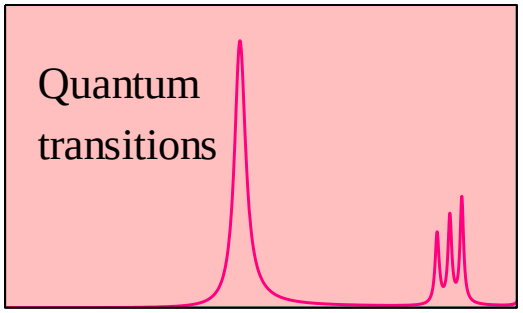
P. Drude, Ann. Phys. 1900



Δσ featureless (increase)
confined carriers
(classical or quantum)



Quantum
transitions



P. Kužel and H. Němec, Adv. Opt. Mater. **7**, 365301 (2019)

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

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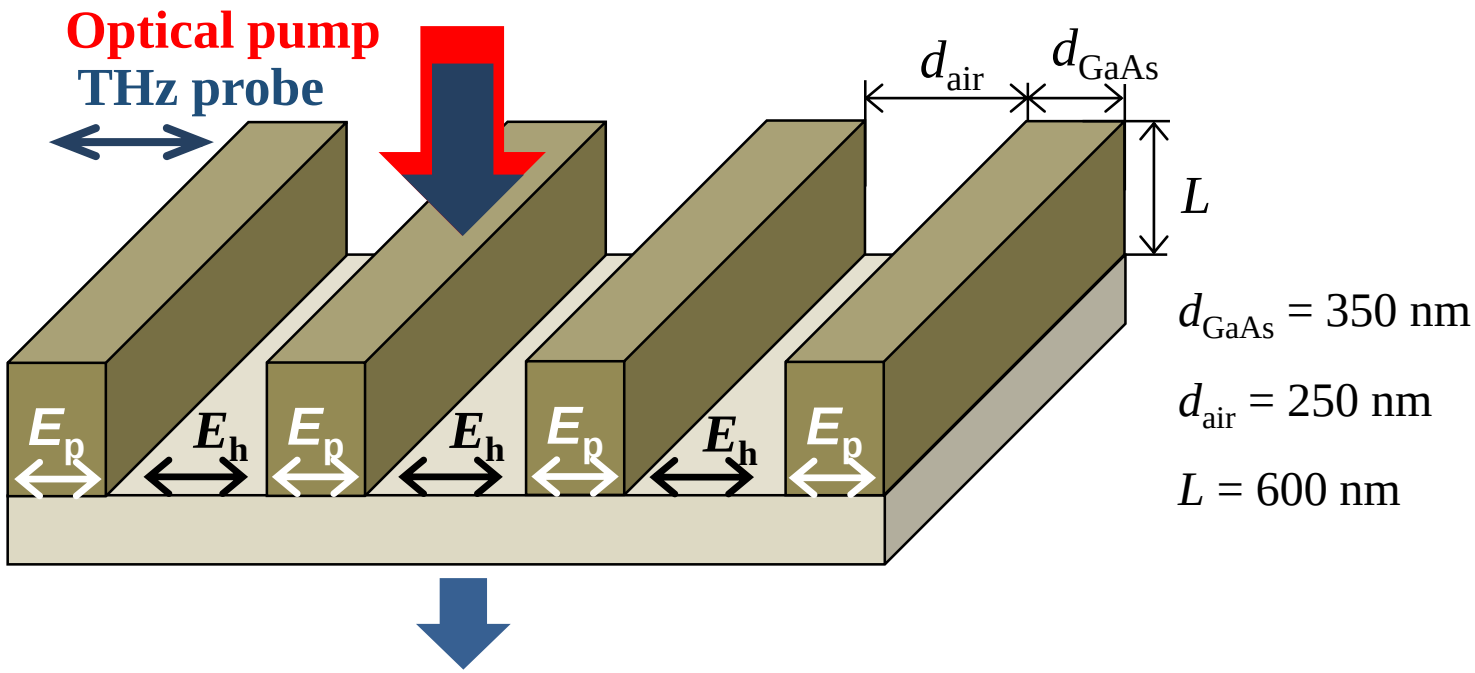
Towards ordered (or uniform) nanostructures

- 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)

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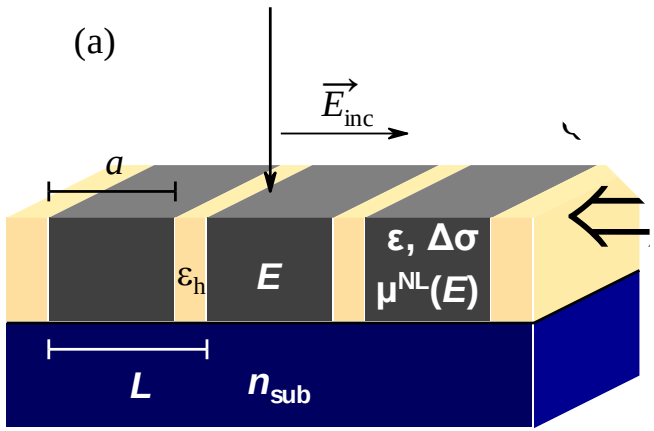
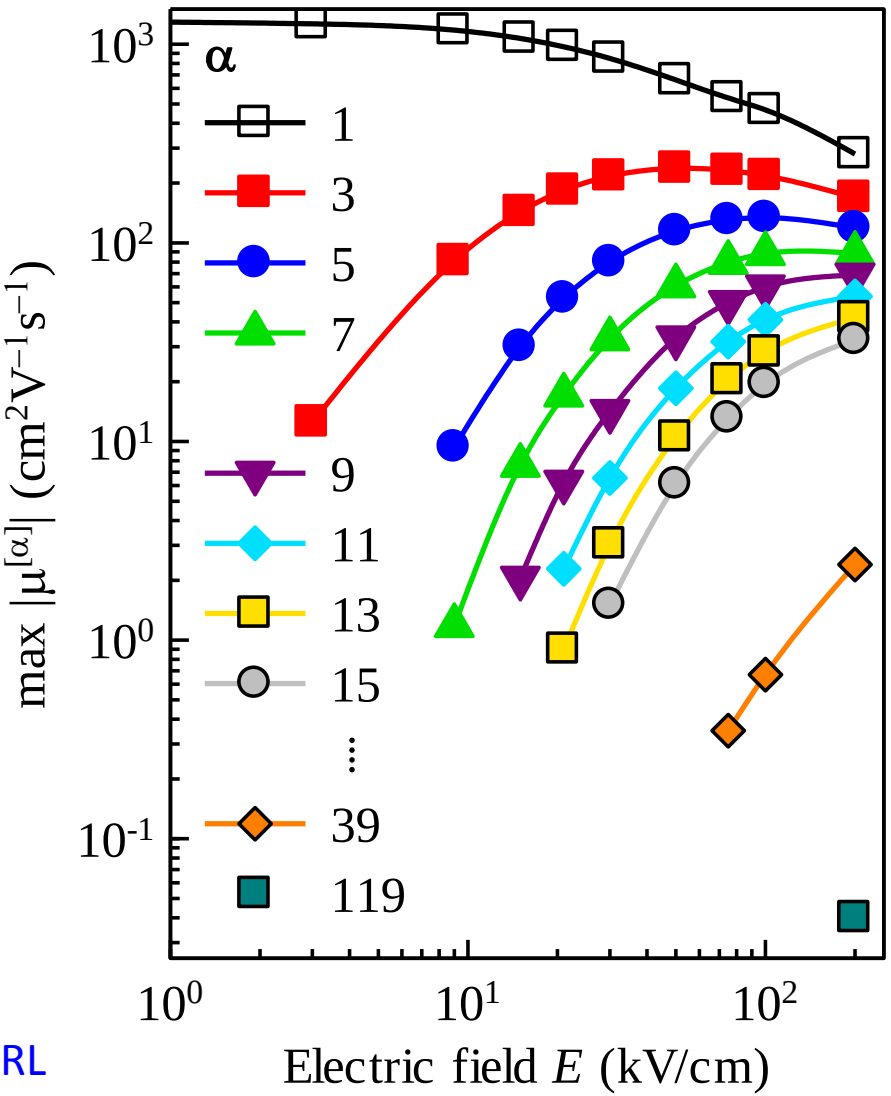
Nonlinear response (to local E) of GaAs nanobars



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



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

J. Kuchařík and H. Němec, submitted to PRL

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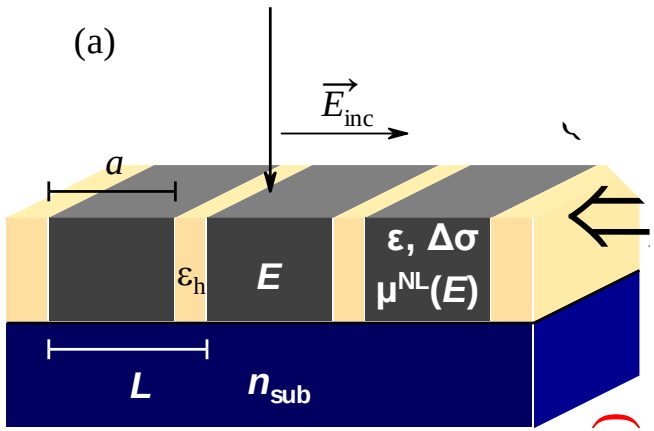
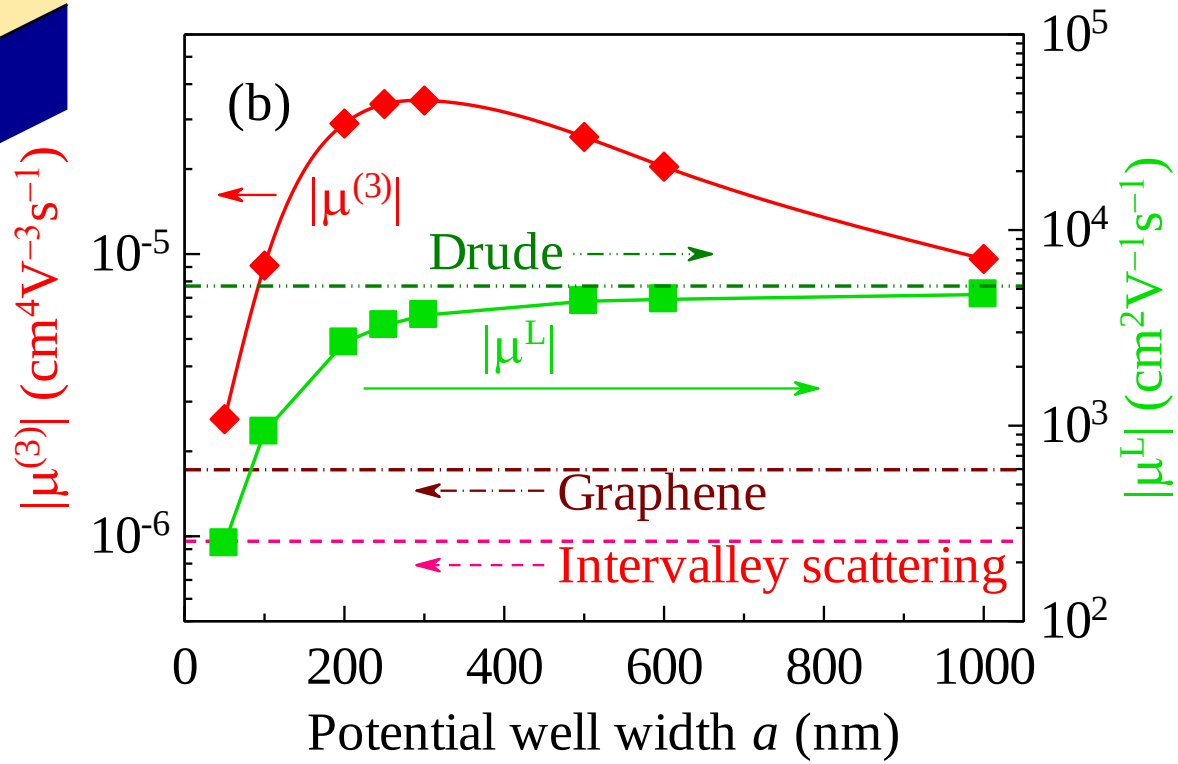
Nonlinear response (to local E) of GaAs nanobars



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

mobility at 0.5 THz:



$a \approx$ 0-1000 nm
GaAs:
m = 0.07
τ = 270 fs

Intervalley scattering: J. Hebling et al., Phys. Rev. B **81**, 035201 (2010).
Graphene: H. A. Hafez, et al., Nature **561**, 507 (2018).

