

# **16th IUVSTA International Summer School on Physics at Nanoscale**



## **Report of Contributions**

Contribution ID: 1

Type: **not specified**

## Spin probes

*Wednesday 9 June 2021 17:30 (1h 45m)*

**Presenter:** Prof. LIPS, Klaus (Helmholtz-Zentrum Berlin)

**Session Classification:** Lectures

**Track Classification:** Spins and spin waves

Contribution ID: 2

Type: **not specified**

## Quantum photonic hybrid systems

*Wednesday 9 June 2021 09:00 (1 hour)*

**Presenter:** Prof. BENSON , Oliver

**Session Classification:** Lectures

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 3

Type: **not specified**

## Spin dynamics/spin waves

*Thursday 10 June 2021 10:30 (1h 30m)*

**Presenter:** Dr HILLEBRANDS, Burkard (Department of Physics and Research Center OPTIMAS, TU Kaiserslautern)

**Session Classification:** Lectures

**Track Classification:** Spins and spin waves

Contribution ID: 5

Type: **not specified**

## **MOCVD structures for optoelectronics**

*Tuesday 8 June 2021 16:00 (1h 30m)*

**Presenter:** Prof. HEUKEN, Michael

**Session Classification:** Lectures

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 6

Type: **not specified**

## Nano-optics / Plasmonics

*Wednesday 9 June 2021 16:00 (1h 30m)*

**Presenter:** Prof. KRENN, Joachim

**Session Classification:** Lectures

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 7

Type: **not specified**

## **Magnetic interfaces and spintronics**

*Thursday 10 June 2021 09:00 (1h 30m)*

**Presenter:** Prof. GAMBARDELLA, Pietro

**Session Classification:** Lectures

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 8

Type: **not specified**

## **Functional and smart materials for electronic and microelectromechanical systems (MEMS)**

*Tuesday 8 June 2021 17:30 (1h 30m)*

**Presenter:** Prof. RIJNDERS, Guus

**Session Classification:** Lectures

**Track Classification:** Surfaces and nanostructures for electronics



Contribution ID: 9

Type: **not specified**

## School kick off

*Tuesday 8 June 2021 15:30 (30 minutes)*

**Presenter:** Dr FEJFAR, Antonín (Institute of Physics, Czech Academy of Sciences)

**Session Classification:** School organization

**Track Classification:** School organization

Contribution ID: 10

Type: poster

## Doping of the hydrogen-passivated Si(100) surface by carborane films studied using density functional theory

Doping is a key process in semiconductor industry, in which the host electronic structure and carrier concentration are modified. When the semiconductor is doped, doping elements with the required electronic properties are introduced into its structure. Dopant introduction processes are either based on diffusion from gaseous phase or on ion implementation, where doping agents are implemented inside the host Si matrix through a high-energy bombardment. However, such a procedure has destructive effects on the structure of the Si matrix, especially near the surface<sup>1</sup>. It is therefore appropriate to be interested in alternative non-destructive methods such as a monolayer doping<sup>2,3</sup> employing chemical reactions to bind a monolayer of dopant-rich molecules onto the surface of the host semiconductor. Such a monolayer can be formed, for example, from dithiocarboranes, i.e. molecules with a large permanent dipole capable of easily forming stable monolayers on a variety of substrates<sup>4–7</sup>.

Here we use Density Functional Theory to investigate the doping of hydrogen-passivated Si(100) substrates through the adsorption of dithiocarborane molecules. We find that dithiocarboranes can both physisorb and chemisorb on the substrate. Chemisorbed structures arise when a S atom in the molecular linker group replaces a surface H atom. We establish the formation of these Si-molecule bonds and characterize their mechanical and thermal stability. Analysis of the calculated electronic structure of adsorbed interfaces shows that carborane adsorption does not result in interface gap states. The band gap in adsorbed junctions is defined by Si states and its magnitude is almost unchanged with respect to the clean Si slab. The large carborane electrostatic dipole results in the downwards shift of Si spectral features by 0.3 eV, reducing the hole injection barrier by this amount with respect to the pristine Si substrate. Molecular dynamics simulations reveal these structural and electronic features to be stable at room temperature. Our work shows that molecular adsorbates having large electrostatic dipoles are a promising strategy to non-destructively dope semiconductor substrates.

### References

1. Chen, W., Qi, D., Gao, X. & Wee, A. T. S. Surface transfer doping of semiconductors. *Progress in Surface Science* 84, 279–321 (2009).
2. Ye, L. et al. Boosting the Boron Dopant Level in Monolayer Doping by Carboranes. *ACS Appl. Mater. Interfaces* 7, 27357–27361 (2015).
3. Veerbeek, J. & Huskens, J. Applications of Monolayer-Functionalized H-Terminated Silicon Surfaces: A Review. *Small Methods* 1, 1700072 (2017).
4. Thomas, J. C. et al. Acid–Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. *ACS Nano* 12, 2211–2221 (2018).
5. Vetushka, A. et al. Adsorption of oriented carborane dipoles on a silver surface: Adsorption of oriented carborane dipoles on a silver surface. *physica status solidi (b)* 253, 591–600 (2016).
6. Baše, T. et al. Carboranedithiols: Building Blocks for Self-Assembled Monolayers on Copper Surfaces. *Langmuir* 28, 12518–12526 (2012).
7. Serino, A. C. et al. Work Function Control of Germanium through Carborane-Carboxylic Acid Surface Passivation. *ACS Appl. Mater. Interfaces* 9, 34592–34596 (2017).

