TCMs TOEO 2025

19-23 October 2025

Rethymno, Crete, Greece

10th International Symposium on Transparent Conductive Materials & 14th International Symposium on Transparent Oxide and Related Materials for Electronics and Optics

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TCM NET

FORTH INSTITUTE OF ELECTRONIC STRUCTURE AND LASER

ARISTOTLE UNIVERSITY OF THESSALONIKI

BOOK OF ABSTRACTS

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Welcome

Dear Colleagues and friends,

We are delighted to welcome you to the 10th International Symposium on Transparent Conductive Materials & 14th International Symposium on Transparent Oxide and Related Materials for Electronics and Optics (TCM-TOEO 2025).

Building on the success of previous conferences held in Crete (2006, 2008, 2010, 2012, 2014, 2016, 2018, 2022), Tokyo (2023) and Leipzig (2024), this year TCM-TOEO 2025 returns to Crete, in Rethymno, Greece, from Sunday 19th to Thursday 23th October 2025, continuing to be a fruitful platform for the development of the metal oxide community with the addition of new topics such as quantum technologies and energy storage devices.

Traditionally, during these events, we have all had the opportunity to meet with dear friends and colleagues from all over the globe and make new ones widening our academic and research horizons. Young researchers advanced rapidly in their fields and past post-docs are now participating as invited speakers. Senior researchers moved forward from academic to industrial research and vice versa, contributing to significant advances in their fields or opening new roads for the next generation of researchers. We have all had the pleasure of following developed careers, fellow scientists moving to more challenging and reputable posts while winning prestigious National and International awards and distinctions. On the other side, we have proudly seen colleagues that despite getting official retirement are still research active, continuing mentoring and training students while disseminating their wisdom to the next generation of young researchers. To all of you the community as a whole and I personally, are deeply grateful.

With this short note, I am proudly welcoming you all to this year’s joint meeting and wish you a scientific, fruitful, and personally pleasant stay.

Warm regards,

Prof. Vassilios Binas

TCM-TOEO 2025 Conference Chair

Program

Sunday, October 19	
16:00-17:30	Registration
Room	Megas Alexandros
17:30-18:00	**Welcome Addresses**
Chairs	**George Kiriakidis & Vassilios Binas**
18:00-18:40	**Plenary 1** **Hideo Hosono** Progress in science and application of transparent oxide semiconductors
18:40-19:20	**Plenary 2** **Lars Österlund** ZnO interfaces: Defects, heterostructures and surface chemistry
19:30-20:30	**Welcome Reception**