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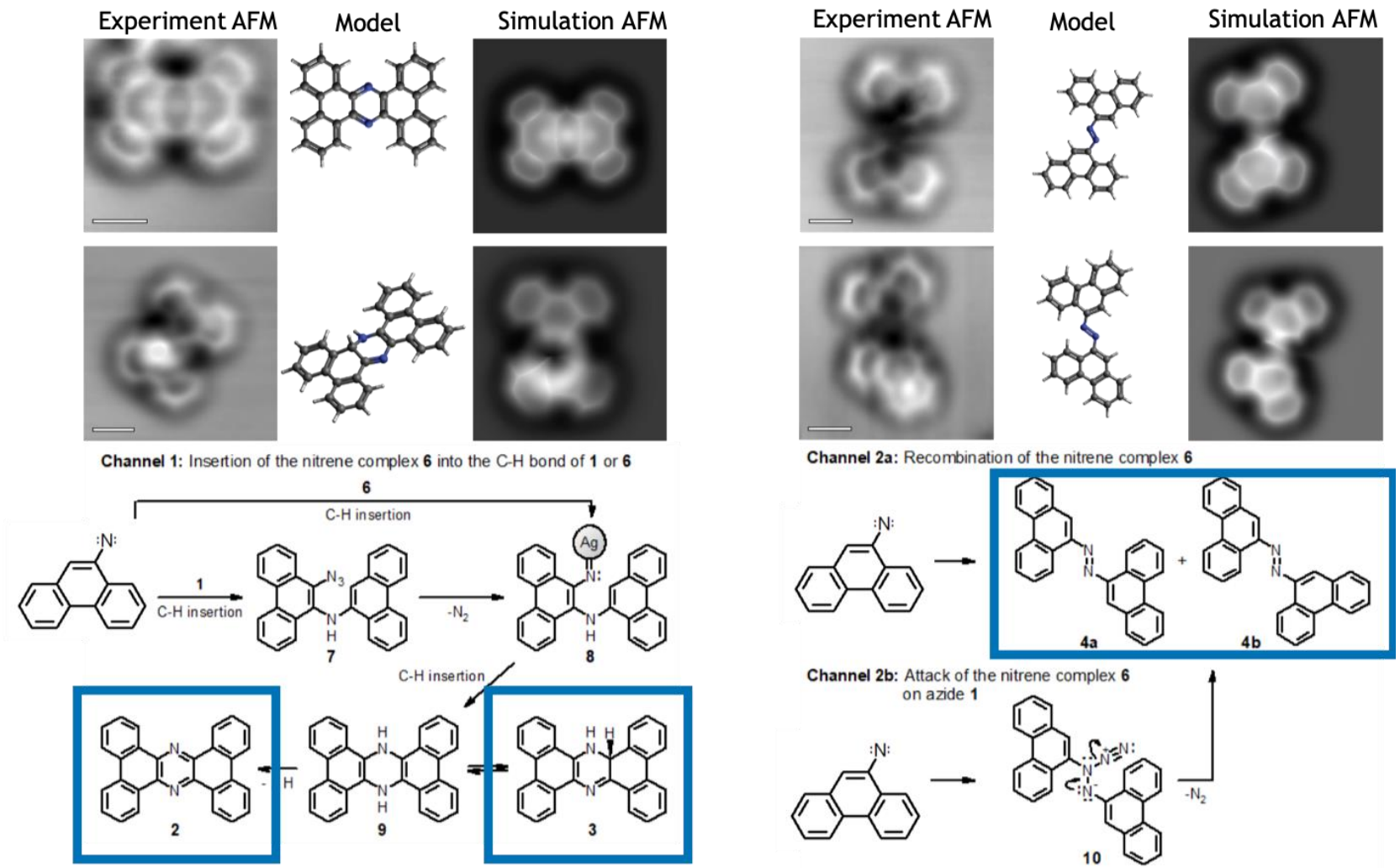
RA2: On-surface synthesis of nitride complexes



J. Hellerstedt et al, Angew. Chem. Int. Ed. ***58*** *(2019) 2266*

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.

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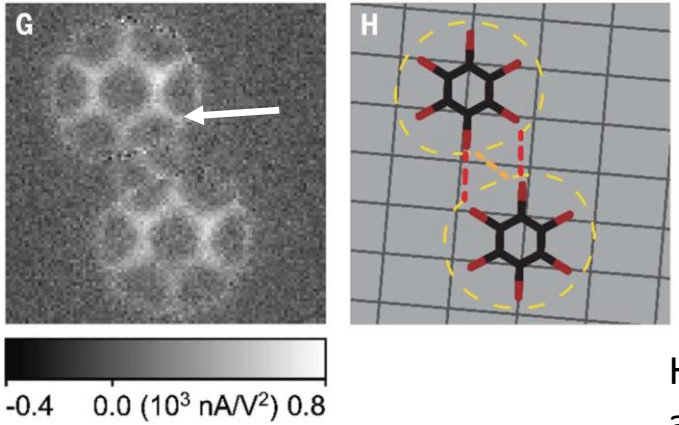
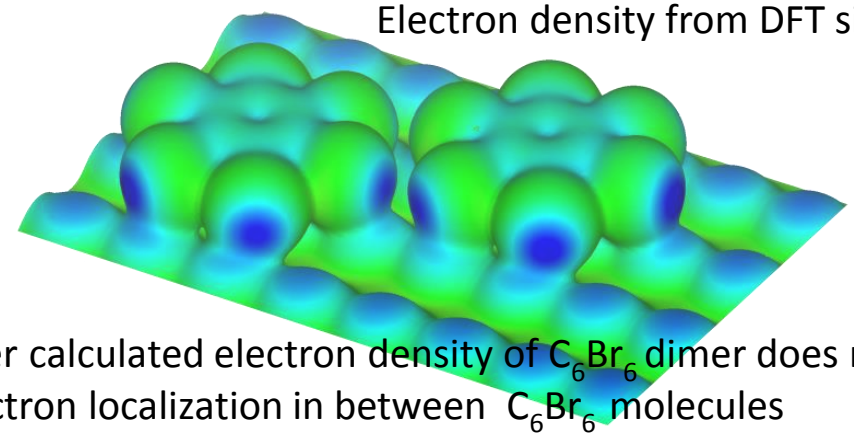
RA2: Can we indeed image non-covalent bonds in SPM ?

Several groups claimed to visualize weak non-covalent (hydrogen, halogen) bonds via appearance of sharp edges in SPM images, see e.g. C_6Br_6 dimer *Zh. Han et al. Science 358,260 (2017).*

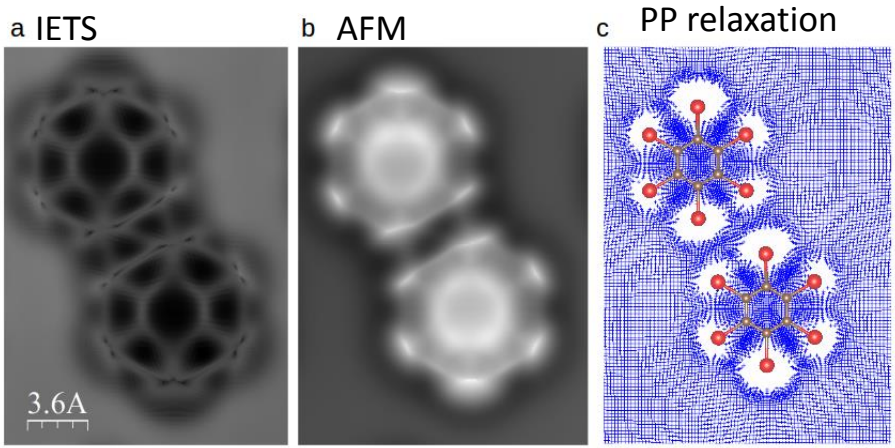


Electron density from DFT simulations



However calculated electron density of C_6Br_6 dimer does not show any electron localization in between C_6Br_6 molecules

SPM simulations with a home-built toolkit of the C_6Br_6 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 **cannot be ascribed to real bonds**.

A. Gallardo, et al. JPCC ***123****, 8379 (2019)*

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RA3: Catalyst-induced doping of Si nanowires

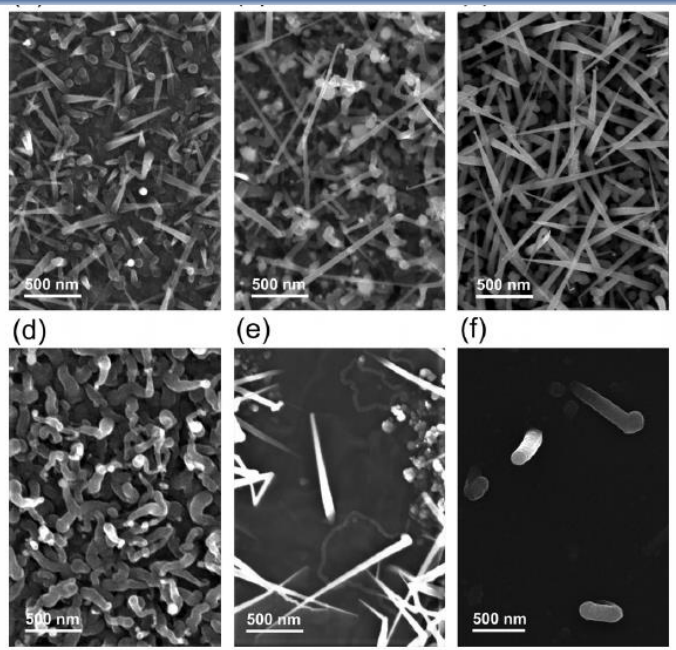

FIG. 1. SEM micrographs of SiNWs catalyzed by different metals: (a) Au, (b) In, (c) Sn, (d) Bi, (e) Pb, and (f) Ga.

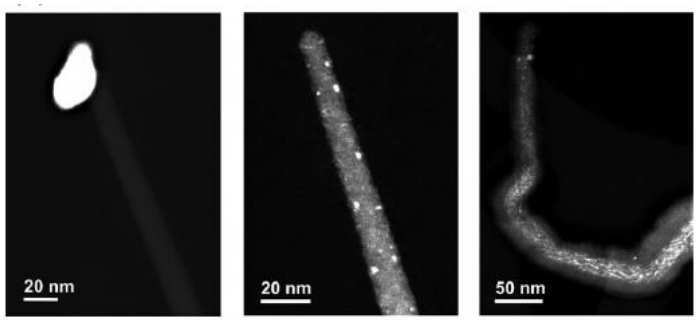

FIG. 2. HAADF imaging in STEM showing the distribution of metal clusters in (a) In-, (b) Sn-, and (c) Bi-catalyzed SiNWs. The bright contrast areas in the images highlight the catalytic metal atoms due to their higher atomic (Z) number than Si.