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**Presenter:** HLADÍK, Martin

**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

## Nanoscale Study of the Hole-selective Passivating Contacts with High Thermal Budget Using C AFM Tomography

One of the ways to solve the rear-contact related limitations of dominant p-type c-Si homojunction solar technology is the implementation of the passivating contact. This type of contact typically consists of a layer stack, where one layer effectively passivates the surface of the Si wafer and another layer acts as a selective contact for one type of the charge-carriers. One of the possible architectures of a selective contact is based on a thin interfacial layer of silicon oxide (SiO<sub>x</sub>) passivating the Si wafer and capped with highly doped poly-Si layer. Integrated at the rear side of p-type solar cells, this type of passivating contact resulted in promising efficiencies above 22% [1]. To further increase the applicability of these contacts, it is necessary to deepen the understanding of the charge-carrier transport mechanism through the layer stack and its changes during annealing, as industrial implementation often requires high-thermal-budget steps.

We investigate hole selective passivating contacts that consist of an interfacial layer of SiO<sub>x</sub> and a layer of boron-doped silicon carbide (SiC<sub>x</sub>). The fabrication process of these contacts involves an annealing step at temperatures above 750°C which crystallizes the initially amorphous layer and diffuses dopants across the interfacial oxide into the wafer to facilitate charge transport, but it can also disrupt the SiO<sub>x</sub> layer necessary for wafer-surface passivation. To investigate the transport mechanism of the charge carriers through the selective contact and its changes during the annealing process, we utilize various characterization methods, such as transmission electron microscopy, micro Raman spectroscopy and Conductive Atomic Force Microscopy. Combining the latter with a sequential removal of material, using the technique known as C-AFM tomography [2], we assemble a tomographic reconstruction of the crystallized layer that reveals the presence of preferential vertical transport channels.

C-AFM tomography revealed the presence of charge-carrier transport channels in the partially crystallized selective SiC<sub>x</sub>(p) layer. Moreover, the density of these channels proved not to be related to the interfacial SiO<sub>x</sub> layer properties or its existence, but only to the degree of crystallinity of the doped selective layer as was shown by performing measurements on the samples without any SiO<sub>x</sub> layer. The first direct visualization of the transport channels through the selective contact proves the importance of the crystallinity of the doped selective layer in the local transport of charge-carriers as well as usefulness of the new microscopical techniques on the up-to-date solar structures and materials.

[1] G. Nogay et al., 'Crystalline Silicon Solar Cells With Coannealed Electron- and Hole-Selective SiC<sub>x</sub>Passivating Contacts', IEEE Journal of Photovoltaics, vol. 8, no. 6, pp. 1478–1485, Nov. 2018, doi: 10.1109/JPHOTOV.2018.2866189.

[2] U. Celano et al., 'Mesoscopic physical removal of material using sliding nano-diamond contacts', Scientific Reports, vol. 8, no. 1, p. 2994, Feb. 2018, doi: 10.1038/s41598-018-21171-w.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 12

Type: poster

## Graphene transparency to underlying surface potential studied by KPFM

During the last decade, an increasing number of papers indicated that 2D materials are transparent to intermolecular interactions [1,2,3]. This phenomenon leads to the fact that electronic properties of underlying surface can penetrate through 2D materials, and was demonstrated by e.g. substrate-governed epitaxial growth on top of a 2D material interfacial layer [2,3].

The strength of electric fields penetrating through the interfacial layer is given by the material combination and number of layers. As a consequence, for example, homoepitaxial growth of LiF on top of graphene interfacial layer is possible with up to 3 ML graphene, whereas GaAs homoepitaxial growth was possible with only 1 ML interfacial graphene [3]. On the other hand, if hexagonal boron nitride is used as an interfacial layer, the possibilities of substrate-governed epitaxial growth are significantly reduced, since it screens the electric fields better than graphene [3].

The transparency to interactions may also bring significant advantage to applications, where special and unstable surface properties are required. Graphene can protect the substrate from degradation while keeping the surface properties given by the substrate [4]. Additionally, being impenetrable to even small ions, this property offers exciting possibilities in designing membranes [1].

In this study, the transparency of graphene to substrate electric fields was visualized and quantified by KPFM (Kelvin Probe Force Microscopy). KPFM is an AFM-based technique for surface electrical characterization that can be used to probe local surface potentials with standard lateral resolution well under 100 nm.

Graphene flakes with 1-3 ML were grown on a Cu foil by CVD. During cooling, a faceted surface was formed under graphene which has been explained by energy minimization principles? [5]. KPFM imaging revealed that different surface facets exhibit different potentials, in agreement with assumptions based on distinct surface energies of these facets. In case of 2 ML graphene, the potential difference between facets sensed by KPFM was reduced by approx. 58 % with respect to 1 ML graphene. The results were also compared with those for CVD graphene grown on Pt. It has shown similar potential difference changes above graphene with the number of layers, pointing to the reproducibility and universality of KPFM-based quantification.

[1] Goshal D. et al., *Langmuir* 35, 38, 12306, (2019)

[2] Kim Y. et al., *Nature* 544, 340 (2017)

[3] Kong W. et al., *Nature Materials* 17, 999 (2018)

[4] Kim G. T. et al., *Advanced Materials* 26, 30, 5166, (2014)

[5] Yi D. et al., *Physical Review Letters* 120, 246101, (2018)

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 13

Type: poster

## Correlative Probe and Electron Microscopy for advanced surface characterization using AFM in SEM system

Scanning electron microscopy (SEM) and atomic force microscopy (AFM) are two of the most used, complementary techniques for surface analysis at the nanoscale. Thus, combining them by integrating a compact AFM into SEM brings novel possibilities for true correlative imaging and advanced multi-modal sample characterization that would be often unfeasible using each imaging modality separately.