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Monday, October 20

Room	Megas Alexandros	
Chair	**Hideo Hosono**	
09:00-09:40	**Plenary 3** **Andreas Klein** Analyzing defect properties in oxides by x-ray photoelectron spectroscopy	
09:40-10:20	**Plenary 4** **Gunnar Westin** Complex structure and composition metal-oxides through solution processing	
10:20-10:50	**COFFEE BREAK**	
Room	**Megas Alexandros**	**Achilles**
Chairs	**Andreas Klein**	**Emmanouil Gagaoudakis**
	Invited Presentations	
10:50-11:20	**Daniel Bellet** Brief overview of metallic nanowire based transparent conductive materials	**Juris Purans** Adaptive chromogenic material for smart windows
11:20-11:50	**Dimitrios A. Koutsouras** Organic materials for bioelectronic devices	**Jiri Rezek** High-power impulse magnetron sputtering as a knob for tailoring transparent conductive oxides
	Oral Presentations	
11:50-12:10	**Markus R. Wagner** From crystal symmetry to heat flow: resolving anisotropic transport in gallium oxide phases	**Jörgen Sweelssen** Tailored liquid-phase chemistry to achieve low-temperature synthesis of $BiVO_4$ for photoelectrochemical water splitting
12:10-12:30	**Marlene Härtel** Industry-scaled DC sputtering of SnZnOx: toward indium-free transparent electrodes for solar cells	**Joon-Ho Oh** Triode plasma approach to low-damage TCO deposition for silicon heterojunction solar cells
12:30-12:50	**Mustafa Göktürk Yazlak** Revealing the incorporation sites and local structure of nickel and selenium in doped copper iodide thin films	**Jan Koloros** Low-resistivity of highly nitrogen-doped p-type Cu_2O thin films prepared by reactive HiPIMS
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Room	Megas Alexandros	
Chair	**Lars Österlund**	
14:50-15:30	**Plenary 5** **Sanjay Mathur** Magnetically Tailored Metal Oxide Thin Films as Efficient Catalysts for Green H_2 and NH_3 Synthesis	
15:30-16:10	**Plenary 6** **Bernd Szyszka** Activation of thin film growth versus plasma damage – the challenge in sputtering of transparent conductors and active semiconductive coatings	
16:10-16:40	**COFFEE BREAK**	
Room	**Megas Alexandros**	
Chair	**Sanjay Mathur**	
16:40-17:20	**Plenary 7** **Darrell Schlom** Reaching beyond Diamond to Sapphire, a 7 eV Semiconductor	
17:20-18:00	**Plenary 8** **Panos Patsalas** Laser growth and processing of materials in the nanotechnology era	
Room	**Megas Alexandros**	**Achilles**
Chairs	**Bernd Szyszka**	**Panos Patsalas**
	Invited Presentations	
18:00-18:30	**József S. Pap** Benchmarking membrane electrode assembly inks with transparent conductive oxides for proton-exchange membrane water electrolysis	**Nikolaos Pliatsikas** Laser processes for colloidal conductive metal nitrides
	Oral Presentations	
18:30-18:50	**Varun Ranade** Real time optical observation of multi-filament formation and electrode remodeling in Ag/SiO_2/Au memristors	**Eleanor Teather** Development of a synthesis route for $YScS_3$, a potential sulfide p-type TCM
18:50-19:10	**Dwight Acosta** A rejuvenation study of WO3 and Re:WO3: thin films deposited on fto substrate using ultrasonic spray pyrolysis	**François Balty** Insight into the morphological instability of metallic nanowires under thermal stress
19:10-19:30	**Nirmal Kumar** Sputter deposited CuO-WO3 nanosized heterojunctions for gas detection	**Ainur Zhussupbekova** Cation engineering and quantum effects in zinc tin oxide films

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Tuesday, October 21

Room	Megas Alexandros	
Chair	**Vasiilios Binas**	
09:00-09:40	**Plenary 9** **Julia Medvedeva** Maximizing electrical conductivity in amorphous oxide semiconductors	
09:40-10:20	**Plenary 10** **George Adamopoulos** Solution-Processed YIZO-based synaptic transistors for neuromorphic applications	
10:20-10:50	**COFFEE BREAK**	
Room	**Megas Alexandros**	**Achilles**
Chairs	**Julia Medvedeva**	**George Adamopoulos**
	Invited Presentations	
10:50-11:20	**Ulrike Kraft** Stretchable conducting polymers and devices for biosensing applications	**Berit Goodge** Advances in electron microscopy for atomic-scale insights to engineer functional oxide thin films
11:20-11:50	**Fabio Cicoira** Repairable, recyclable, and stretchable electronic materials	**Tomas Kubart** Reactive high power impulse magnetron sputtering of oxide thin films
	Oral Presentations	
11:50-12:10	**Doga Selin Memikoglu** Two-Layer ITO metallization in transparent electronics	**Atsushi Shimizu** High sensitivity H_2 gas sensor gas sensor utilizing large on/off ratio of amorphous In-Ga-Zn-O thin film transistor
12:10-12:30	**Brian Walls** Optical anisotropy of pristine and reduced V_2O_5(010)	**Ekaterine Chikoidze** Two-dimensional electron (2DEG) and hole (2DHG) gases onto β-Ga_2O_3
12:30-12:50	**Ling Lu** Hyper-gap transparent conductor & superconductor	**Maria de la Luz Olvera** Transparent and conductive codoped-ZnO thin films (IGZO, IAZO, AGZO) deposited by ultrasonic chemical spray technique
12:50-14:50	**LUNCH BREAK**	

