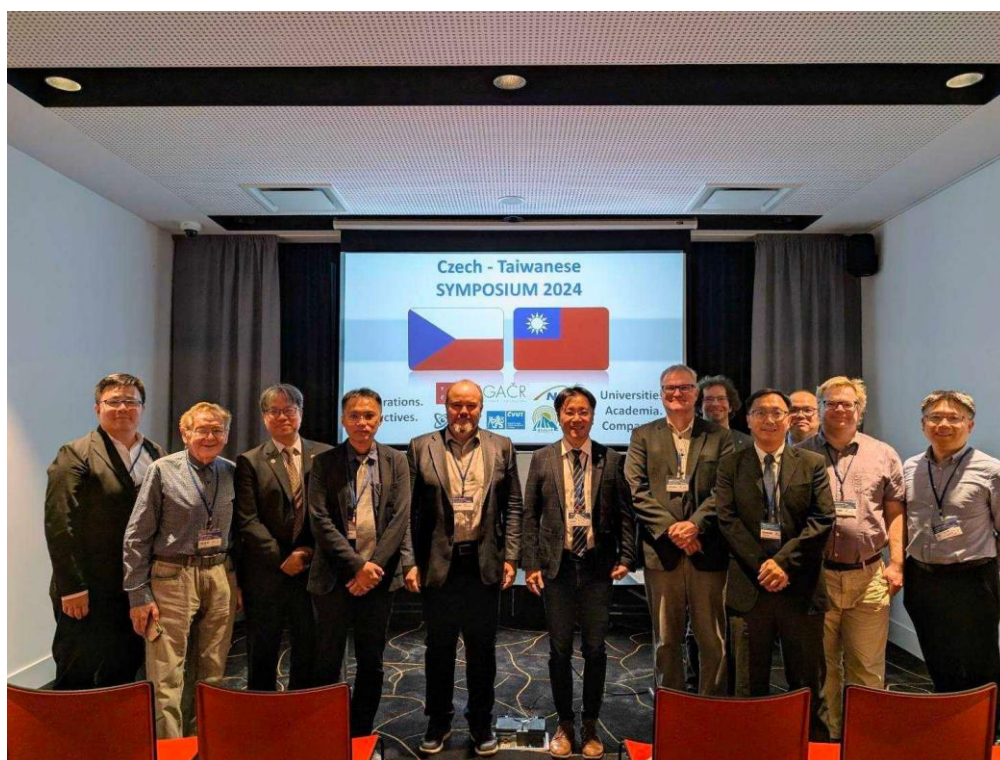


# **2025 Annual Meeting of the Physical Society of Taiwan –**

## **Taiwan-Czech Republic Joint Workshop: Scientific Analysis**

### **Methods and Industrial Collaboration**



The collaboration between Taiwan and the Czech Republic in scientific research has been marked by strong exchanges and joint projects supported by the National Science and Technology Council (NSTC) of Taiwan and the Czech Science Foundation (GACR). Building upon the success of the Czech-Taiwan Bilateral Forum held at NANOCON 2024 in Brno, Czech Republic (<https://www.nanocon.eu/en/czech-taiwanese-symposium/>), this year's Taiwan Physics Annual Meeting in 2025 has invited Czech researchers to Taiwan for further exchanges and to share their research achievements. The Taiwan-Czech Republic Joint Workshop will be held in Kaohsiung, covering research topics that span from fundamental science to industrial applications. This event also offers the Czech participants an in-depth understanding of Taiwanese physics research, allowing them to bring back insights to the Czech Republic and foster more comprehensive research collaborations.



## Program Committee

**Prof. RNDr. Bohuslav Rezek, Ph.D.**

*Czech Technical University in Prague, Czech Republic, EU*

**Prof. Hua Shu Hsu**

*Department of Applied Physics, National Pingtung University, Taiwan*

**Prof. Chien-Cheng Kuo**

*Department of Physics, National Sun Yat-Sen University, Taiwan*

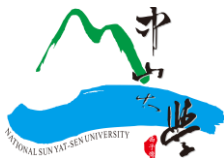
**Dr. Yen-Fa Liao**

*Associate Researcher, National Synchrotron Radiation Research Center (NSRRC), Taiwan*