LiteScope is produced by the NenoVision company and represents a compact AFM, which is designed to be integrated into a large variety of SEMs in a plug-and-play manner. In general, the strength of the AFM-in-SEM hybrid system lies in combining the AFM modes (3D topography, electrical, mechanical and magnetic measurements) with SEM capabilities (fast imaging with wide resolution range, chemical analysis, surface modification using FIB/GIS etc.). Further benefits include precise AFM tip navigation by SEM to the region of interest, roughness evaluation and in-situ conditions, which is essential for sensitive samples and minimizes sample handling. Uniquely, LiteScope design enables simultaneous acquisition and correlation of AFM and SEM data by NenoVision's proprietary technique called Correlative Probe and Electron Microscopy (CPEM).

CPEM functionates in a way that the electron beam and AFM tip keep a constant offset and remain static during the image acquisition. The scanning movement is conducted by a piezo scanner that carries the sample. This ensures simultaneous SEM and AFM data collection in the same coordinate system and with identical pixel size. The resulting 3D CPEM view can combine multiple channels, both from AFM and SEM, enabling thorough sample analysis and clear data interpretation for specific applications.

In conclusion, the AFM-in-SEM strategy benefits from the complementarity of both techniques alongside significant savings both in time and resources. Also, it opens completely new possibilities for advanced data correlation and measurements in variety of industrial and research applications, such as semiconductors, material-, biological- and earth-sciences.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics



Contribution ID: 15

Type: poster

## Influence of primary beam energy on localized surface plasmon resonances mapping by STEM-EELS

STEM-EELS has become a standard technique to map localized surface plasmon resonances (LSPR), which are collective oscillations of free electrons in metal nano- and microstructures. Despite that many works dealing with EELS measurement of LSPR have been published over the last 15 years, there has been no experimental work discussing the experimental conditions during the measurement. Therefore, we have experimentally studied the influence of the primary beam energy and the collection semi-angle on the localized surface plasmon resonances measurement by STEM-EELS to make an instructive overview for the beginners in the field [1].

We took a series of 3 rods and do the STEM-EELS measurement at the primary beam energy of 300 keV, 120 keV, and 60 keV. The best results in terms of the best signal-to-background ratio are obtained using a medium primary beam energy, in our case 120 keV. The primary beam energy should be high enough to suppress the scattering in the sample and at the same time should be low enough to avoid the appearance of relativistic effects. In the case of too high primary beam energy, for example 300 keV, the relativistic effects [2] in the supporting membrane play a non-negligible role and lead to a higher intensity of the background. However, the advantage of the 300 keV electron beam is a lower scattering probability resulting into a better signal to noise ratio in the case of spatial EEL maps of LSPR modes. We note that in the case of a better monochromatization of the primary electron beam (far below 0.1 eV), the elastic part of the background would be significantly reduced which should lead to much better signal to background ratio at lower primary beam energies.

### References:

- [1] M Horák and T Šikola, *Ultramicroscopy* **216** (2020), p. 113044.
- [2] M Horák and M Stöger-Pollach, *Ultramicroscopy* **157** (2015), p. 73.

### Acknowledgement:

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 16

Type: poster

## Spin Wave Normalization Towards all Magnonic Circuits

The key enabling factor for Spin Wave (SW) technology utilization for building ultra-low power circuits is the ability to energy efficiently cascade SW basic computation blocks. SW Majority gates, which constitute a universal gate set for this paradigm, operating on phase encoded data are not input output coherent in terms of SW amplitude. Thus, their cascading requires information representation conversion from SW to voltage and back, which is by no means energy effective. In this paper, a novel conversion free SW gate cascading scheme is proposed that achieves SW amplitude normalization by means of a directional coupler. After introducing the normalization concept, we utilize it in the implementation of three simple circuits and, to demonstrate its bigger scale potential, of a 2-bit inputs SW multiplier. The proposed structures are validated by means of the Object Oriented Micromagnetic Framework (OOMMF) and GPU-accelerated Micromagnetics (MuMax3). Furthermore, we assess the normalization induced energy overhead and demonstrate that the proposed approach consumes 1.25x to 1.5x less energy when compared with the transducers based conventional counterpart. Finally, we introduce a normalization based SW 2-bit inputs multiplier design and compare it with functionally equivalent SW transducer based and 16nm CMOS designs. Our evaluation indicates that the proposed approach provided 1.34x and 6.25x energy reductions when compared with the conventional approach and 16nm CMOS counterpart, respectively, which demonstrates that our proposal is energy effective and opens the road towards the full utilization of the SW paradigm potential and the development of SW only circuits.

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**Presenter:** MAHMOUD, Abdulqader (Delft University of Technology)

**Session Classification:** Posters

**Track Classification:** Spins and spin waves

Contribution ID: 17

Type: **not specified**

## **Lunch/Excursion**

*Thursday 10 June 2021 12:00 (2 hours)*

**Session Classification:** Teaming

Contribution ID: **18**

Type: **not specified**

## **Dinner**

*Wednesday 9 June 2021 19:15 (1 hour)*

**Session Classification:** Teaming

Contribution ID: **19**

Type: **not specified**

## **Lunch/Volleyball**

**Session Classification:** Posters

Contribution ID: **20**

Type: **not specified**

## **Dinner**

*Tuesday 8 June 2021 19:00 (1 hour)*

**Session Classification:** Teaming

Contribution ID: **21**

Type: **not specified**

## Student mixer

*Tuesday 8 June 2021 20:00 (1h 30m)*

Hands-on experiments with Amazing Theatre of Physics (in Czech “Úžasné divadlo fyziky (UDIF)”  
)