Room	Megas Alexandros	
Chair	**Elisabetta Comini**	
14:50-15:30	**Plenary 11** **Chris Van de Walle** Hydrogen in indium oxide and gallium oxide	
15:30-16:10	**Plenary 12** **Wen Ruitao** Electrochromic materials for visible and near infrared light modulation	
16:10-16:40	**COFFEE BREAK**	
Room	**Megas Alexandros**	
Chair	**Tetsuya Yamamoto**	
16:40-17:20	**Plenary 13** **Norifumi Fujimura** Novel chemical vapor deposition process of ZnO and Ga_2O_3 films by nonequilibrium atmospheric pressure N_2/O_2 Plasma	
17:20-18:00	**Plenary 14** **Holger von Wenckstern** Creation of material libraries of wide and ultra-wide bandgap conductive oxides by combinatorial pulsed laser deposition	
Room	**Megas Alexandros**	**Achilles**
Chair	**Chris Van de Walle**	**Wen Ruitao**
	Invited Presentations	
18:00-18:30	**Dalibor M. Stanković** Transparent electrodes and semiconductor materials for electrocatalysis applications	**Maria Kandyla** Micro/nano-structures of transparent oxides by laser processing for optoelectronics and smart surfaces
	Oral Presentations	
18:30-18:50	**Jonas Elz** The plasma plume deflection and target surface roughness during pulsed laser deposition of functional oxides	**Amaury Baret** Heuristic approach to the fundamental optical constants of silver nanowire networks: experiments and theory
18:50-19:10	**Emmanouil Gagaoudakis** Flexible, printed absorbers for shielding against microwave radiation	**Liam Morgan** QM/MM Investigations of defects in MgO and their use as a model system for high-Tc Superconductivity

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19:10-19:30	**Ke Li** Extrinsic doping mechanism in Sb_2O_5 as a promising n-type transparent conducting oxide	**Måns Mattsson** Full subgap defect density of states in p- and n-type metal oxide transistors
19:30-19:50	**Mona Tréguer-Delapierre** Oxidation-resistant Cu-based nanowires transparent electrodes activated by an exothermic reaction	A. Chebotareva Electrical Properties of Heterostructure Metal - Polyarylene Ether Ketone Copolymer - TCO

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Wednesday, October 22

Room	Megas Alexandros	
Chair	**Norifumi Fujimura**	
09:00-09:40	**Plenary 15** **Elisabetta Comini** From Sensing to Energy: Metal Oxide Nanostructures for Green Technologies	
09:40-10:20	**Plenary 16** **Tetsuya Yamamoto** Materials Design of High Carrier Transport Oxide Films for Various Applications	
10:20-10:50	**COFFEE BREAK**	
Room	**Megas Alexandros**	**Achilles**
Chair	**Holger von Wenckstern**	**Emmanouil Gagaoudakis**
	Invited Presentations	
10:50-11:20	**Junjun Jia** Switching the Transparency of Semiconductor Thin Films	**Ilya Sytjugov** Nanomaterials for Semi-Transparent Photovoltaics and Transparent Wood
11:20-11:50	**Spyros Kassavetis** Colloidal Metal Oxides for Printed Electronics	**P. Mazzolini** Challenges and perspectives in r-GeO_2 heteroepitaxy
	Oral Presentations	
11:50-12:10	**Maria del Mar Rodriguez** Protection of Transparent Electrodes based on metallic nanowires by nitrides deposited by Plasma-Enhanced ALD	**Ryotaro Nakazawa** Direct observation of the density of in-gap states of In_2O_3:H thin films and the origin of instability of thin film transistors
12:10-12:30	**Minseok Kim** New evaluation method on various gas barrier performances using functional oxide films (1); O_2 or H_2O barrier properties	**Sabine Heusing** Electrospun fiber coatings as new transparent conductive coatings
12:30-12:50	**Anthony Sanderse** Surface activation of $BiVO_4$ for improved performance in alkaline photoelectrochemical water splitting	**Sandra Montag** Uncovering the element-specific interatomic distances throughout the Cu(Br,I) alloy system
12:50-14:50	**LUNCH BREAK / POSTER SESSION II**	