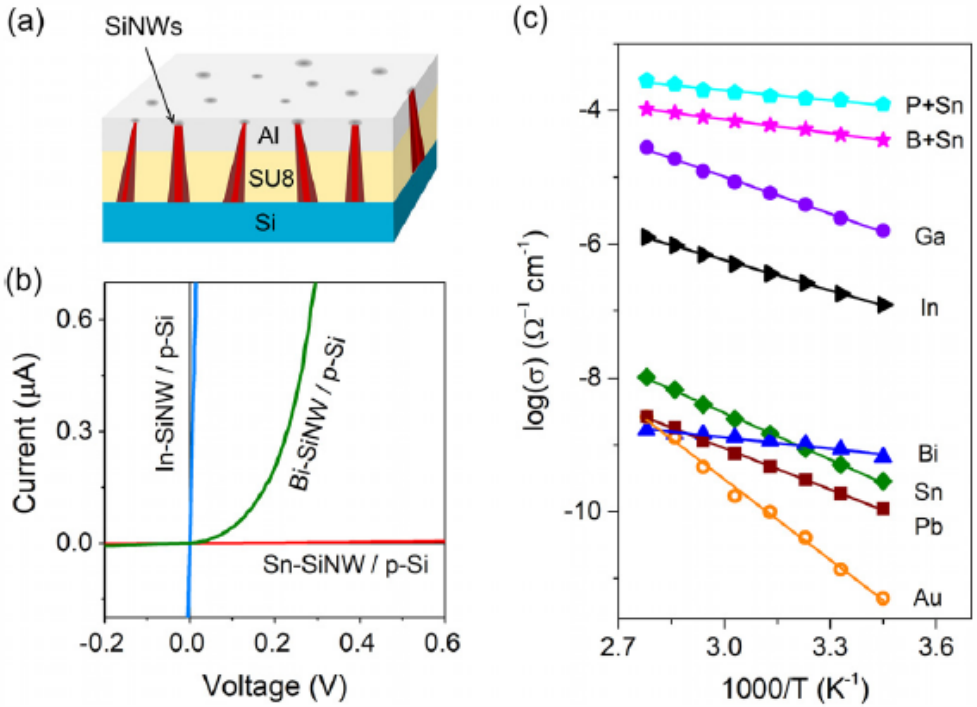

FIG. 3. Schematic picture of a SiNW-based electrical device. (a) Schematic image of a SiNW device using an array of SiNWs embedded in a dielectric SU8 epoxy layer which is sandwiched in between a Si substrate (n-type or p-type doped) and a top Al contact. (b) Current-voltage characteristics of Sn-catalyzed 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 at al. APL 114, 132103 (2019)

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RA3: 3D graphen superstrings

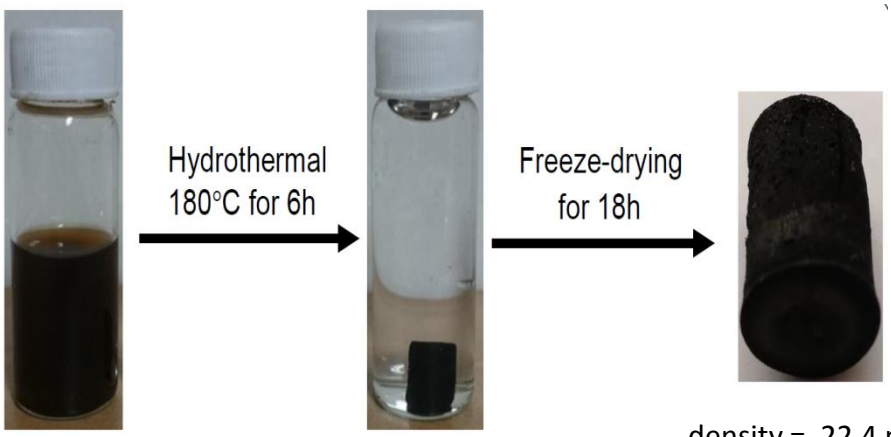
Fabrication of 3D graphene aerogels

1. Hydrothermal reduction of graphene oxide

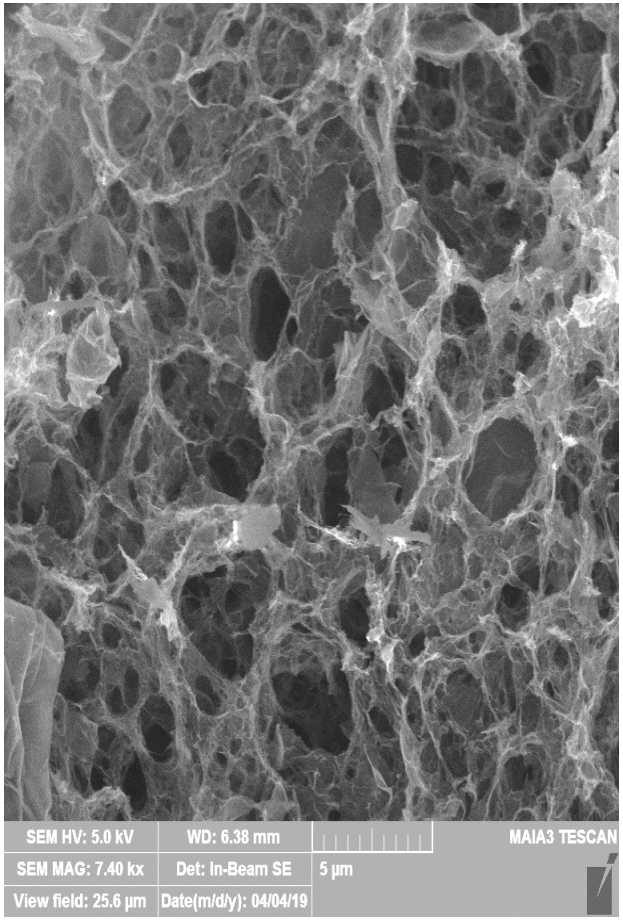
- Self assembly of reduced graphene oxide
- Chemical coupling of individual graphene sheets
- Reduced 3D graphene contains oxygen groups

2. High-temperature annealing at 1300 °C

- Oxygen and defect removal
- Fabrication of free-standing 3D graphene aerogels



density = 22.4 mg/cm^{-3}



Šilhavík et al., manuscript in preparation

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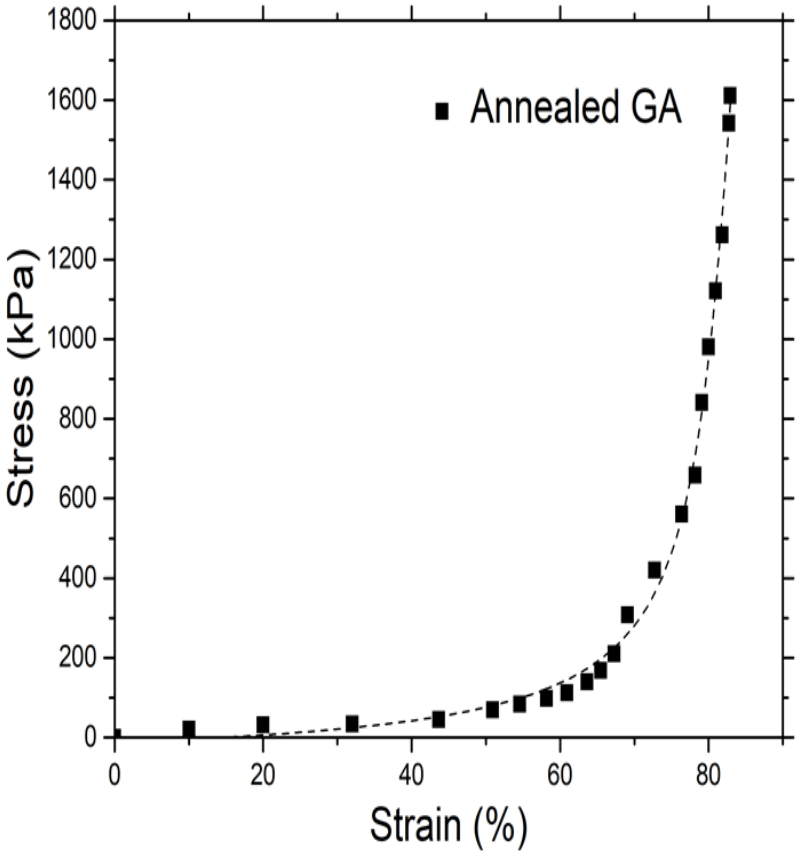
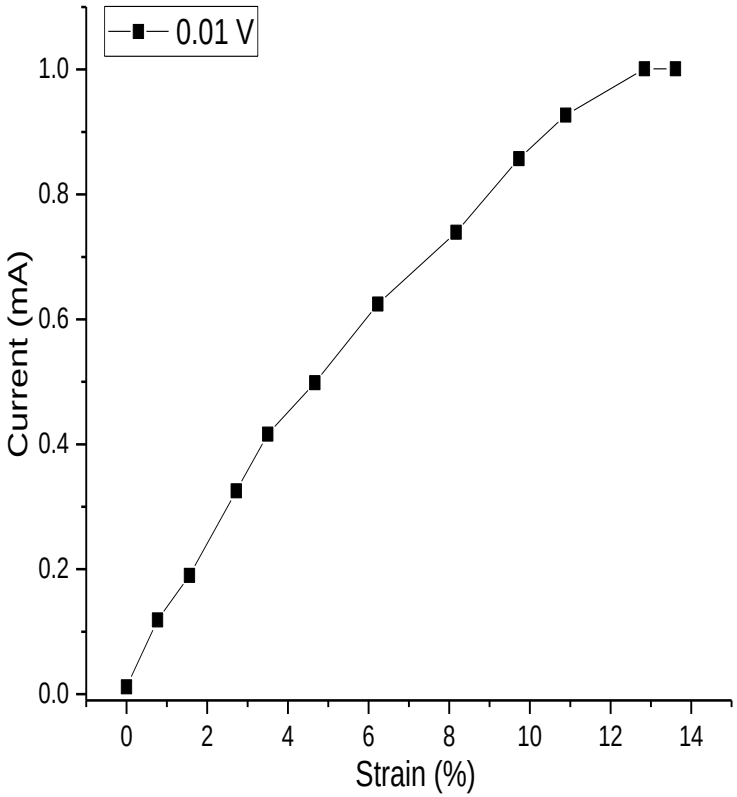
RA3: 3D graphen superstrings