**Session Classification:** Teaming

Contribution ID: 22

Type: **not specified**

## Evening programme

*Wednesday 9 June 2021 20:15 (1 hour)*

Physics at Dance, together with PONEC theater

**Session Classification:** Teaming



Contribution ID: **23**

Type: **not specified**

## **Lunch/Volleyball**

*Wednesday 9 June 2021 10:30 (3 hours)*

Contribution ID: 24

Type: **poster**

## Structural coloration metasurface

Color filters enable photosensors to obtain spectral composition of incoming radiation, be it to mimic human vision or to separate analytical signals. Efforts to increase the resolution of these photosensors lead to decrease in size of individual picture elements –pixels, which places increasing demands on the color filter technology. Conventional color filters operating on the principle of absorption of light in organic pigments are frequently used, but they are no longer meeting growing requirements of increasing sensor resolution. Within our research, we use nanostructures to separate light by wavelength and thus create structural coloration. We present a novel approach to separate colors which utilizes manipulation of radiation polarization using half-wave plate nanostructures and promises extremely small pixel size of only 300 nm. The presented color filter is first modeled and optimized through numerical simulations and then manufactured using nanofabrication methods. The designed metasurface could not however be fabricated. The optical response of substitute nanostructures of approximately similar dimensions is verified using optical spectroscopy in far field and shows successful color filtration despite exhibiting wide transmission peak.

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 25

Type: **poster**

## The scanning time-resolved Kerr microscope

In recent days, magnetic materials, structures, and devices are getting more popular, especially those related to spintronics. Research and development of such magnetic samples require a way to observe magnetization with good spatial and temporal resolution. Most dynamic changes of magnetization are realized in nanoseconds or even faster. If we can detect these dynamic processes, we can reveal many exciting magnetization features and add the fourth dimension to our experiments. We introduce a scanning Kerr microscope working in two modes: static and dynamic. In static mode, our microscope detects a direction of magnetization in a variable magnetic field. In dynamic mode, we use a pump-probe method to reach a temporal resolution and observe a fast evolution of magnetization.

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**Session Classification:** Posters

**Track Classification:** Spins and spin waves

Contribution ID: 26

Type: poster

## Label-free and charge-sensitive second harmonic imaging of giant vesicle hydration

A biological membrane forms a dynamic and complex barrier between compartments of the living cell and its environment. However, its *in vivo* studies are difficult because it consists of a high variety of lipids and proteins and is continuously reorganized by the cell. Giant unilamellar vesicles (GUVs) are a powerful model system of the cell membrane due to their comparable size and membrane curvature. The majority of studies carried out on GUVs utilize fluorescence microscopy in combination with fluorescent markers. However, these methods of membrane imaging typically neglect molecular level details. As a consequence, there is virtually no knowledge on the role of membrane hydration, even though it is clear that without water lipid bilayer membranes cannot exist. A recent improvement in imaging throughput has resulted in the construction of a second harmonic imaging device that can non-resonantly and dynamically image interfacial water molecules [1,2]. This microscope was subsequently used to image the hydration of macroscopic free-floating membranes in aqueous solutions [3]. Here, we envision to extend our approach to SH image the interfacial hydration of GUVs. By varying the ionic strength of the adjacent solutions and lipid composition of the vesicles, we show that the non-resonant SH response of water molecules aligned by charge–dipole interactions with charged lipids can also be used as a label-free probe of membrane structure of GUVs.

[1] Carlos Macias-Romero et al., Optics express, 2014, 22 (25), 31102–31112.

[2] Carlos Macias-Romero et al., Science, 2017, 357 (6353), 784–88.

[3] Orly B. Tarun et al., PNAS, 2018, 115 (16), 4081–4086.

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 27

Type: **poster**

## Switching of Confined Antiskyrmions Under Circular Magnetic Fields

Magnetic antiskyrmions may occur in cases where the magnetic chirality is anisotropic. In another word, DMI with opposite signs along two perpendicular directions can stabilize antiskyrmions [1]. They were theoretically predicted in certain tetragonal materials with D2d symmetry [2]. This topological spin structure plays a crucial role in low dimensional magnetic systems, where topological features dominate their magnetic and dynamic properties. Utilizing micromagnetic simulations, we investigate the dynamics and switching of confined topological spin textures, in particular antiskyrmions. The ability of a controlled switching of the polarity of these objects is essential for their potential applications in novel devices. First, after stabilizing a single skyrmion in a magnetic nanodisk, we study the dynamics and switching of an antiskyrmion under the application of a circular magnetic field. We show that the antiskyrmion can be switched with a minimum field amplitude of  $H_0 = 40$  kA/m. This threshold amplitude depends on materials parameters. The results show that the proposed circular field is also capable of switching of an antiskyrmionium to another antiskyrmionium with different polarity and the switching is favored for materials with a smaller damping parameter.

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**Session Classification:** Posters

**Track Classification:** Spins and spin waves

Contribution ID: 28

Type: **poster**

## **A Multicomponent System by Chemical Transformation: 4,4'-biphenyl-dicarboxylic Acid on Ag(001)**

Molecular self-assembly is an atomically precise approach for the fabrication of organic layers with tailored functionality. We present multi-component molecular phases of 4,4'-biphenyl dicarboxylic acid self-assembled on Ag(001) and their transformations for sub-monolayer and full monolayer coverages are followed by LEEM, STM, and XPS. Specific mixtures of intact, partially-, and fully dehydrogenated molecules are associated with k-uniform tilings.

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**Presenter:** CECHAL, Jan (CEITEC BUT)

**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 29

Type: poster

## Atomic scale control and visualization of topological quantum phase transition in $\pi$ -conjugated polymers driven by their length

Using topological band theory and by means of density functional theory, tight-binding and GW calculations, we can show that polymers near the topological transition point can transition from a trivial quantum phase to a non-trivial one. This transition between two insulators must proceed via closure of the electronic gap.