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	Megas Alexandros	
Chair:	**George Adamopoulos**	
14:50-15:30	**Plenary 17** **Clark Bright** Metallic thin films: Back to the future	
15:30-16:10	**Plenary 18** **Pedro Barquinha** Beyond the pixel: oxide TFTs shaping smart, sustainable systems	
16:10-16:40	**COFFEE BREAK**	
	Megas Alexandros	
Chair	**Nektarios Lathiotakis**	
16:40-17:20	**Plenary 19** **Yiannis Deligiannakis** Precision engineering of functional NanoOxides at industrial scale: from lab scale research to the TRL ladder	
17:20-18:00	**Plenary 20** **Volker Sittinger** Sputtering technologies for the deposition of transparent conductive oxides on large areas	
Room	**Megas Alexandros**	**Achilles**
Chair	**Yiannis Deligiannakis**	**Volker Sittinger**
	Oral Presentations	
18:00-18:20	**Peter Russell** Computational prediction of $Cd_2Sb_2O_7$ as a candidate TCO	**Keisuke Ide** Fast solution of inverse problems on IGZO transistor characterization via tandem neural network
18:20-18:40	**Petr Novák** Structural properties of Ga_2O_3 thin films grown via dc-pulsed magnetron sputtering using a liquid gallium target	**Stefanie Frick** Transparent conductive Cu diffusion barriers: A 2-dimensional combinatorial screening study on the In-Zn-O system
18:40-19:00	**Romain Claes** Exploring the Sb (V) oxides: transport and defect properties of ASb_2O_6 (A = Mg, Ca, Sr, Ba, Cd)	**Taiga Kurihara** New evaluation methods on various gas barrier performances using functional oxide films (2); Hydrogen gas barrier properties
19:00	**Gala Dinner**	

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Thursday, October 23

Room	Megas Alexandros
Chair	**Pedro Barquinha**
09:00-09:40	**Plenary 21** **John Robertson** Deep acceptor polarons in a-TeO_2 and hydrogen-induced Instabilities in IGZO
	Invited Presentations
09:40-10:10	**Nektarios Lathiotakis** First-principles study of carbon-doped Cu_2O and lead-free A_2ZrX_6 defect perovskites for optoelectronic applications
	Oral Presentations
10:10-10:30	**Karsten Fleischer** Spray pyrolysis of ternary oxides – the case of Cu_xCrO_2 and a-$ZnSnO_3$
10:30-10:50	**Dimitra Katerinopoulou** Photocatalytic materials for a greener tomorrow
10:50-11:20	**COFFEE BREAK**
Room	**Megas Alexandros**
Chair	**Vassilios Binas**
11:20-11:40	**Tomoya Suzuki** Mechanism of epitaxial growth of rutile-type GeO_2 by PLD
11:40-12:00	**Yang Chen** Ambient-Stable p-Type transparent CuI thin-film transistors via room-temperature pulsed laser deposition
	Invited Presentations
12:00-12:30	**Seohan Kim** Advanced applications of wide bandgap semiconductors with hybrid structures
12:30	**Awards / Closing Remarks**

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Oral Presentation

Progress in Science and Application of Transparent Oxide Semiconductors

Hideo Hosono[1,2]