Compression of 3D graphene aerogels





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

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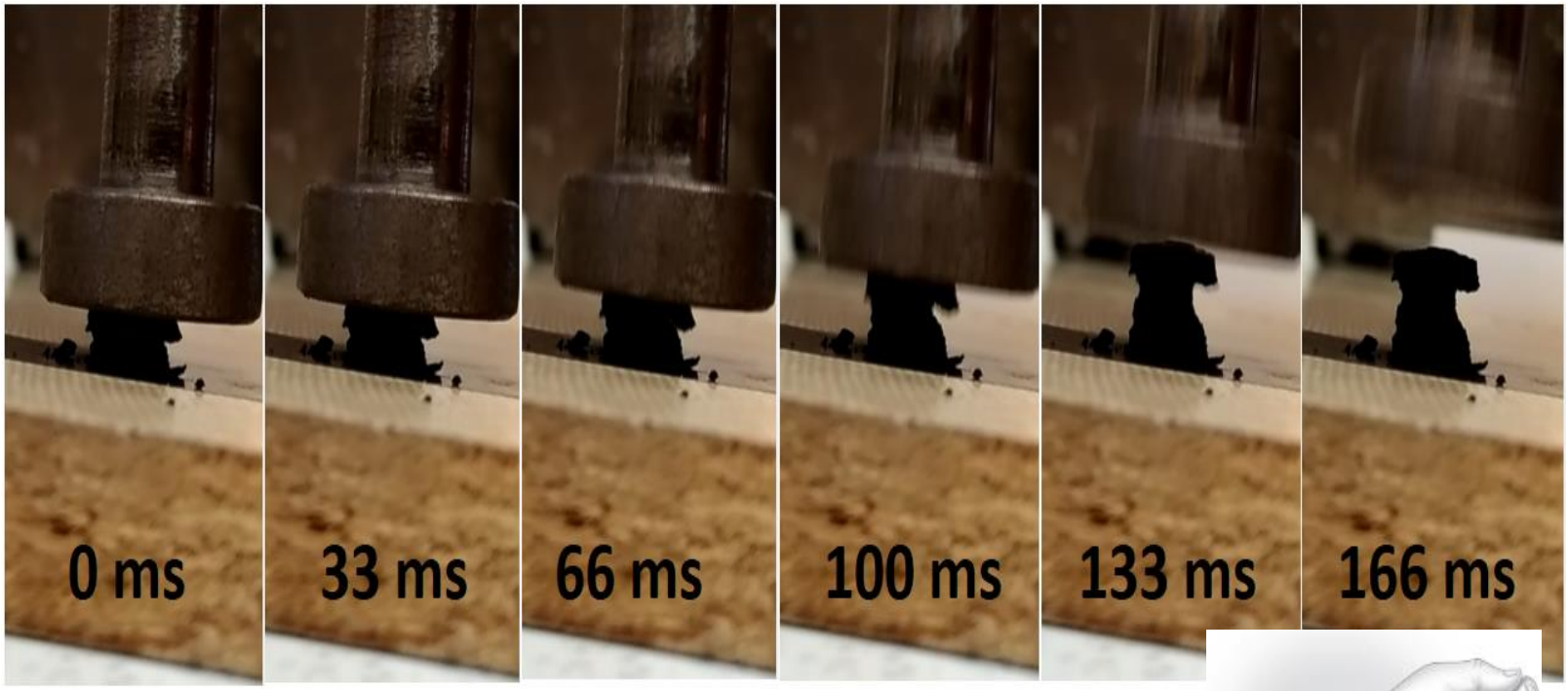
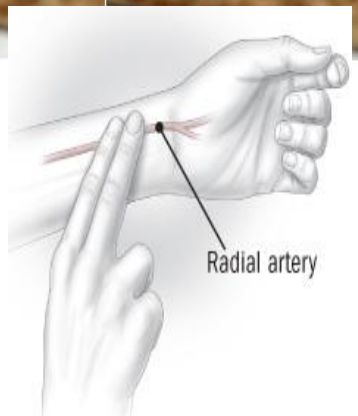
RA3: 3D graphen superstrings

3D Graphene Superelastic Spring



Fast response < 1 ms

Application: Electromechanical heart rate measurement



Šilhavík et al., manuscript in preparation

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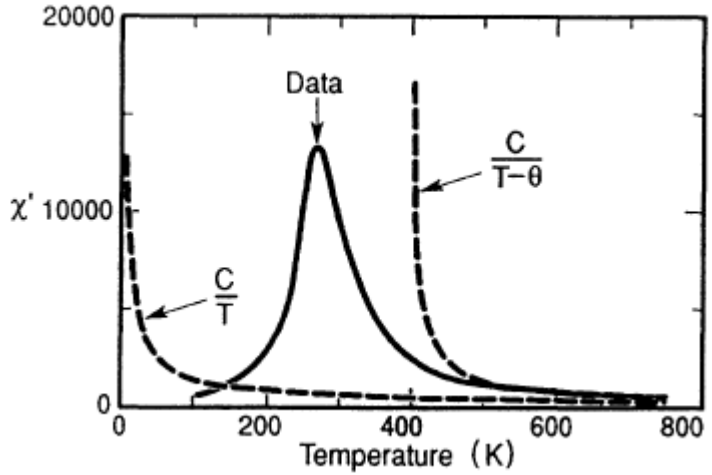
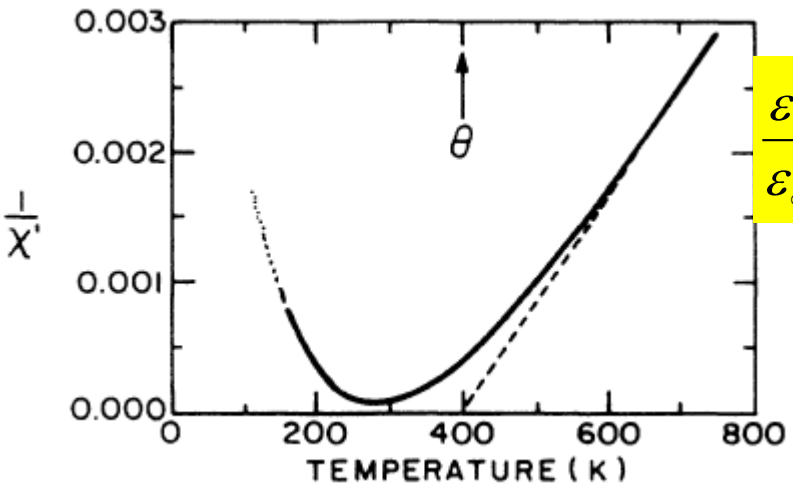
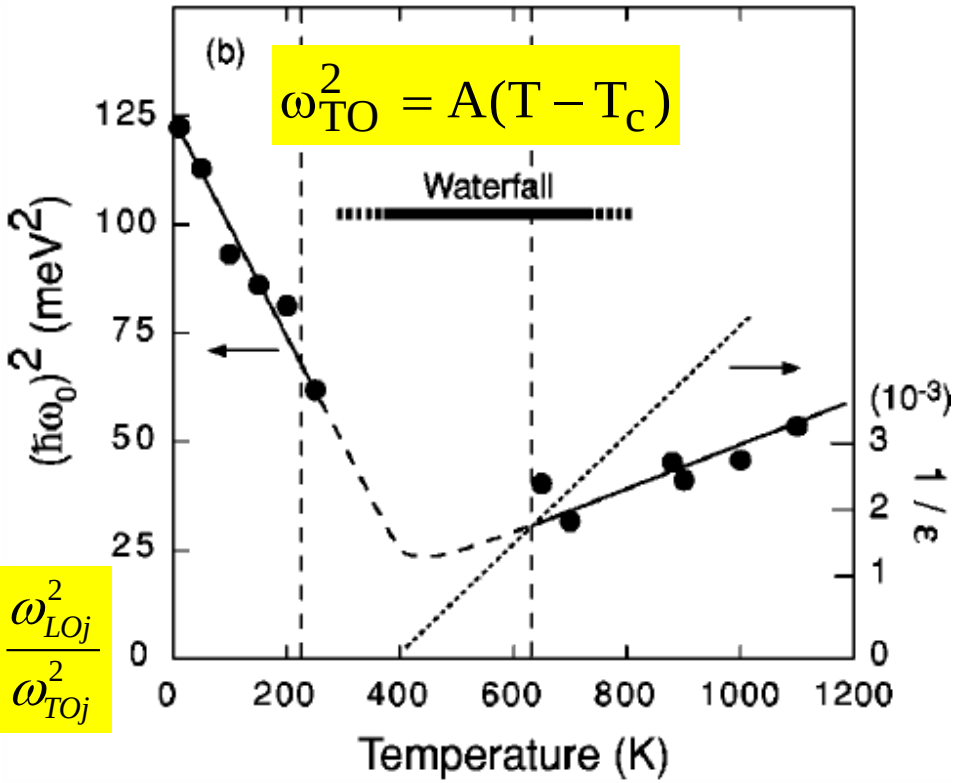
RA4: Curie-Weiss law and soft phonon behavior in relaxor feroelectrics

Viehland *et al.* PRB **46**, 8003 (1992)





$$\frac{\varepsilon_0}{\varepsilon_\infty} = \prod_j \frac{\omega_{LOj}^2}{\omega_{TOj}^2}$$



Wakimoto *et al.* PRB **298**, 224102, (2002)

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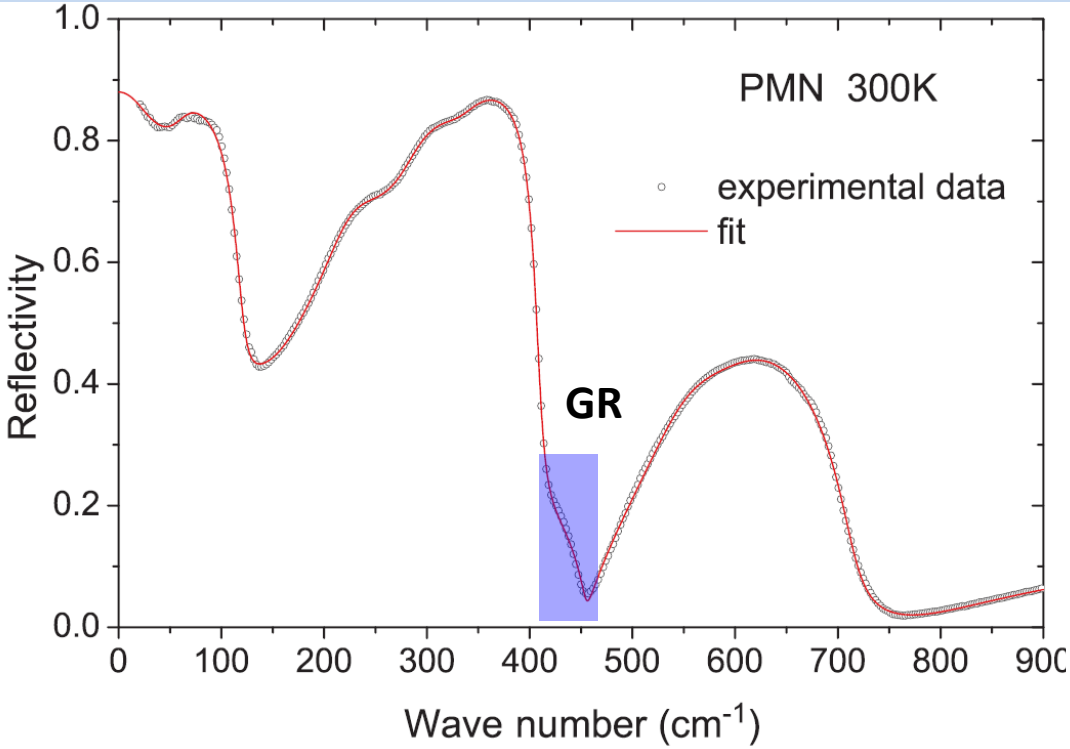
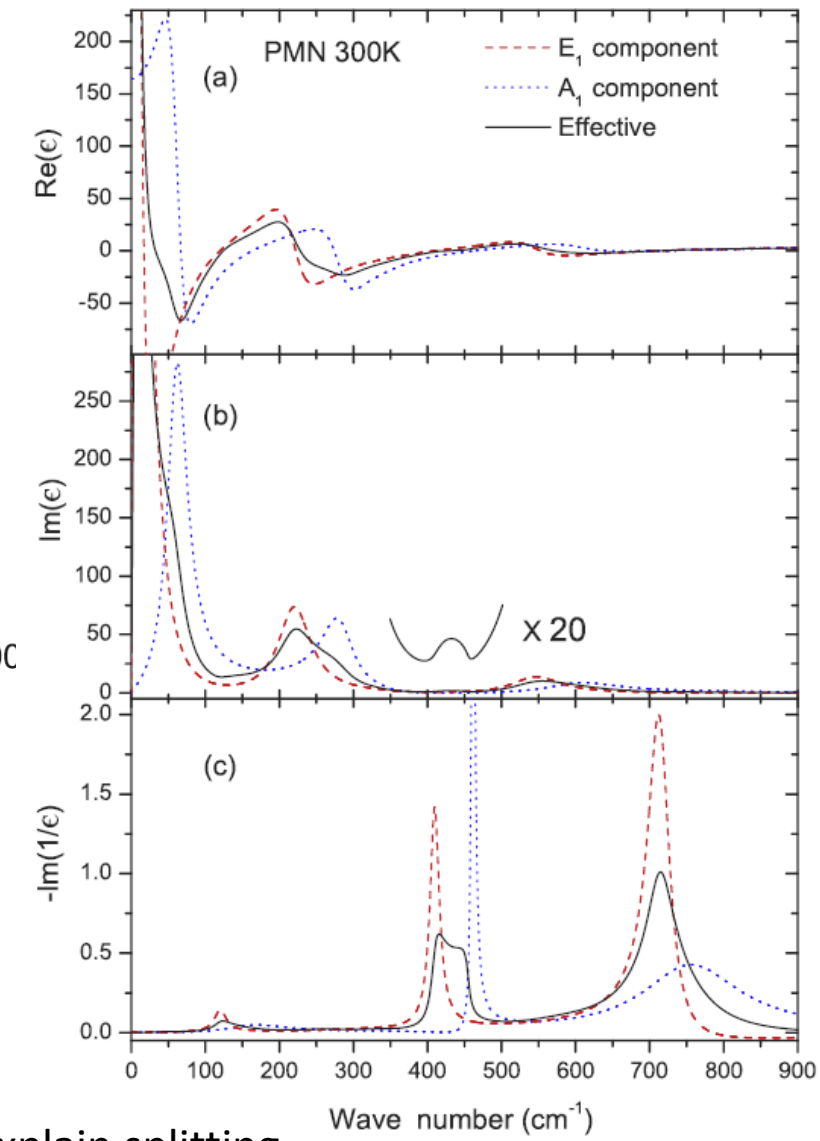
EMA: $Pb(Mg_{1/3}Nb_{2/3})O_3$ at room temperature