By employing on-surface synthesis with custom-designed precursors on a pristine Au(111) surface, we produce polymers which consist of 1D, linearly-bridged acene moieties. These polymers feature narrow bandgaps (being in the proximity of the transition point) and in-gap zero-energy edge states, when in the topologically non-trivial phase close to the topological transition point. We also reveal the important role played by a polymer's length in order to achieve an atomic scale control over the quantum phase transition between the two different topological quantum classes in one of the polymers[1-3].

### References:

- [1] Sánchez-Grande, A. et al. Angew. Chem. Int. Ed. 58, 6559 (2019).
- [2] Cirera, B., Sánchez-Grande, A., de la Torre, B. et al. Tailoring topological order and  $\pi$ -conjugation to engineer quasi-metallic polymers. Nat. Nanotechnol. 15, 437–443 (2020).
- [3] Gonzalez Herrero, H. et al. Atomic scale control and visualization of topological quantum phase transition in  $\pi$ -conjugated polymers driven by their length. arXiv preprint arXiv:2105.00025 (2021)

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**Presenter:** EDALATMANESH, Shayan

**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 30

Type: poster

## Composition-Gradient-Mediated Semiconductor–Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers

The semiconductor–metal transition (SMT) enables multiple applications of one single material, especially in modern devices. How to control it remains one of the most intriguing questions in material physics/chemistry, especially in two-dimensional layered materials. In this work, we report realization of SMT in  $\text{MoS}_2\text{--xOx}$  bilayers, driven by the concentration gradient of the chalcogen atom across the van der Waals (vdW) gap of the disordered bilayers. Using the cluster expansion method, we determined that either semiconducting (stable) or metallic states (metastable) can be realized in  $\text{MoS}_2\text{--xOx}$  bilayers with the same composition. Machine learning analysis revealed that the concentration gradient of the chalcogen atom across the vdW gap is the leading fingerprint of SMT, with structural distortion induced by atom mixing being a significant secondary factor. The electronic origin of the SMT is the broadening of the Mo  $d_{z^2}$  and O  $p_z$  bands, accompanied by the redistribution of the d electrons. This in-vdW-gap composition-gradient-driven SMT phenomenon also applies to  $\text{MoSe}_2\text{--xOx}$  and  $\text{MoTe}_2\text{--xOx}$  bilayers. The present work provides an alternative mechanism of SMT and demonstrates that the composition gradient across the vdW gap in the bilayer materials can be another degree of freedom to tune the band gaps without introducing extrinsic elements. Our findings will benefit the material design for small-scale and energy-efficient electronic devices.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics



Contribution ID: 31

Type: poster

## AN ATOMISTIC STUDY OF TWIN BOUNDARY MIGRATION BY THE MOTION OF DISCONNECTION

### Abstract:

The deformation twinning in hcp crystals have been extensively researched nowadays due to the dominant role it plays in the plastic deformation and strengthening mechanisms of materials. The twin boundary migration plays a significant role in the microstructure evolution of metallic materials. The knowledge of migration mechanisms under applied stress can be considered as a basis for the development of nanostructured materials with improved mechanical properties. The deformation twinning in magnesium is a complex phenomenon and is still under intensive study. The most common twinning mode in hcp metals is takes place in  $\{10\text{-}12\}$  planes [1] and this mode accommodates tensile deformation along with  $[0001]$  direction. Some less common twinning modes such as  $\{11\text{-}26\}$  and  $\{11\text{-}22\}$  are also observed in Mg [2].

In the present work, we highlight the atomic-level study of the migration of  $\{11\text{-}26\}$  twin boundaries by conducting molecular dynamic simulation using of LAMMPS [3] using the embedded atom methods (EAM) potential developed by Sun et. al. [4]. The visualization software OVITO [5] is used to realize the dynamic display in our study [5]. Simulation shows the formation of twinning disconnection in  $\{11\bar{2}6\}$  twin boundary with subsequent gliding along this plane. Twinning disconnections are accumulated in simulation block with formation of basal pyramidal interfaces. Electron backscatter diffraction analysis and TEM analysis were performed to verify the simulated results.

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5. A. Stukowski, Modell. Simul. Mater. Sci. Eng. 18 (2010) 015012.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 32

Type: poster

## Real time electron microscopy of formation of low-dimensional materials

Full understanding of nanostructures' formation is a key for engineering of their physical properties. At nanoscale, this is a very challenging task. Electron microscopy is conventionally used for post-growth analysis of the fabricated nanostructures, and the growers have therefore no choice than perform time-consuming numerous experimental runs with uncertain results. These are often combined with other post-growth techniques, and the growth mechanism is deduced from these correlative experiments. In this regard, real-time in-situ microscopy has become inevitable tool for deducing the growth mechanisms, which is well documented in case of 1D nanostructures (nanowires) using transmission electron microscopy [1]. However, TEM has a very limited usecase due to the requirements posed on the samples. In our work, we have focused on using SEM, and were able to demonstrate several successful experiments dealing with the growth of nanowires (both out-of-plane and in-plane) and, recently, 2D materials. Note that the latter is hardly possible in TEM. We will show different approaches to in-situ electron microscopy, demonstrating the versatility of SEM for this kind of research.

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[2] Kolibal, M. et al., Nano Letters 2016, 16, 4880.