**Organizers:** The Physics Society of Taiwan, Taiwan



**Hosted by:** National Sun Yat-Sen University, Taiwan



**Sponsors:**

National Science and Technology Council, Taiwan

Czech Science Foundation (GACR), Czech Republic





## Programs

| Thursday, January 16, 2025 |  |
|----------------------------|--|
| Chair: Prof. Hua-Shu Hsu   |  |
| Time                       | Session  |
| 09:00 – 09:10              | <p><b>Opening Speech</b></p> <p><b>Prof. Chia-Ming Kuo</b></p> <p><i>President of the Physical Society of Taiwan, Taiwan</i><br/> <i>Department of Physics, National Central University, Taiwan</i></p> <p><b>Prof. RNDr. Bohuslav Rezek, Ph.D. (Online)</b></p> <p><i>Head of Physics department at the Faculty of Electrical Engineering, Czech Technical University in Prague, Czech Republic, EU</i><br/> <i>Senior researcher at the Department of Thin films and Nanostructures, Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic, EU</i></p> |
| 09:10 – 09:25              | <p><b>FFMD simulations, AFM and CD analyses of chiral helicene assembly on ZnO polar and non-polar facets</b></p> <p><i>Egor Ukraintsev, Ph.D., Czech Technical University in Prague, Czech Republic, EU</i></p>   |
| 09:25 – 09:40              | <p><b>Optical spectroscopy and surface properties of intrinsic and doped nanocrystalline ZnO thin films deposited by pulsed laser deposition on interdigitated electrode</b></p> <p><i>Mgr. Zdeněk Remeš, Ph.D., Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic, EU</i></p>   |
| 09:40 – 09:55              | <p><b>Thermal Plasma Effect on the ZnO Properties - Comparison of the Nano(Micro)rods and Single Crystal Wafer</b></p> <p><i>Mgr. Maksym Buryj, Ph.D., Institute of Plasma Physics of the Czech Academy of Sciences, Prague, Czech Republic, EU</i></p>  |
| 09:55 – 10:10              | <p><b>Spectroscopic studies on freestanding transition metal oxides films</b></p> <p><i>Dr. Shih-Wen Huang, Swiss Light Source, Paul Scherrer Institut, Villigen PSI 4232, Switzerland, EU</i></p>   |



## Programs

|                           |  |
|---------------------------|--|
| 10:10 – 10:30<br>(20 min) | <b>Coffee break</b>  |
| 10:30 – 10:45             | <b>Oxygen vacancy in atomic metal oxide clusters demonstrate outstanding oxygen reduction activity</b><br><i>Prof. Tsan-Yao Chen, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan</i>   |
| 10:45 – 11:00             | <b>Unraveling the Spatial Asynchronous Activation Mechanism of Oxygen Redox-involved Cathode for High-voltage Solid-state Batteries</b><br><i>Dr. Shu-Chih Haw, National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan</i>  |
| 11:00 – 11:15             | <b>Hard X-ray Photoelectron Spectroscopy (HAXPES) for Semiconductor Research</b><br><i>Dr. Yen-Fa Liao, National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan</i>  |
| 11:15 – 11:30             | <b>Revealing Changes in the Electronic Structure of Electrocatalysts for Artificial Photosynthesis via In Situ HERFD-XAS and XES</b><br><i>Dr. Chia-Shuo Hsu, National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan</i>  |
| 11:30 - 12:15             | <b>Industry Forum</b><br><b>Dr. Nan-Hung Yeh (葉南宏)</b><br><i>Manager of Advanced Battery Technologies/ Chief Cell Designer/ Process development/ Project manager, E-One Moli Energy (能元科技)</i><br><b>Dr. Hao-Wen Liu (劉浩汶)</b><br><i>Research Scientist, Lee Chang Yung Chemical Industry Corporation(李長榮化學工業股份有限公司)</i> |



## Egor Ukraintsev

Assistant professor

Czech Technical University in Prague, Czech Republic



Egor Ukraintsev was born in Ekaterinburg, Russia in 1981. Since 2024 he became Czech citizen. He received Ph.D. degree in physics from Moscow State University in 2007 on the study on intermolecular interactions by atomic force microscopy. From 2008 to 2018 he was a researcher in the Institute of Physics, Czech Academy of Sciences. In 2019-2023, he was a research fellow at Faculty of Electrical Engineering, Czech Technical University in Prague. Since 2023 he has become an assistant professor there. He is the author or co-author of two book chapters, more than 50 journal articles, 2 international patent applications, 1 utility model and many contributions in proceedings. His research interests include characterization and modification of material and surface properties by correlative microscopy and spectroscopy (atomic force microscopy, Kelvin probe, electron emission, infrared and Raman spectroscopy) and development of novel atomic force microscopy methods.