$$\frac{2}{3}\frac{\epsilon_\perp - \epsilon_{\rm eff}}{\epsilon_\perp + 2\epsilon_{\rm eff}} + \frac{1}{3}\frac{\epsilon_\parallel - \epsilon_{\rm eff}}{\epsilon_\parallel + 2\epsilon_{\rm eff}} = 0$$

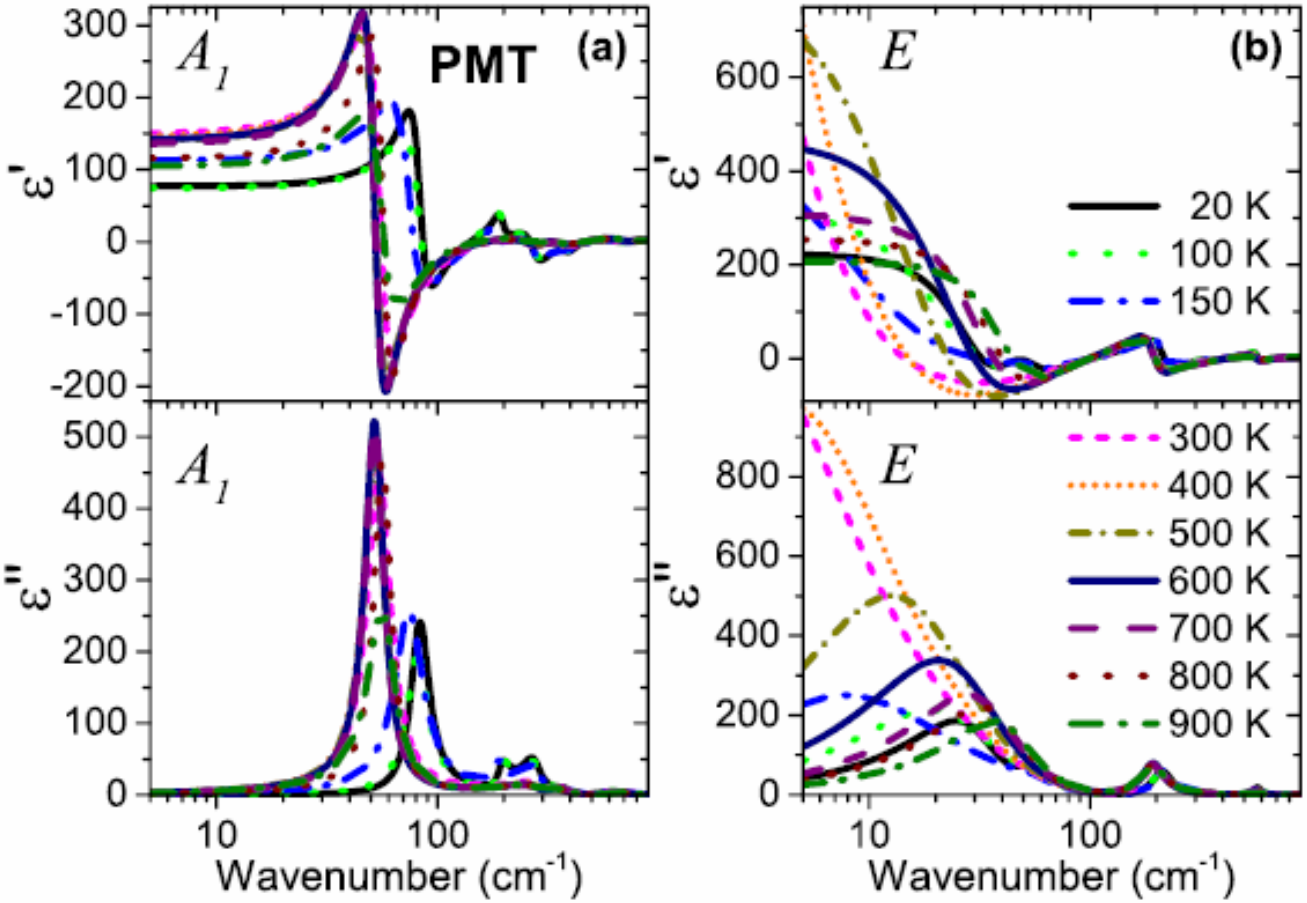
$$\epsilon_\parallel = \epsilon_{\parallel,\infty}\prod_{j=1}^{3}\frac{(\omega^2_{{\rm A}_1,{\rm LO}j} - \omega^2 - i\omega\gamma_{{\rm A}_1,{\rm LO}j})}{(\omega^2_{{\rm A}_1,{\rm TO}j} - \omega^2 - i\omega\gamma_{{\rm A}_1,{\rm TO}j})}$$

$$R = \left|\frac{\sqrt{\epsilon_{\rm eff}} - 1}{\sqrt{\epsilon_{\rm eff}} + 1}\right|^2$$

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)

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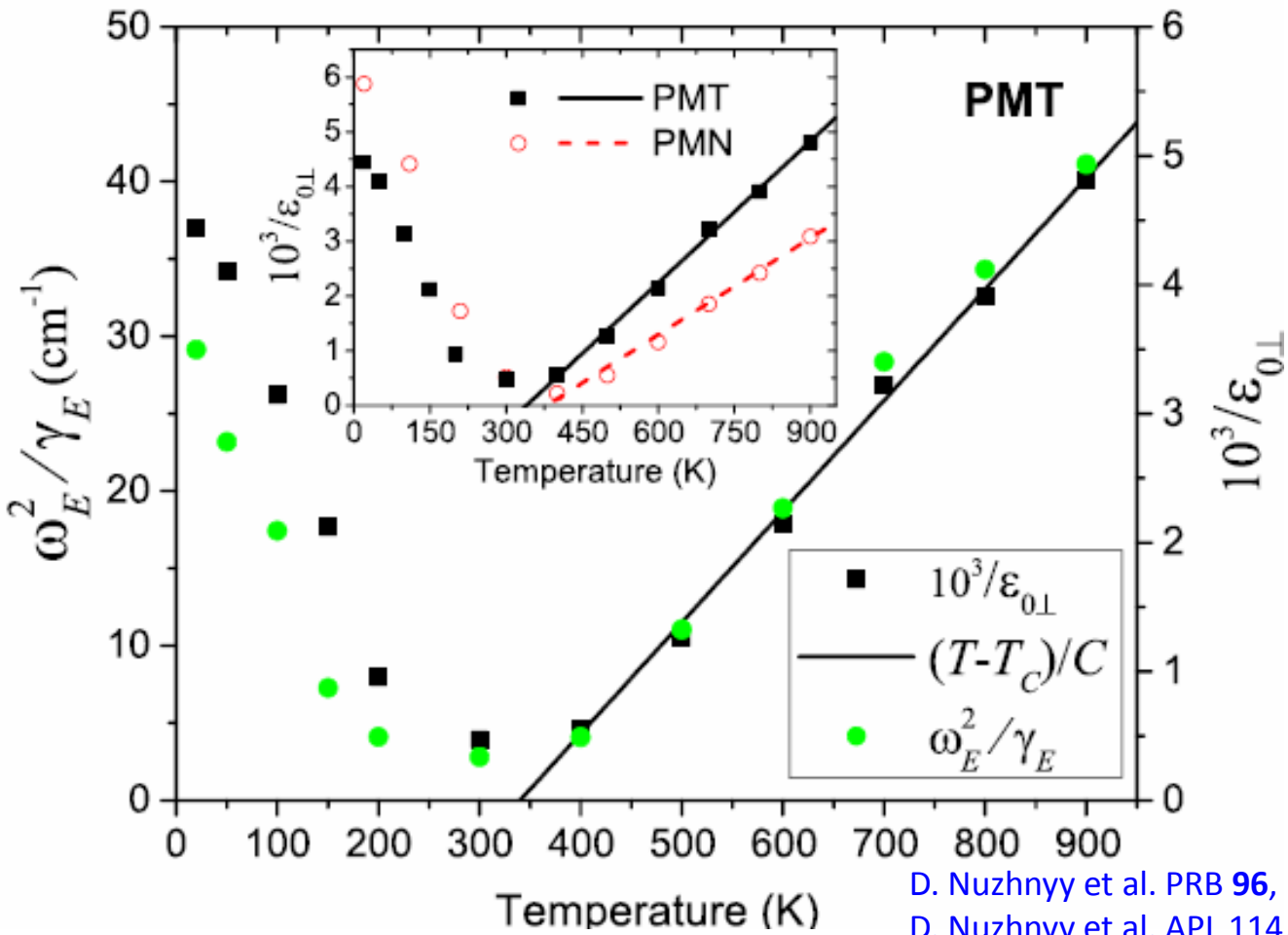
MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY

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)