[3] Kolibal, M. et al., J. Phys. Chem. Lett. 2020, 11, 6498.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 33

Type: poster

## InGaN/GaN quantum wells: correlations between cathodoluminescence properties and V pit characteristics

InGaN/GaN quantum well (QW) structures are commonly used in LEDs and laser applications [1]. Under certain growth conditions, hexagonal V shaped pits (V pits) are formed. These V pits may enlarge during the growth and their density is connected with density of dislocations containing a screw component. These V pits have large impact on optical properties of the samples [2]. Therefore, statistical quantities concerning V pits (like density, sizes, ...) are of great importance. If they are obtained, they can be correlated with luminescence properties of the sample and provide deeper insight into physics of InGaN/GaN quantum well structures.

Scanning electron microscope (SEM) is standard equipment for studying surface defects of different samples. In the case of InGaN/GaN, a common type of defects are V pits. To obtain relationship between the V pit density, sizes, etc. and properties of the samples, automatic V pit finding in the SE image is required. Automatic finding of V pits by blob detection as well as automatic fitting of cathodoluminescence (CL) spectra is carried out by CV2 library for Python. This contribution shows correlations between CL properties and V pit statistical quantities as the motivation for using Python in the image analysis.

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[2] T. Vaněk et al., J. Cryst. Growth. 565 (2021) 126151.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 34

Type: poster

## Vacuum Rabi splitting of a dark plasmonic cavity mode revealed by fast electrons

Recent years have seen a growing interest in strong coupling between plasmons and excitons, as a way to generate new quantum optical testbeds and influence chemical dynamics and reactivity. Strong coupling to bright plasmonic modes has been achieved even with single quantum emitters. Dark plasmonic modes fare better in some applications due to longer lifetimes, but are difficult to probe as they are subradiant. Here, we apply electron energy loss (EEL) spectroscopy to demonstrate that a dark mode of an individual plasmonic bowtie can interact with a small number of quantum emitters, as evidenced by Rabi-split spectra. Coupling strengths of up to 85 meV place the bowtie-emitter devices at the onset of the strong coupling regime. Remarkably, the coupling occurs at the periphery of the bowtie gaps, even while the electron beam probes their centre. Our findings pave the way for using EEL spectroscopy to study exciton-plasmon interactions involving non-emissive photonic modes.

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 35

Type: poster

## Properties of yellow band in MOVPE grown GaN layers

Nitride semiconductors became the second most important semiconductor material after silicon in the last two decades. Many daily used devices, such as blue light emitting diodes or high electron mobility transistors in electronic devices, are based on nitride semiconductors. Despite the nitride devices mass production, there are many open questions and not well understood phenomena which have to be solved.

One of the open question is the origin of different defect bands in luminescence spectra. Epitaxially grown GaN layers contain in their luminescence spectra very fast excitonic band and also different kinds of defect bands, which have mostly slow decay time. Fast decay time without any slow components is necessary for many scintillation applications. Especially defect band with the maximum emission around 2.2 eV (called yellow band) has very slow decay time (microsecond range) and needs to be suppressed in fast scintillators.

In our previous work [1], we have shown that different technological parameters during Metal Organic Vapour Phase Epitaxy (temperature, carrier gas, etc.) influence properties of yellow band quite significantly. In this work, we continue to study properties of yellow band of GaN layers grown with different parameters (different precursor and carrier gas). Photoluminescence and other measuring techniques are used for investigation of yellow band properties. Origin of yellow band will be discussed.

[1] T. Hubáček et al., J. Cryst. Growth 531 (2020) 125383.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 36

Type: poster

## Nanocomposites of PMMA and rose-like BiOCl nanostructure: Synthesis and characterization

Nanocomposites of PMMA: BiOCl with different concentrations of BiOCl (5, 10, 15 wt%) were prepared by using simple solution cast technique. Prepared nanocomposites as well as BiOCl nanostructure characteristics were examined by using XRD, FESEM and EDAX. Morphology reveals that the developed nanostructure of the filler (BiOCl) is of rose like geometry, which composed of dozens rapidly grown nanosheets of thickness 53nm. Uniform distribution and tight adherence of nanoparticles with PMMA matrix has also been confirmed through FESEM images. It is witnessed that the surface morphology changes from smooth to rough with increase in weight ratio of filler might be due to particle-particle interaction dominance over matrix-particle interactions. Further the newly emerged sharp peaks in the XRD pattern confirm the presence of nano-BiOCl crystallites within the polymeric matrix. The obtained results reflect that the properties of polymer nanocomposites depend upon the type of nanomaterial such as shape, concentration, size, and interaction with polymer matrix, which find its application in optical devices, fuel cells, and chemical sensors.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 37

Type: **poster**

## Role of Urbach energy in material science

Defect states in semiconductors are one of the main focuses of all semiconductor studies. Many different approaches are used to determine the defect's origin, character and densities. One of the often overlooked semiconductor's parameters related to the defect states is the Urbach energy. It is an easily accessible measure of material disorder. Here, the process of obtaining the Urbach energy and the information which can be gained from it will be discussed.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 38

Type: poster

## In-situ SEM study of surface guided ZnSe nanowires grown by CVD

Surface-guided planar nanowires show a lot of promise for integration into practical devices [1], but that is conditioned upon understanding their synthesis in detail. In this work, we investigate the VLS growth of ZnSe nanowires by chemical vapor deposition, guided by the steps on annealed M-plane sapphire substrate [2].