### **FFMD simulations, AFM and CD analyses of chiral helicene assembly on ZnO polar and non-polar facets.**

Egor Ukraintsev<sup>1\*</sup>, Pin-Qian Yang<sup>2</sup>, Hua Shu Hsu<sup>2</sup>, Bohuslav Rezek<sup>1</sup>

<sup>1</sup>*Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic*

<sup>2</sup>*Department of Applied Physics, NPTU University, Pingtung, Taiwan*

*\* Presenter: Egor Ukraintsev, E-mail: ukraiego@fel.cvut.cz*

**Abstract:** Interaction of organic molecules with semiconductor surfaces is key to many applications from energy conversion to electronic sensors and catalysis. Despite the importance of [7]-helicene as a small chiral molecule, its interactions with zinc oxide (ZnO) nanomaterials that are prospective in photocatalysis and spintronics have not yet been sufficiently explored. Here, the impact of surface polarity of different ZnO facets on P/M-[7]-helicene adsorption is studied both experimentally by atomic force microscope (AFM), circular dichroism (CD), and theoretically by force field molecular dynamics (FFMD). Nonpolar ZnO surfaces cause self-assembly into layered nanoislands with characteristic 4 nm layer thickness.





Polar O-face ZnO surface causes the formation of similar nanoislands, while polar Zn-face ZnO surface is practically clean with few circular objects. CD measurements do not detect the presence of sub-monolayer helicene structures but reflect ZnO slab orientation. FFMD simulations help reveal the effect of surface dipole electric field orientation on helicene self-assembly. The results thus show a way for controlling the assembly of [7]-helicene and other chiral molecules for diverse applications.

**Keywords:** Carbon nanostructures, molecular adsorption, polar and non-polar surfaces, helicene molecules, ZnO, AFM, CD, MD simulations

## 1. Introduction

Nanoparticles (NPs) are widely used for different applications. Usually, NPs do not have a well-defined surface; each individual NP may have several different surface facets. The interaction between different surface facets and adsorbing molecules can vary significantly. For example, the same material can form different structures on substrates with the same composition [1-4]. In this work, we present the results of adsorption experiments, conducted theoretically by force field molecular dynamic simulations (FFMD) and experimentally by atomic force microscopy (AFM), with chiral molecules on low-index ZnO surfaces.

## 2. Results and Discussion

Figure 1 shows the result of adsorption experiments of single P-[7]-helicene molecules on four low-index ZnO surfaces. Individual helicene molecules tend to adsorb on Zn-face and  $(10\bar{1}0)$  ZnO surfaces, while they tend to repel from O-face ZnO surfaces and float within the unit cell on  $(10\bar{2}0)$  ZnO surfaces. Similar results were obtained in simulations with 100 helicene molecules.

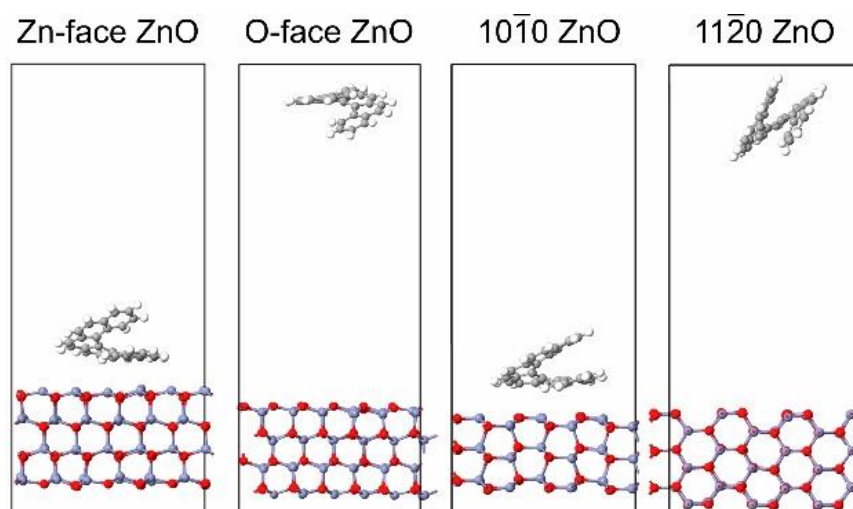


Fig. 1. The result of simulation adsorption experiments of single P-[7]-helicene molecules on 4 ZnO surfaces.



Figure 2 shows the result of adsorption experiments and formation of helicene nanostructures on different ZnO surface facets. The results for both chiral molecules, P-[7]-helicene and M-[7]-helicene, were very similar on all low-index ZnO surfaces. Zn-face ZnO surfaces were practically clean after deposition of P-[7]-helicene and M-[7]-helicene, only some aggregates were found. Nanoislands with characteristic thickness  $\sim 4$  nm were found on O-face and both non-polar surfaces. In many cases on O-face ZnO surface a taller object was found in the middle of helicene nanolayer.