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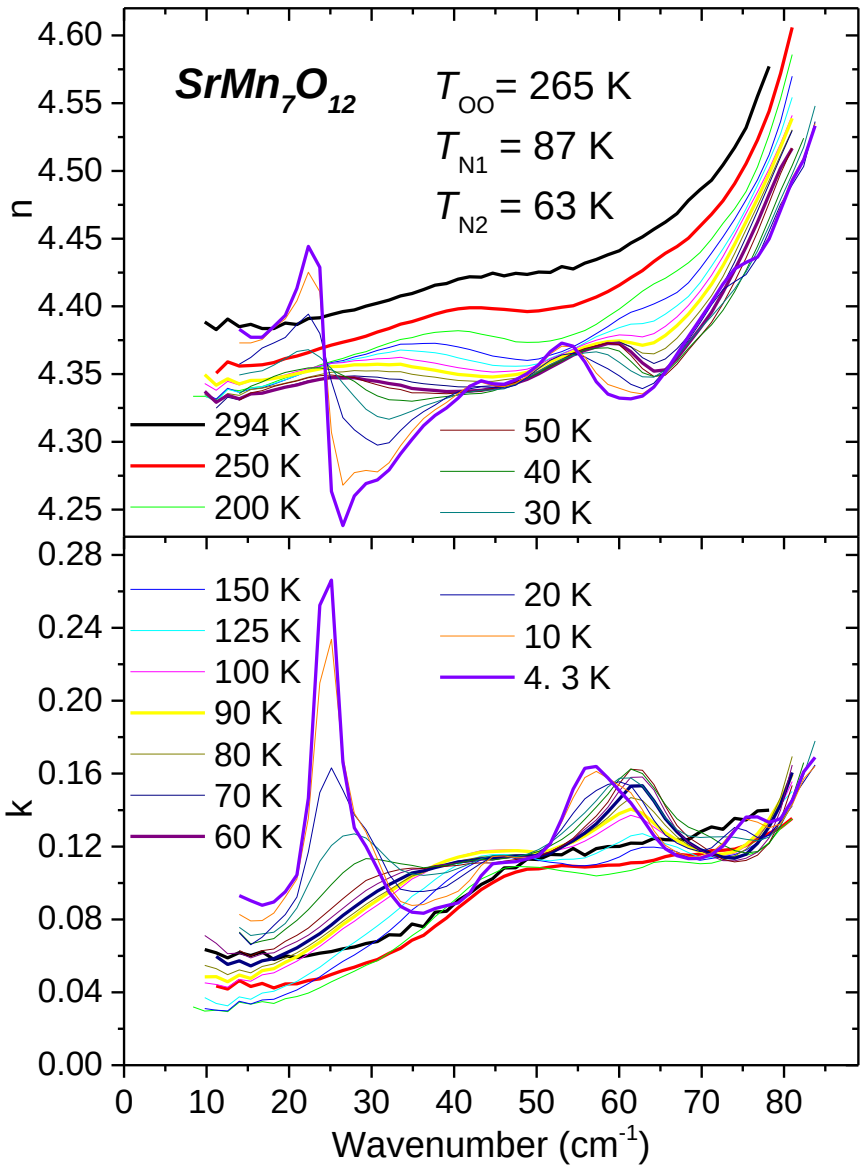
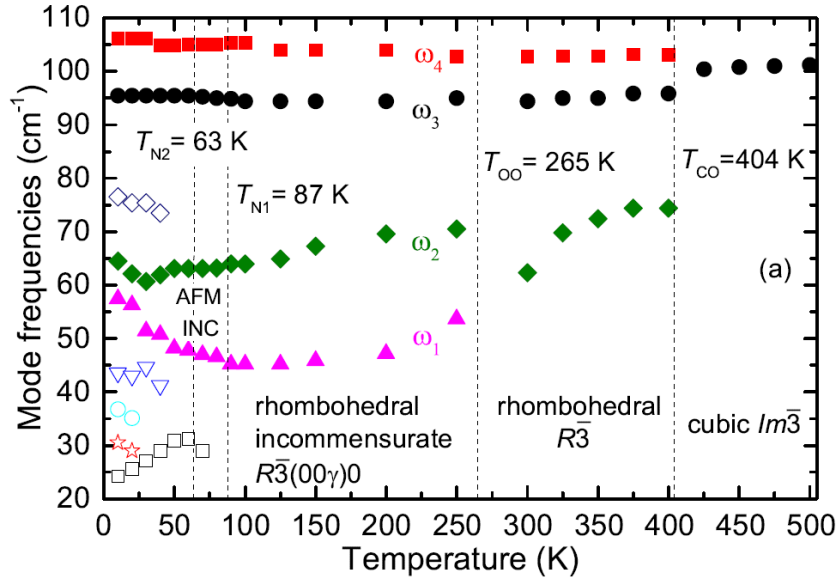
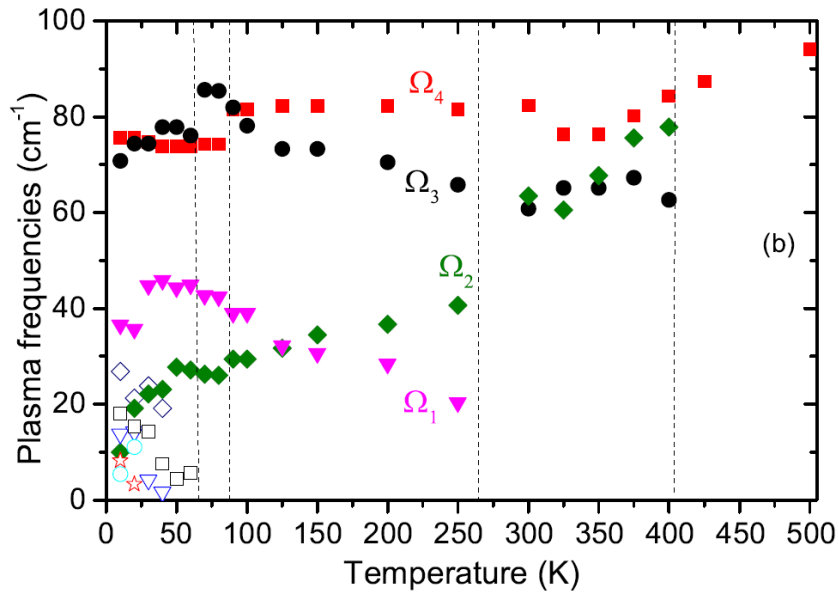
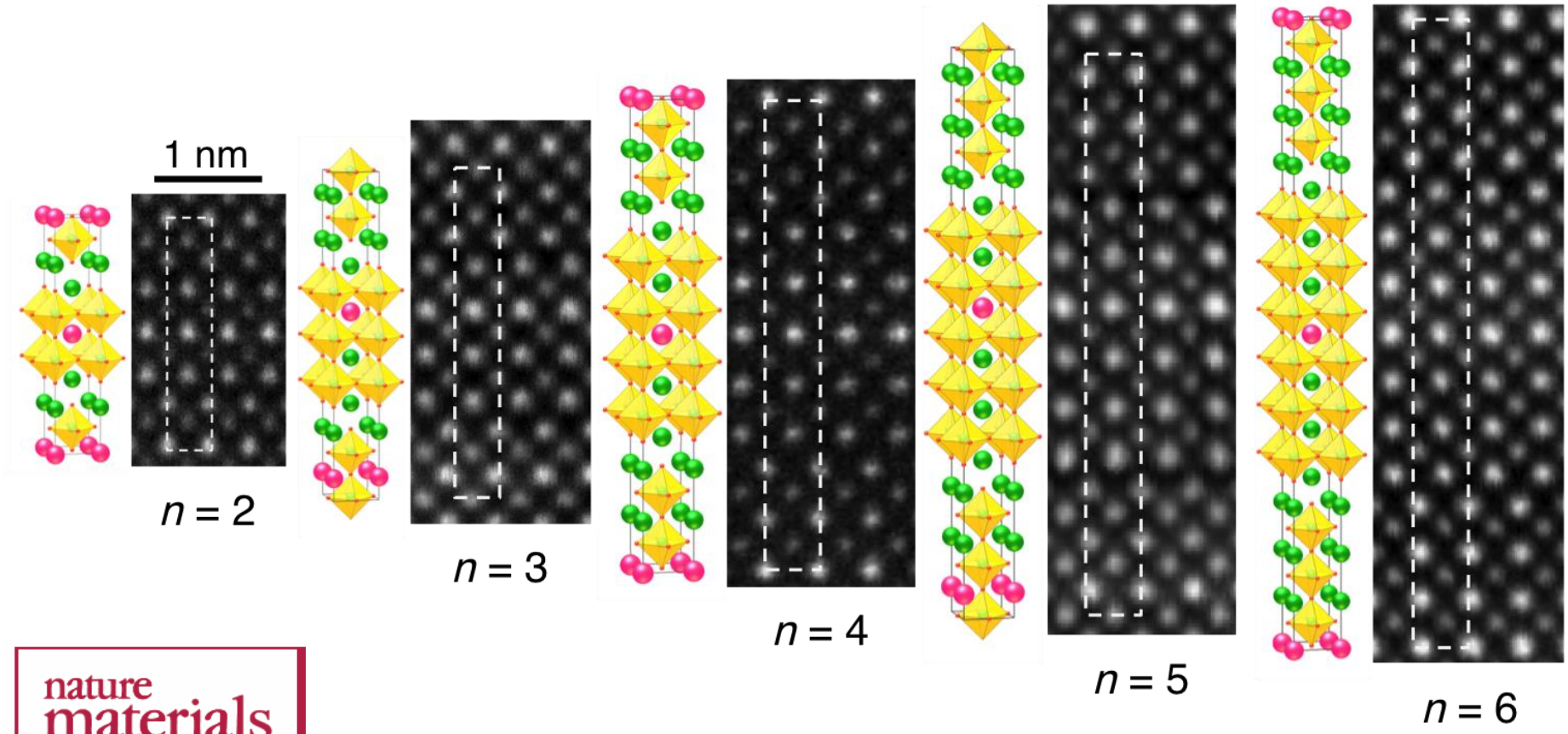
Electromagnons in THz spectra of $SrMn_7O_{12}$