We have developed a reactor compatible with SEM and, although the experimental conditions differ from the standard CVD growth, it successfully mimics the conditions in conventional furnaces while allowing us to use standard detection systems since the chamber is kept at high vacuum. SEM enables us to directly study the growth kinetics and for the first time, we can directly observe the growth behavior previously predicted by ex-situ and theoretical approaches [3]. Interestingly, we have also observed effects of the electron beam on the synthesis.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics



Contribution ID: 39

Type: **poster**

## Comparative study of monocrystalline and polycrystalline gold plasmonic nanorods

Plasmonic antennas are often fabricated by lithographic patterning of a thin metallic film and its properties are then intimately related to the quality of the resulting structures. Here we compare two kinds of thin gold films: polycrystalline thin film deposited by magnetron sputtering, and chemically synthesized monocrystalline gold platelet. Both metallic substrates were used to fabricate plasmonic nanorods using focused ion beam lithography. The resulting nanorods were characterized by scanning transmission electron microscopy and electron energy loss spectroscopy.

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 40

Type: poster

## Free energy QM/MM simulations of on-surface reaction pathways

On-surface chemistry represents a fast-growing field allowing to synthesize molecular structures not available by traditional wet chemistry. In combination with high-resolution scanning probe technique providing the unprecedented spatial resolution, individual products of reactions can be precisely identified. Nevertheless, a deep understanding of the reaction mechanism under the conditions imposed by the substrate remains unknown.

Widely adopted energy reaction path techniques will only describe the potential energy landscape at zero Kelvin, while the free energy landscape at given temperature enables a more appropriate description of the reaction. Such simulations including temperature effect include the effect of entropy, vibrations modes, concerted motion, etc.

Consequently, such simulations avoid local minima and allows to explore different states, revealing lower energy pathways. We will present QM/MM simulations of strain-induced isomerization in one-dimensional metal-organic chains on Cu(111) surface [1]. The simulation demonstrates the importance of the temperature effect on proper description of the reaction mechanism.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 41

Type: poster

## Structural Details of a Prototypical Organic-Inorganic Interface: CuPc on $\text{In}_2\text{O}_3(111)$

Indium oxide ( $\text{In}_2\text{O}_3$ ) is a ubiquitous material in OLEDs and photovoltaics due to an ideally matched optical transmission window and metal-like conductivity at room temperature when doped with Sn (as ITO). When  $\text{In}_2\text{O}_3$  is paired with organic materials, a nearly universal fabrication step is the introduction of a thin organic buffer layer to improve the charge injection efficiency from  $\text{In}_2\text{O}_3$  to the organic active layers. Using a combination of STM, nc-AFM, and local spectroscopy (STS), we probe the adsorption structure and density of states (DOS) at the prototypical copper phthalocyanine (CuPc)- $\text{In}_2\text{O}_3$  interface. We focus on the stoichiometric (111) surface but also investigate the effects of dissociated water coadsorbed in UHV. STM/AFM imaging reveals single CuPc molecules adsorb in a flat, slightly tilted geometry in three symmetry-equivalent orientations. Increasing the coverage leads to (densely packed) 1D chains oriented along the  $\langle 110 \rangle$  directions. With increasing coverage up to 1 ML, first, a  $(2 \times 2)$  and then a  $(1 \times 1)$  superstructure is found. Finally, differential conductance ( $dI/dV$ ) measurements reveal the energetic positions of the HOMO and LUMO states which are critical for improving charge injection.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 42

Type: poster

## Lipid membrane phase transitions involve structural redistribution of interfacial water

Morphological transitions of lipid membranes are thought to depend primarily on the chain length diversity of its components. However, the role of different lipid head groups, their counter ions and hydrating water molecules in the close proximity of the membrane on the gel-to-liquid phase transition of lipid is mostly unknown. We employed second harmonic (SH) scattering measurements to probe asymmetric distribution of water molecules between the lipid leaflets. Measurements on the same acyl chain length and single lipid component liposomes consisting of 1,2-dimyristoyl-sn-glycero-3-phosphate (sodium salt) (DMPA), 1,2-dimyristoyl-sn-glycero-3-phospho-L-serine (sodium salt) (DMPS), 1,2-dimyristoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) (DMPG), 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and 1,2-dimyristoyl-3-trimethylammonium-propane (chloride salt) (DMTAP) showed a significant lipid hydration alteration as a function of temperature. More specifically, we observed a > 20% increase in the second harmonic intensity at the phase transition temperature for liposomes made of charged lipids. Zwitterionic DMPC lipids on the other hand, display only smaller (~ 8%) changes. This data implied that an increasing number of water molecules anisotropically oriented towards surface normal above the phase transition and the charge state of the lipids play key role on the gel-to-liquid phase transition. Our data demonstrate that lipid phase transitions not only lead to structural changes in the bilayer itself but also in the adjacent aqueous phase.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 43

Type: poster

## Direct assessment of the acidity of individual surface hydroxyls on $\text{In}_2\text{O}_3(111)$

Non-contact atomic force microscopy is a versatile tool to investigate properties of individual atoms or molecules. Here we report a novel approach to determine the acidity of individual surface hydroxyls, which is directly linked to the proton affinity (PA) of the involved O atoms. The PA - the tendency to gain or lose a proton - is crucial *e.g.* in acid-base catalysis and the electro- and photocatalytic splitting of water.