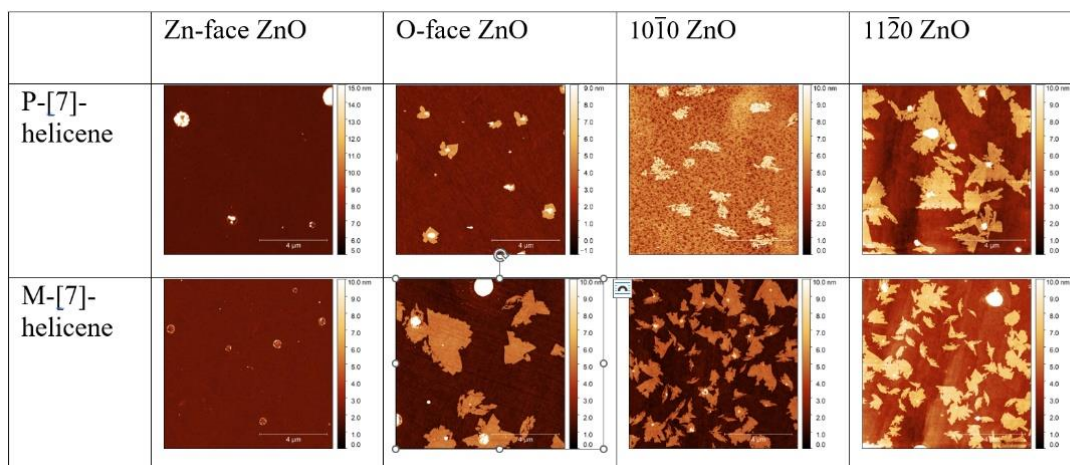


Fig. 2. The result of adsorption experiments of P- and M-[7]-helicene molecules on 4 different ZnO surfaces.

CD measurements did not detect the presence of sub-monolayer helicene structures but did reflect ZnO slab orientation and asymmetry. With further setup and parameter tuning, CD shows prospects for detecting chiral molecule assembly on ZnO.

### 3. Conclusions

The adsorption of P- and M-[7]-helicene, chiral molecules, on various ZnO surfaces with different surface polarity was studied experimentally by AFM and theoretically by classical MD. Experimental results show that both a single P-[7]-helicene molecule and a group of 100 P-[7]-helicene molecules are attached to Zn-face and (10 $\bar{1}$ 0) ZnO surfaces, while they tend to repel from O-face ZnO surfaces and float within the unit cell on (10 $\bar{2}$ 0) ZnO surfaces.

High-resolution AFM topography measurements were employed to study the morphology of helicene molecules on four low-index ZnO surface facets. Results show very similar behavior for both chiral molecules, P-[7]-helicene and M-[7]-helicene. Zn-face ZnO surfaces were practically clean after deposition of P-[7]-helicene and M-[7]-helicene, with only some aggregates found. Nanoislands with a characteristic thickness of  $\sim 4$  nm were observed on O-face and both non-polar surfaces, with taller objects often present in the middle of the nanolayer.



Such nanoislands made from chiral molecules can be considered as quantum dots and as a new type of spin-polarized nanomaterial. Polar ZnO O-face and both nonpolar surfaces may be ideal for creating chiral quantum dots. Similar to thiorphan [1], the well-defined self-limited nanometer thicknesses of the observed dense molecular layers serve as examples of novel ultrathin nanostructured two-dimensional (2D) molecular nanomaterials.

## References

- [1] E. Ukraintsev, H. Hematian, and B. Rezek, “Polarization Controlled Assembly of Ultrathin Thiorphan Nanostructures on ZnO Surface Facets,” *Langmuir*, vol. 39, no. 5, pp. 1764–1774 (2023), doi: 10.1021/acs.langmuir.2c02393.
- [2] H. Hematian, E. Ukraintsev, and B. Rezek, “Strong Structural and Electronic Binding of Bovine Serum Albumin to ZnO via Specific Amino Acid Residues and Zinc Atoms,” *ChemPhysChem*, cphc.202100639 (2021), doi: 10.1002/cphc.202100639.
- [3] B. Rezek et al., “Microscopic Study of Bovine Serum Albumin Adsorption on Zinc Oxide (0001) Surface,” *Phys. Status Solidi A*, vol. 218, no. 6, 2000558 (2021), doi: 10.1002/pssa.202000558.
- [4] E. Ukraintsev, B. Rezek, A. Kromka, A. Broz, and M. Kalbacova, “Long-term adsorption of fetal bovine serum on H/O-terminated diamond studied in situ by atomic force microscopy,” *Phys. Status Solidi B*, vol. 246, no. 11–12, pp. 2832–2835 (2009), doi: 10.1002/pssb.200982257.