[1]*Institute of Science Tokyo, Yokohama ,Japan*
[2] *National Institute for Materials Science, Tsukuba, Japan*

Two decades have passed since the first TCM conference. Transparent contact represented by ITO was only the major function for application before 2 decades. During the past 2 decades, distinct progress has been made both in science and application. The representative progress is seen in transparent oxide semiconductor in which Fermi level is controllable. Many n-type new materials are reported and carrier doping may be understood by computational approach For device application, oxide TFTs has grown to a hot topic in electronics. IGZO-TFTs are now widely used as the switching transistor of flat panel displays. Further oxide TFTs are attracting attention for memory application utilizing extremely low-off current.[1,2]

In his talk, I mainly introduce the progress in our research on transparent oxide semiconductors (Fig.1) along with current challenges:

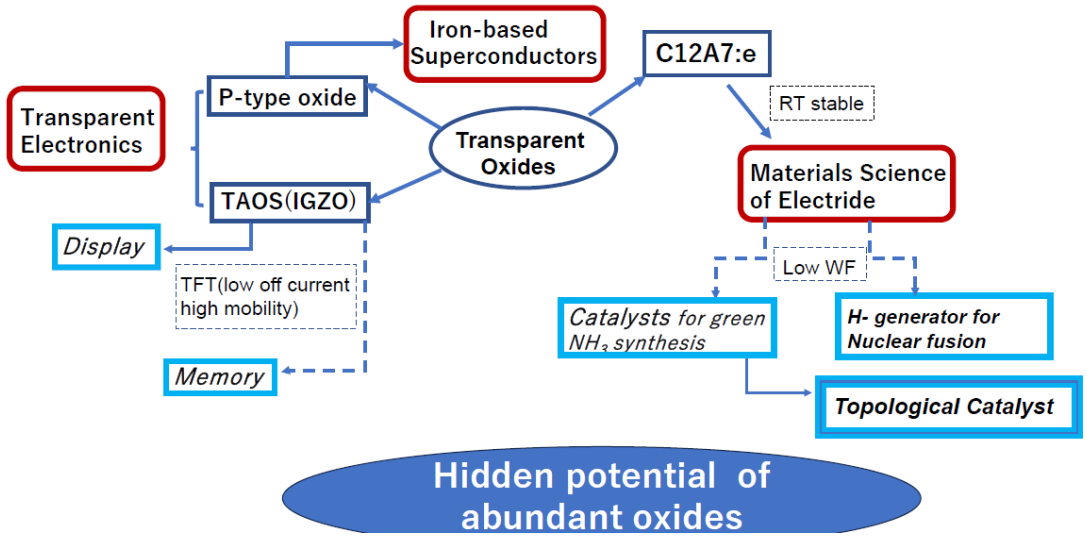

Fig.1 Frontier opened from transparent oxide research

1) Hosono and Kumomi (edited) Amorphous Oxide Semiconductors: IGZO and Related Materials for Display and Memory, Wiley 2022.
2) Kuo, Hosono, Shur and Jiang, Oxide Thin Film Transistors, Wiley, 2024

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ZnO interfaces: Defects, heterostructures and surface chemistry

Lars Österlund[1], Fredric G. Svensson[1], Bozhidar I. Stefanov[2], Seohan Kim[1,3]

[1] *Dept. Materials Science and Engineering, The Ångström Laboratory, Uppsala University, P.O. Box 34, 75103 Uppsala, Sweden.*
[2] *Department of Chemistry, Faculty of Electronic Engineering and Technologies, Technical University of Sofia, 8 Kliment Ohridski Blvd, 1756 Sofia, Bulgaria.*
[3] *Department of Materials Science and Engineering, Pusan National University, Busan, 46 241, South Korea.*