The testcase of this study is the stoichiometric  $\text{In}_2\text{O}_3(111)$  surface, which has four inequivalent surface O atoms  $\text{O}_S(\alpha-\delta)$ . Water dissociation leads to a pair of OH groups: the surface  $\text{O}_S\text{H}(\beta)$  and the water  $\text{O}_W\text{H}$ . The remaining surface O atoms  $\text{O}(\alpha, \gamma, \delta)$  can be protonated via manipulation with the tip. We probe the strength of their H bond with a functionalized tip of a nc-AFM via  $F(z)$ -spectroscopy and find quantitative agreement with density-functional theory (DFT) calculations. By relating the results to known PAs of gas-phase molecules, we can calibrate our data and determine the PA of different surface sites of  $\text{In}_2\text{O}_3(111)$  with atomic precision. Measurements on hydroxylated  $\text{TiO}_2$  and zirconia extend our method to other oxides. The trends of the site-specific PA values agree well with the expectations based on area-averaging techniques.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 44

Type: poster

## 4,4'-biphenyldicarboxylic acid on Ag(111)

Self-assembly of organic and metal-organic species is a thrilling field, which exploits the mechanisms of supramolecular chemistry to build complex molecular entities [1]. Recently, this field has been tried at surfaces [2], where multiple two-dimensional structures with various functional properties can be synthesized. At the time, there is abundant information on resulting thermodynamically stable molecular architectures on diverse substrates, but the knowledge of how intermediate kinetically trapped states form and how, in general, self-assembly processes develop in time is still deficient. The use of a complementary experimental approach may shed some light on those yet unanswered questions. In this work we present an investigation of 4,4'-biphenyldicarboxylic acid (BDA) self-assembly on an Ag(111) single crystal, which, along with our previous studies [3-6], aims at generalizing the knowledge on BDA self-assembly at relevant noble-metal substrates. Utilizing Scanning Tunneling Microscopy, X-ray Photoelectron Spectroscopy and Low Energy Electron Microscopy/Diffraction (LEEM/LEED), we reveal the structures of transitional and final BDA molecular phases forming on Ag(111). Furthermore, we demonstrate real-time observations of the temperature-dependent phase transitions. Such a multicomponent analysis allows us building up a comprehensive picture of the BDA behavior on the Ag(111) surface.

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- [5] Kormoš, L., et al. *Nature Communications*, 2020, 11, 1856;
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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics

Contribution ID: 45

Type: **poster**

## **Influence of deposition angle on fabrication of plasmonic gold nanocones**

Gold nanocones can show several plasmonic resonances and can be used to enhance light-matter interactions or for location-specific plasmonic sensing. Their fabrication often utilizes so-called self-shading effect, which occurs during metal film evaporation into circular nanowells. We present a view on the fabrication of ordered arrays of gold nanocones using electron beam lithography and electron beam evaporation. Lateral position of the substrate during the evaporation influences the symmetry of the fabricated nanocones and that off-axis deposition forms asymmetric structures. Our findings help to identify limits for production of wafer-scale arrays and also suggests new fabrication possibilities for more complicated structures such as mutually connected nanocones for electrically addressable chips.

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**Session Classification:** Posters

**Track Classification:** Nanophotonics / Plasmonics

Contribution ID: 46

Type: poster

## Limiting factors in Photovoltaic-Electrochemical cell development for syngas production

### Abstract:

One of the ways to reduce the CO<sub>2</sub> concentration in air is to convert it to any valuable product(s), such as fuels. This can be achieved by employing photo-electrochemical route. However, this is an energy intensive technique and almost 50% cost of fuel production goes into the applied electrical power. The success of this technique can be achieved if the applied power is derived from a source that is (1) cheap, (2) non-toxic (3) renewable and (4) up scalable. Wind and solar photovoltaics are good candidates to serve this purpose. With sharp decrease in the price of PV energy, especially record low auction values (0.027\$/kWh!), it is a very attractive power source. We have looked into various types of catalysts Zn, porous Zn, Cu-In, and estimated the Faradaic efficiencies of the production of hydrogen (H<sub>2</sub>) and carbon-monoxide (CO) from CO<sub>2</sub> splitting in a electrochemical cell. We made various types of solar PV power sources, i.e., modules made from a-Si/a-Si/nc-Si triple junction cells, a-Si/nc-Si tandem cells and silicon heterojunction solar cells. Comparing the current voltage characteristics of the electrochemical cells and PV modules, we estimated solar to fuel conversion efficiency of CO over 3% for Zn and porous Zn catalysts for CO<sub>2</sub> splitting. We tried as a demonstration a PV wired electrochemical cell with Cu-In catalyst, which produced very small quantity of CO and the STF efficiency was below 1%. The coupling loss was observed with the wired connection which affects the product efficiency. The solution to this problem can be found by reducing the operational voltage and equi-balance current flows in these two devices.

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**Session Classification:** Posters

**Track Classification:** Surfaces and nanostructures for electronics



Contribution ID: 47

Type: **poster**

## **Analysis of GaN and AlN growth on SiC using Synchrotron Radiation.**

High-resolution and high surface-sensitive in-situ core-level photoelectron spectra will be presented and briefly discussed.

The main purpose of the work is to study the intricate and complex phenomena occurring at the surface and interface during the growth mechanism of Ga, Al, GaN on SiC, including the analysis of heterostructures. All the processes are followed in-situ by photoelectron spectroscopy using synchrotron radiation.

To have an overview and reasonable understanding of the several processes involved, a careful fitting and chemical state assignments and detailed analysis of core-level spectra are of great importance. For that purpose, FitXps and Casa XPS are employed.

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## XPS using Ag L $\alpha$ radiation and dual peak analysis of the same element for layer thickness determination

X-ray Photoelectron Spectroscopy is frequently used method for elemental and chemical analysis of surfaces and ultra thin films. By using proper model, the method is also able to obtain information about morphology, for example thickness of ultra thin films. Information depth is dependent on energy of incident X-ray radiation, therefore it is twice higher in case of using Ag L $\alpha$  (2984.3 eV) than standard Al K $\alpha$  (1486.6 eV). In presented work, we studied possibilities of using Ag L $\alpha$  X-ray radiation for determination of Al<sub>2</sub>O<sub>3</sub> layer thickness. The layers were deposited on silicon substrate by Atomic Layer Deposition and analysed by Kratos Axis Supra spectrometer in Czech-NanoLab research infrastructure.

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