## Zdenek Remes

Senior Scientist

FZU - Institute of Physics of the Czech Academy of Sciences  
Na Slovance 1999/2, 182 00 Prague 8, Czech Republic



PhD. in solid state physics from the Faculty of Mathematics and Physics, Charles University in Prague (1999), postdoctoral fellowships at the University of Hasselt (Belgium) and TECHNION - Israel Institute of Technology, Haifa (1999-2004). Assistant Professor at the Czech Technical University in Prague (since 2013) and Senior Researcher at the FZU - Institute of Physics of the Czech Academy of Sciences with h-index 30 and 203 published documents according to Scopus (November 2, 2024). An expert in solid state optical spectroscopy (UV-visible-NIR absorption, photocurrent, photoluminescence, FTIR, Raman), optical and electrical properties of thin films, bulk and surface electronic states in thin films, nanoparticles and hybrid nanostructures, kinetic processes of charge and energy transfer in solar cells, diodes and sensors.

### **Optical spectroscopy and surface properties of intrinsic and doped nanocrystalline ZnO thin films deposited by pulsed laser deposition on interdigitated electrodes**

Zdenek Remes<sup>1\*</sup>, Neda Neykova<sup>1,2</sup>, Sergii Chertopalov<sup>1</sup>, Gabriel Vanko<sup>1</sup>, Egor Ukraintsev<sup>2</sup>, Bohuslav Rezek<sup>2</sup>, Jaroslav Bruncko<sup>3</sup>, Hua Shu Hsu<sup>4</sup>

<sup>1</sup>*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

<sup>2</sup>*Faculty of Electrical Engineering, Czech Technical University, Prague, Czech Republic*

<sup>3</sup>*International Laser Centre, Slovak Centre of Scientific and Technical Information, Bratislava, Slovak Republic*

<sup>4</sup>*Department of Applied Physics, National Pingtung University, Pingtung, Taiwan*

\* Presenter: Zdenek Remes, E-mail: [remes@fzu.cz](mailto:remes@fzu.cz)

Zinc oxide (ZnO) is a low-cost and environmentally friendly material with unique optical properties and a variety of nano and microstructures. These properties impose challenges for applications in energy conversion, scintillators, photocatalytic wastewater treatment, electrochemical energy storage, and sensing.



In our previous work, we presented results on nanocrystalline ZnO thin films prepared by reactive magnetron sputtering of a Zn target in a pure oxygen atmosphere. We demonstrated that plasma hydrogenation effectively suppresses ZnO defects, significantly increasing electrical conductivity and exciton-related UV luminescence. We observed good room-temperature stability of the plasma-hydrogenated ZnO nanocrystals in air, but rapid degradation at elevated temperatures.

In this study, nominally undoped and doped (Co, Al, In, Ga) nanocrystalline ZnO thin films were pulsed laser deposited (PLD) on commercial interdigitated gold electrodes (MicruX Technologies, Spain) and tested using optical, photocurrent, and impedance spectroscopy. Surface properties were characterized by Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM).

To further investigate surface-related effects, we employed a custom-built inductively coupled plasma (ICP) 13.56 MHz reactor with up to 300 W RF discharge power and exposed ZnO samples to the ICP plasma.

This work was supported by the Czech Science Foundation (project no. 24-10607J), the Operational Programme Johannes Amos Comenius, funded by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (SENDISO—CZ.02.01.01/00/22\_008/0004596), and the Slovak Research and Development Agency (project no. APVV-23-0083).

**Keywords:** *solid-state material growth and synthesis, and its electrical and optical characterizations, semiconductor/optoelectronic-related devices physics, fabrication, and characterizations and performances, electronic transport in semiconductor, thin films and heterostructures*



## Dr. Maksym Buryi

Head of the Plasma Chemical Technologies Department

Institute of Plasma Physics of the Czech Academy of Sciences



- 2014 - Ph.D. in Physics in Czech Technical University in Prague
- 01.05.2022-31.12.2023 – Head of group at the FZU – Institute of Physics of the Czech Academy of Sciences (CAS)
- 01.01.2024- – Head of Department at the Institute of Plasma Physics CAS.