Strained thin films of $(SrTiO_3)_{n-1}(BaTiO_3)_1SrO/DyScO_3$



nature materials

N.M. Dawley at al. Nature Materials (2019) DOI: 10.1038/s41563-019-0564-4

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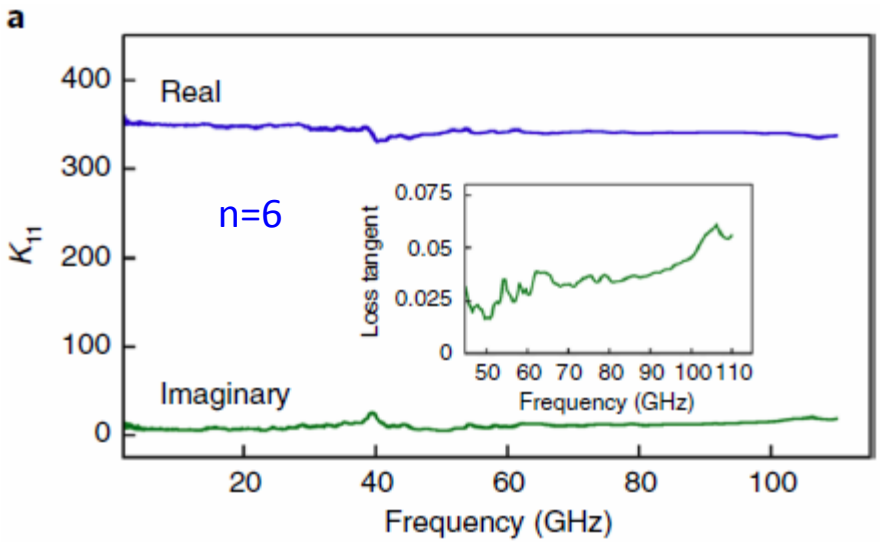
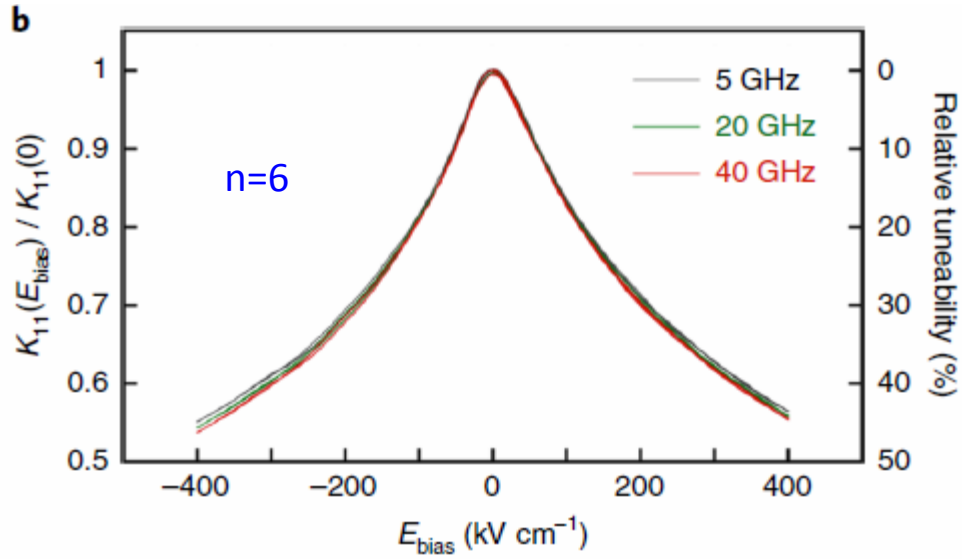
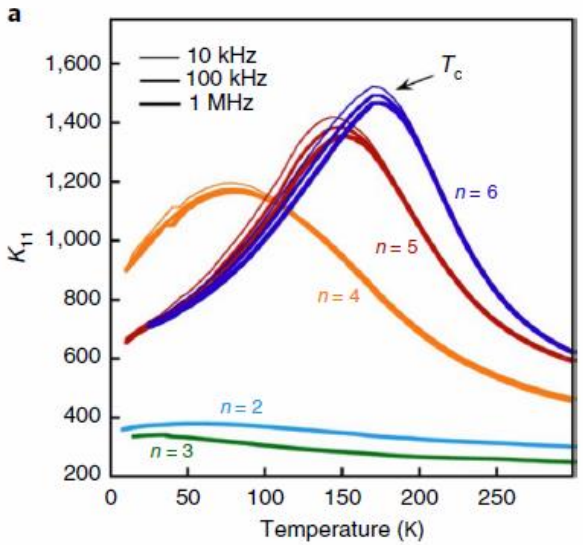
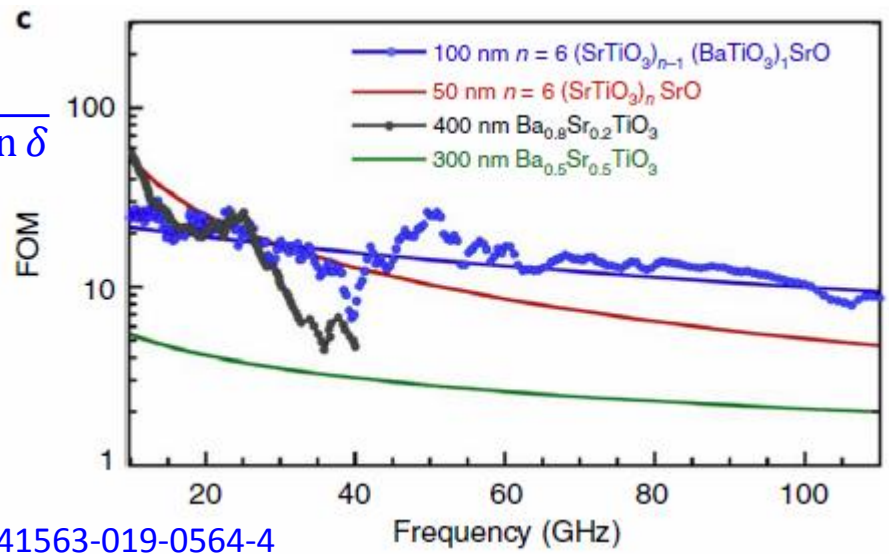






$$FOM = \frac{\Delta k}{k \cdot \tan \delta}$$



N.M. Dawley at al. Nature Materials (2019) DOI: 10.1038/s41563-019-0564-4

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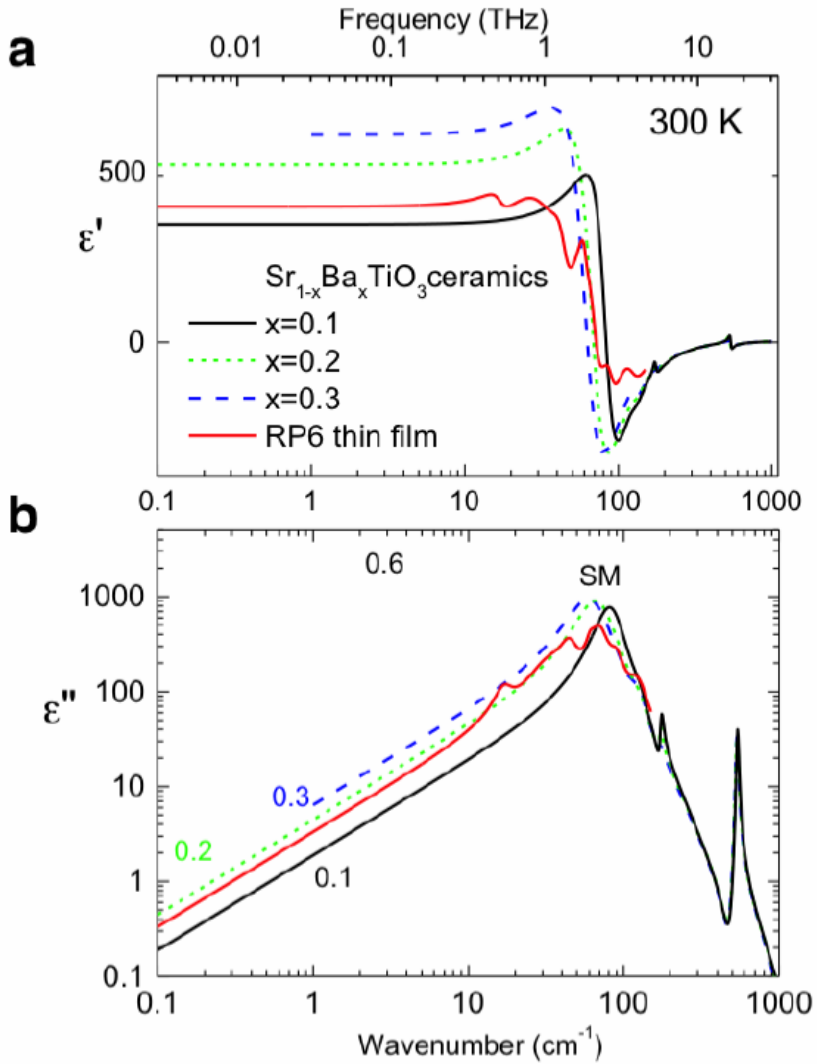
Strained thin films of $(SrTiO_3)_{n-1}(BaTiO_3)_1SrO/DyScO_3$



nature materials

N.M. Dawley at al. Nature Materials (2019) DOI: 10.1038/s41563-019-0564-4

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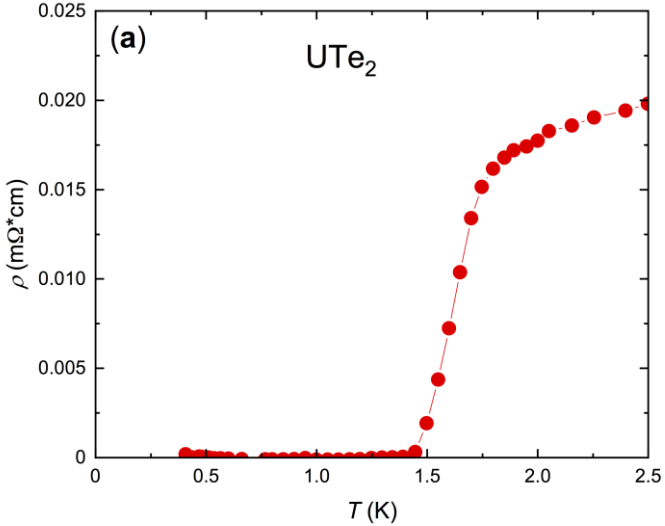
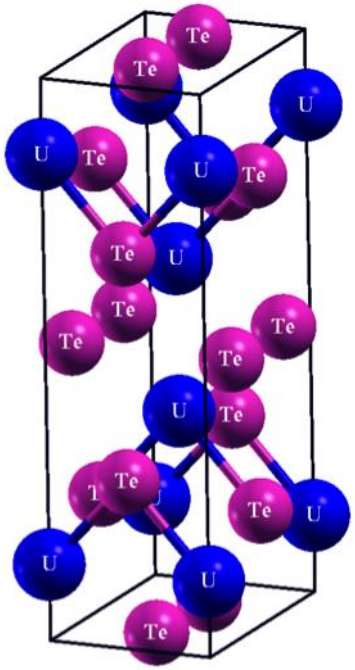
RA5: Anisotropic unconventional superconductor UTe_2

Exp.: S. Run,..., J. Paglione, N. Butch, Science (2019)

- *Immm*
  (bco, inversion)

Space group #71
U-chains along
a-[100]-axis

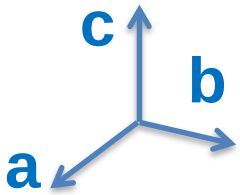


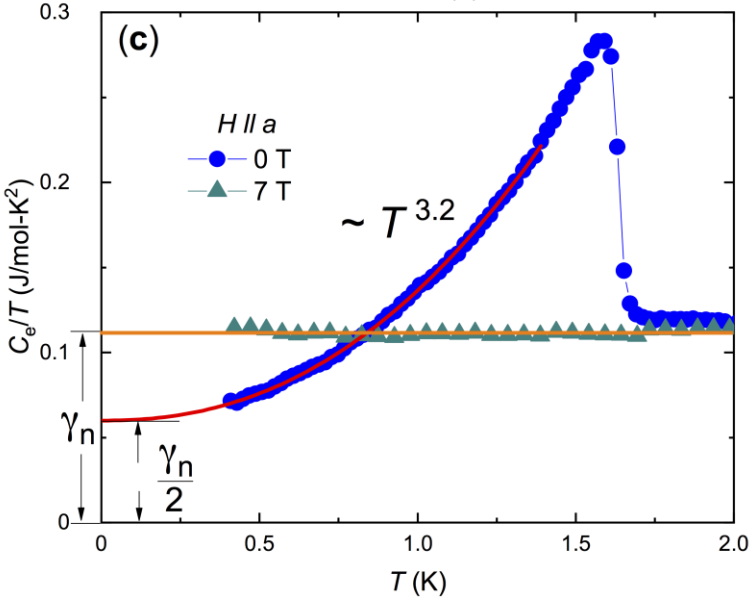


Superconductivity,

- T_c=1.7K
- residual C_V/T as $T \to 0$

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





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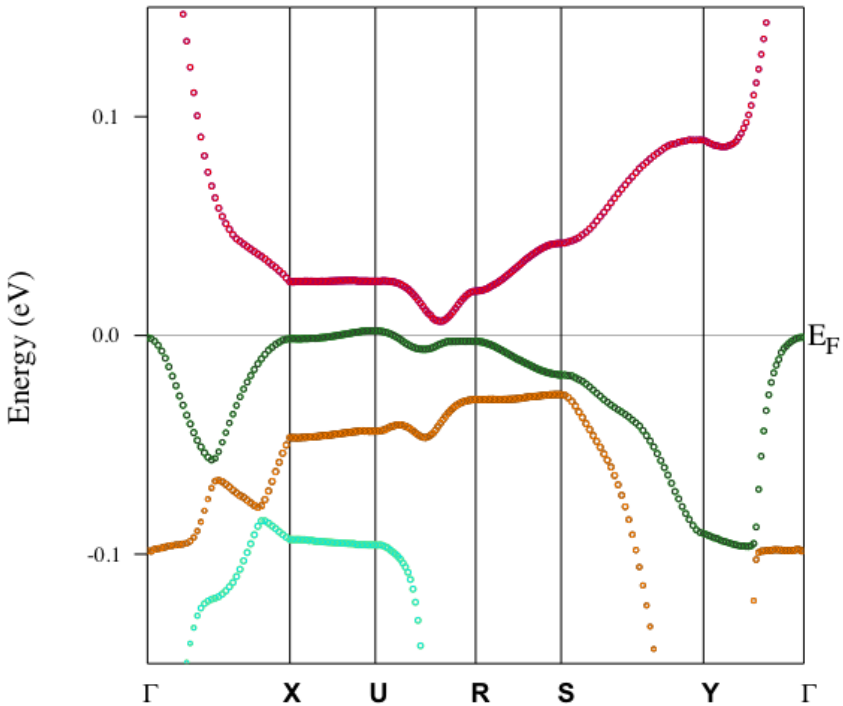
MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY

RA5: Electronic structure of UTe_2

Normal phase: Curie susceptibility with the local moment ~3 μ_B

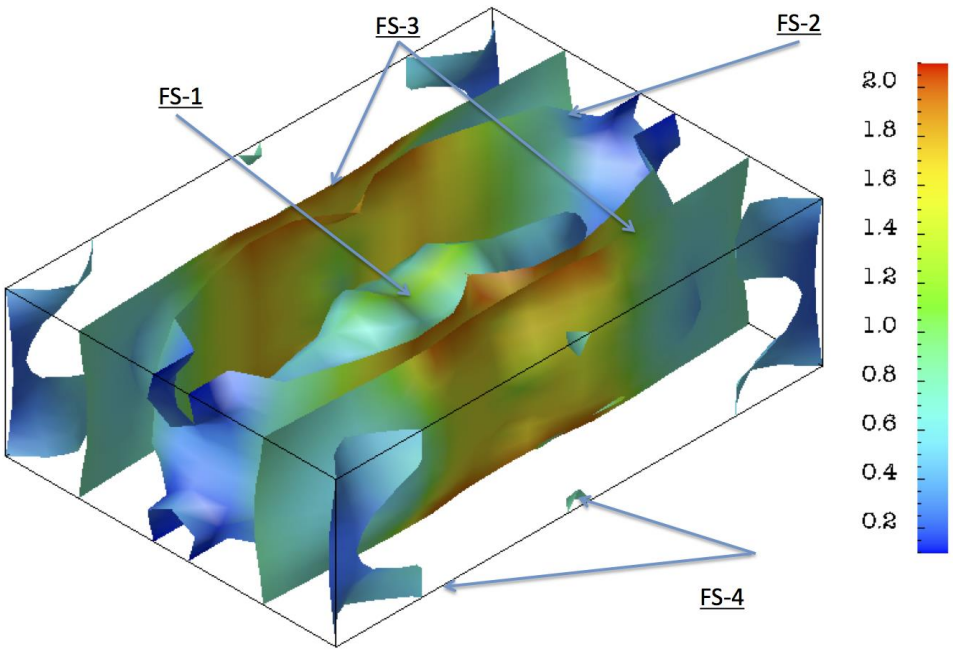
No magnetic order

Non-magnetic
DFT+orbital polarization



Semi-metallic
13 meV hybridization band gap

Ferromagnetic DFT+OP
Metallic and strongly anisotropic



Nesting ~(0,π/b,0)
FM becomes unstable

A. B. Shick and W. E. Pickett, Phys. Rev. B 100, 134502 (2019)

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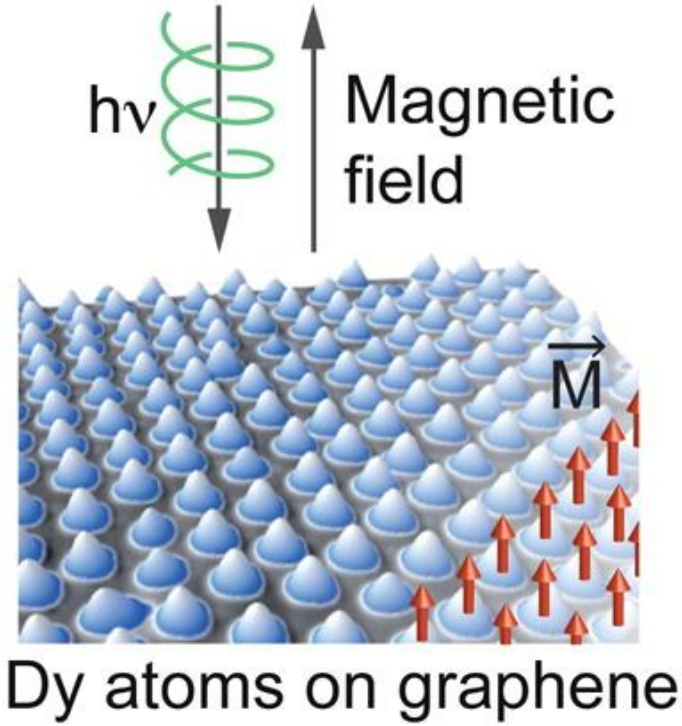
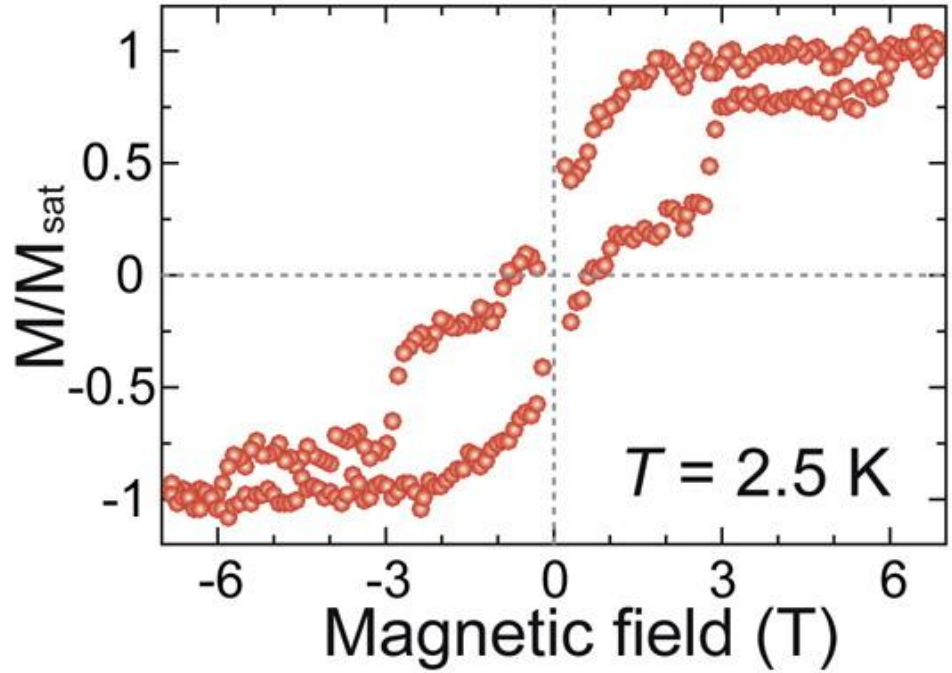
Search for ultra-high density data storage media ~100 Tbit/in^2

R. Baltic *et al.*, Nano Lett. (2016)





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

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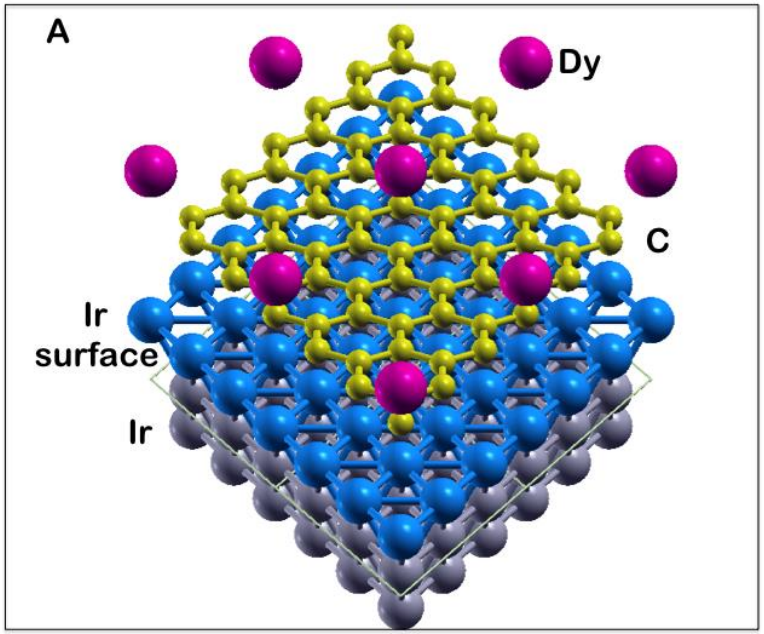
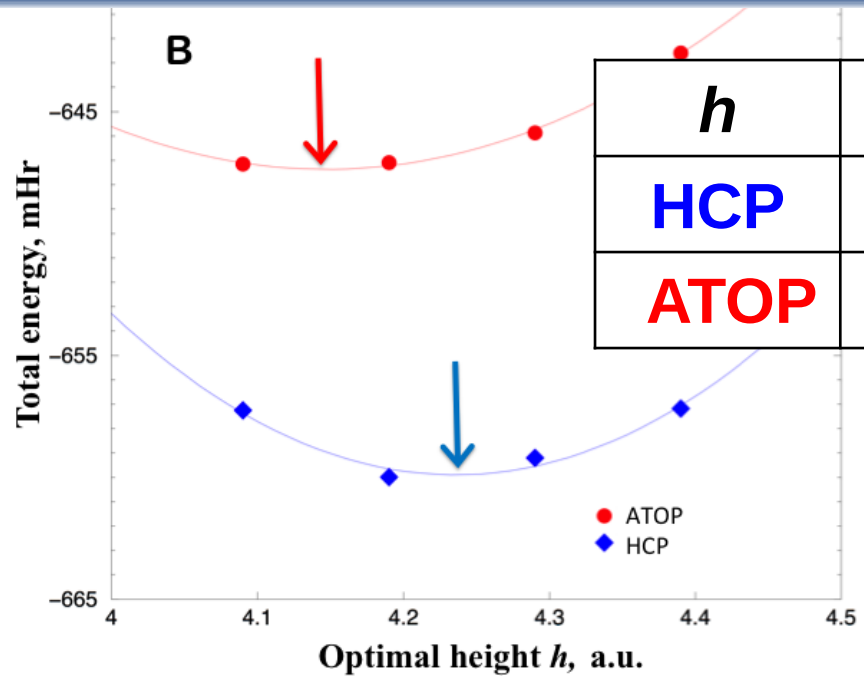
RA5: DFT+U+Hubbard-I calculations of Dy@GR/Ir(111)





h	a.u.
HCP	4.24
ATOP	4.15

	$\langle M_S \rangle$	$\langle M_L \rangle$	$\langle M_S \rangle + \langle M_D \rangle$	R_{LS}	MAE, meV
"HCP"	3.78	5.81	4.53	1.28	7.1
"ATOP"	3.63	5.72	4.52	1.27	5.6
XMCD Exp.	2.4±0.2	3.9±0.2	3.0±0.2	1.31±0.15	> 0

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

A. B. Shick, A. Yu. Denisov, JMMM **475**, 211 (2019).

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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!

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