Fields of interest. Plasma chemical technologies, nanomaterials engineering, EPR and luminescence spectroscopies.

Projects. Principal Investigator (PI) and Co-PI of the Czech Science Foundation projects in 2020-2024: No. 20-05497Y (Accomplished. Evaluation: Excellent); No. 24-12872S (2024-2026); No. 24-14580L (Bilateral with Poland; 2024-2026).

Awards. Otto Wichterle Prize (2021) by the Czech Academy of Sciences for outstanding achievements in the field of inanimate nature sciences. Medal of the Ministry of Education, Youth and Sports for the outstanding teaching and scientific activities (2023).

Scientific metrics (SCOPUS). Author and co-author of 103 papers in peer-reviewed journals (1207 citations). Hirsch index,  $H = 21$ . Member of international advisory committee of two conferences (EIRODIM and ICDIM).

### Thermal Plasma Effect on the ZnO Properties - Comparison of the Nano(Micro)rods and Single Crystal Wafer

Maksym Buryi<sup>1\*</sup>, Tomáš Hostinský<sup>1</sup>, Brenda Natalia Lopez Niño<sup>1</sup>, Bohuslav Rezek<sup>2</sup>, Jaroslav Kuliček<sup>2</sup>, Andrey Prokhorov<sup>1,4</sup>, Jakub Volf<sup>4</sup>, Zdeněk Remeš<sup>4</sup>, Júlia Mičová<sup>3</sup>

<sup>1</sup>Plasma Chemical Technologies Department, Institute of Plasma Physics of the Czech Academy of Sciences, Prague, Czech Republic

<sup>2</sup>Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic

<sup>3</sup>Institute of Chemistry of the Slovak Academy of Sciences, Bratislava, Slovak Republic

<sup>4</sup>Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

\*Presenter: Maksym Buryi, E-mail: buryi@ipp.cas.cz\*



An increasing number of applications is using zinc oxide (ZnO) nanosystems. Therefore, ZnO-based nanostructures appear on the top of the worldwide research and development. Its broad bandgap reaching a value of about 3.3-3.5 eV, high exciton binding energy of about 60 meV, and ultrafast luminescence timing (decay time is about 400-500 ps in the case of excitonic emission) make it especially attractive for the time-of-flight (TOF) positron emission tomography, especially when combined with other materials like CsPbBr<sub>3</sub>. Another scientific and industrial application for ZnO and/or CsPbBr<sub>3</sub> is in solar cells and other renewable energy sources.

It is well known that luminescence and charge carrier mobility can be altered by doping with different ions and/or post-growth treatments such as annealing in different atmospheres and plasma processing. Erbium doping, air annealing, and separate hydrogen plasma treatment have proven to be the efficient techniques leading to modification of ZnO characteristics. However, nothing is known about Er doping at larger concentrations (1-30%) and concomitant hydrogen plasma treatment combined with the earlier air annealing or vice versa. The current work attempts to address every aspect of the doping and post-growth treatment of ZnO nano- and microrods, seeking ways to improve luminescence efficiency.

The factors influencing the photophysics of luminous materials are typically point defects of different origins. These may have a complicated genesis, particularly at a heterostructure's edge. To understand their effect on ZnO-based structures, the approach is to first examine the ZnO substrate. Second, the ZnO nano- and microrods will be scrutinized to comprehend the unique characteristics of the ZnO surface, particularly with regard to boundary, charge, and energy transfer.

Notably, it is uncertain how the Zn- or O-face along the <0001> axis or the Zn and O combination along the <1010> (or similar) axis of ZnO would affect the situation. To reveal the impact of the ZnO facet on the ZnO surface properties, specific techniques will be used, including photoluminescence, radioluminescence, electron paramagnetic resonance, X-ray diffraction, scanning electron microscopy, and atomic force microscopy.

## Acknowledgements

The financial support of the Czech Science Foundation project No. 24-12872S and the program “Strategy AV 21” of the Czech Academy of Sciences, specifically work package VP 27 - Sustainable Energy (Renewable energy resources and distributed energy systems), are gratefully acknowledged.

**Keywords:** ZnO nano(micro)rods, Thermal plasma treatment, Luminescence, Electron Paramagnetic Resonance, Point defects



## Shih-Wen Huang

Scientist

Paul Scherrer Institut, Switzerland



I specialize in synchrotron-based spectroscopic and scattering techniques, including soft x-ray absorption, resonant elastic /inelastic scattering, resonant, as well as time-resolved x-ray scattering/spectroscopy. My research focuses on exploring strongly correlated electron systems with emergent properties.

### Spectroscopic studies on freestanding transition metal oxides films

Shih-Wen Huang<sup>a</sup>

<sup>a</sup> *Swiss Light Source, Paul Scherrer Institut, Villigen PSI 4232, Switzerland*

Freestanding oxide films have recently attracted enormous attention due to their nanometer-scale thickness that allows explorations of material properties toward quasi two-dimensional (quasi-2D) limits without the influence of supporting substrates. In this talk, I will present our recent studies on freestanding SrTiO<sub>3</sub> (STO). STO exhibits the quantum paraelectric behavior in bulk form, and it becomes ferroelectric when strained. Our x-ray diffraction measurements on freestanding STO (STO\_FS) films reveal that STO\_FS loses its cubic structure at room temperature and becomes tetragonal when the thickness is less than 20 nm. The structure instability modifies the Ti-O pd hybridization, causing the valence of Ti ion to deviate from the nominal 4+ values. The refined lattice parameters from XRD show no measurable strain effect at room temperature, and the THz time-domain spectroscopy suggests that STO\_FS becomes polar at a temperature as high as 85 K.





## Tsan-Yao Chen

Professor

Department of Engineering and System Science,  
National Tsing Hua University, Hsinchu, Taiwan



Chen Tsan-Yao is the Professor at National Tsing Hua University. With over 10 years of expertise in materials characterization and 6 years specializing in electronic device failure analysis (focusing on MEMS and ICs) using Synchrotron Light Source techniques at NSRRC, Taiwan, he conducts foundational research on materials for green energy applications. His work includes fuel cells, CO<sub>2</sub> conversion, and water pollutants sensing, in collaboration with renowned research teams from Russia, the USA, Italy, Japan (SPRING-8), and the UK. Professor Chen leads projects funded by both academic and industrial, focused on physical chemistry research and environmental sensing technologies. Heading a team dedicated to nanocrystal design and fabrication for energy conversion applications, his group specializes in atomic cluster decoration techniques to enhance catalyst redox performance. This interdisciplinary, multi-scale approach to heterogeneous catalysis addresses emerging real-world challenges in green energy.

### Oxygen vacancy in atomic metal oxide clusters demonstrate outstanding oxygen reduction activity

Tsan-Yao Chen<sup>a†</sup>, Sheng Dai<sup>b\*</sup>, Jyh-Pin Chou<sup>c</sup>, Kuan-Wen Wang<sup>d</sup>, Alice Hu<sup>e</sup>

<sup>a</sup> Department of Engineering and System Science, National Tsing Hua University, Hsinchu 30013, Taiwan

<sup>b</sup> School of Chemistry & Molecular Engineering, East China University of Science and Technology, Shanghai 200237, P.R. China

<sup>c</sup> Department of Physics, National Changhua University of Education, Changhua, Taiwan

<sup>d</sup> Institute of Materials Science and Engineering, National Central University, Taiwan

<sup>e</sup> Department of mechanical and biomedical engineering, City University of Hong Kong

Hierarchical structured heterogeneous catalyst comprising atomic metal oxide clusters with high contents of oxygen vacancy (O<sup>V</sup>) and the carbon or Co oxide supported metal / oxide nanoparticle (NPs) is developed for electrocatalytic application. Such a catalyst processes a



collaboration between  $O^V$ s and the neighbouring atoms in the electrochemical reaction. With this characteristic, the reaction kinetics of all steps are simultaneously operated consequent leading to a quantum leap on the current density and stability of the redox reaction. Apart from using noble metals, atomic scaled Co oxide clusters ( $CoO_x^a$ ) were employed. Those clusters are decorated in surface defect regions of Co oxide supported Pd nanoparticles ( $CoO_x^a$ -Pd) by using self-aligned nanocrystal growth followed by ultra-high-speed quench reaction with strong reduction agent. The decorated  $CoO_x^a$  localize electrons from the neighbouring atoms and thus boost the activity of  $CoO_x^a$ -Pd in ORR. With a proper reaction time and loading control, the  $CoO_x^a$ -Pd enhance its mass activity by 340 times as compared to that of commercial Pt catalysts in an alkaline electrolyte of 1.0M KOH.



## Dr. Shu-Chih Haw

Assistant Scientist

National Synchrotron Radiation Research Center (NSRRC)



Dr. Shu-Chih Haw holds a Ph.D. in Science and Technology of Synchrotron Light Sources from National Tsing Hua University and is currently an assistant scientist specializing in soft X-ray absorption spectroscopy. Dr. Haw's research centers on strongly correlated materials, with a particular focus on advanced materials for lithium-ion batteries, employing cutting-edge spectroscopic techniques.

### **Unraveling the Spatial Asynchronous Activation Mechanism of Oxygen Redox-involved Cathode for High-voltage Solid-state Batteries**

Shu-Chih Haw<sup>a</sup>

<sup>a</sup> National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan

Li-rich layered oxides (LRLO) exhibit significant potential for use in all-solid-state lithium batteries (ASSLBs) owing to their high capacities and wide range of operating voltages. However, the practical application of LRLO in ASSLBs is hindered by the severe failure of carrier transport at the solid–solid interface, which subsequently limits the electrochemical activity of these batteries. Here, the spatially asynchronous activation mechanism of the LRLO in ASSLBs is presented. A spectroscopic study extending from the surface into the bulk interior of LRLO indicates that the activation kinetics of anionic oxygen prefers hysteretic delivery over uniform delivery and fast transition metals (TMs) activation. This spatial hetero activation is dominated by the failure of carrier transport at the interface, which is induced by microstructural defects in the composite cathode. This study is expected to facilitate the microstructural design of high-performance LRLO-based ASSLBs.



## Yen-Fa Liao

Associate Scientist

National Synchrotron Radiation Research Center (NSRRC)



Dr. Yen-Fa Liao is a beamline scientist at the National Synchrotron Radiation Research Center specializing in the application of synchrotron techniques, with a particular focus on Hard X-ray Photoelectron Spectroscopy (HAXPES). He is in charge of the construction, development, and optimization of the HAXPES end station, where he utilizes HAXPES to investigate the electronic structures of semiconductor materials.

### Hard X-ray Photoelectron Spectroscopy (HAXPES) for Semiconductor Research

Hsiu-An Liu<sup>a</sup>, Ya-Hsin Cheng<sup>a</sup>, and Yen-Fa Liao<sup>a</sup>

<sup>a</sup> National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan

We have established a new Hard X-ray Photoelectron Spectroscopy (HAXPES) experimental end station at the Taiwan Photon Source (TPS), specifically designed for semiconductor research. The high penetration capabilities of the hard X-rays in this technique provide a significant advantage for investigating semiconductor devices and multilayer systems, particularly the electronic structure of the inner layers and interfaces of semiconductor devices.

One of our primary research objectives is to analyze the interfaces within semiconductor devices to enhance their efficiency and operational stability. Utilizing HAXPES, we can detect the distribution of interface elements and chemical shifts, offering valuable insights into the factors that influence semiconductor performance and strategies for optimization.

Additionally, developing an in situ/operando setup for semiconductor devices will be a crucial focus of our research at the HAXPES experimental end station. This capability will enable us to monitor and understand the dynamic physical characteristics of devices under actual operating conditions.



## Dr. Chia-Shuo Hsu

Assistant Scientist

National Synchrotron Radiation Research Center (NSRRC)



Dr. Chia-Shuo Hsu earned a Ph.D. in Chemistry from National Taiwan University and is currently an assistant scientist with a focus on X-ray absorption spectroscopy and X-ray emission spectroscopy. Dr. Hsu's research is centered on elucidating the complex processes of electron transfer and catalyst functionality during reactions. This work facilitates the identification of critical factors that influence the performance, durability, and selectivity of electrocatalysts.

### **Revealing Changes in the Electronic Structure of Electrocatalysts for Artificial Photosynthesis via In Situ HERFD-XAS and XES**

Chia-Shuo Hsu<sup>a</sup>

<sup>a</sup> *National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan*

Artificial photosynthesis is a promising method for energy storage and CO<sub>2</sub> conversion into fuel. To minimize energy consumption, it is crucial to utilize electrocatalysts that exhibit high activity, selectivity, and stability. Achieving an optimal catalyst necessitates a comprehensive understanding of its reaction mechanisms. Recent advancements in in-situ experimental techniques have significantly enhanced our ability to investigate these mechanisms. Our research concentrates on analyzing transition metal-based catalysts through high energy resolution fluorescence-detected X-ray absorption spectroscopy (HERFD-XAS) and X-ray emission spectroscopy (XES). These techniques facilitate a thorough examination of how transformations in the catalyst's symmetry center during reactions affect catalytic activity. Additionally, they provide valuable insights into the electronic structure changes that occur during catalyst reconstruction, which influence product selectivity, as well as the impact of the catalyst's bonding environment on its stability. Ultimately, these insights aid in the rational design of more efficient electrocatalysts.

**Keywords:** *X-ray spectroscopy, electrocatalyst, In-situ methodology*