In many applications, such as electrodes and thin films in heterogeneous (photo/electro)catalysis, solid-state sensors, and batteries, the surface chemistry of ZnO is crucial. Defects are known to significantly influence the physicochemical properties of ZnO. Lattice vacancies and adsorbed surface species, originating from the synthesis, can modify and inhibit the intrinsic ZnO properties. Here, we present results on the interfacial properties of nanostructured ZnO prepared by commonly employed wet-chemical methods, providing molecular evidence of the role of defects and precursors on the ensuing surface chemical properties. We provide molecular evidence of two opposing effects on the catalytic activity that occur during heat-treatment of ZnO in oxidizing conditions: Reduction of site-inhibiting synthesis residues (increasing the reaction rate), and reduction of active lattice defect sites (decreasing the reaction rate). We show that by careful "engineering", the ZnO interface can be purposefully adjusted to control which kind of defects that are exposed and remove unwanted synthesis residues.[1]

Further, we show that by controlling the ZnO interface properties, Cu-Zn oxide heterojunction can be prepared by photo-decomposition of the chelated Cu(II) species $[Cu(EDTA)]^{2+}$resulting in photocatalysts with markedly enhanced activity compared to corresponding Cu-Zn oxide structures containing a higher concentration of defects and synthesis residues.[2] The results are attributed to more efficient electron-hole separation in purposefully synthesized Cu_2O@ZnO due to well-developed interfaces.

Our results show the importance of careful synthesis and pre-treatment methods to prepare ZnO materials with desired interfacial properties for catalytic and optoelectronic applications.

[1] Fredric G. Svensson, Erik Djurberg, Seohan Kim, Gunnar Westin, and Lars Österlund, *Effect of surface impurities and lattice defects on the photocatalytic activity of ZnO nanoparticles*, in manuscript.
[2] Fredric G. Svensson, Erik Djurberg, Yige Yan, Seohan Kim, Jiri Henych, Jakub Tolasz, Frederic Dappozze, Stephane Parola, Chantal Guillard, Bozhidar I. Stefanov, and Lars Österlund, *Preparation of copper-zinc oxide pn-heterojunction catalysts by photo-deposition of $[Cu(EDTA)]^{2+}$ complexes over ZnO nanorods with well-developed interfaces*, submitted.

Analyzing defect properties in oxides by x-ray photoelectron spectroscopy

Andreas Klein
Technical University of Darmstadt, Electronic Structure of Materials, 64287 Darmstadt, Germany

Defects and dopants are the key to understand and manipulate the properties of functional ceramics. Despite their importance, the knowledge about defect properties is mostly qualitative and based on separate concepts for the different possible charge compensation mechanisms. A combined quantitative treatment of the different charge compensation mechanisms is highly desirable and could pave the way for predicting material properties. Quantitative information on defect properties, such as their energy levels which determine the valence state, can directly be used for quantitative defect models but are still barely available from experiment. X-ray photoelectron spectroscopy (XPS) has the potential to fill this gap, as it provides simultaneous information on the valence states and on the position of the Fermi energy, which are intimately connected with each other. The technique is able to directly determine charge transition levels of dopants without any assumptions and model comparison and can be applied to doping concentrations even below 1%. As XPS is element specific, it can also be applied to materials in which more than a single dopant species is present. The presentation will give an overview on how defect properties can be analyzed with XPS. Experimental solutions for the challenge of measuring highly insulating samples will be demonstrated with examples from electronic, ionic and mixed ionic-electronic conductors and piezoelectric materials. The extend to which defect energy levels depend on concentration and the possibility to transfer defect energy levels between materials will be discussed. For some cases, the experimentally obtained defect properties will be compared with those calculated by means of density functional theory.

Complex structure and composition metal-oxides through solution processing

Gunnar Westin

Department of Chemistry-Ångström, Uppsala University, 75121 Uppsala, Sweden

Abstract. Solution based processing routes have gained much interest for the preparation of complex nano-structured materials. Benefits are found in the simple processing routes to complex composition and structure materials, allowing for large-scale, low cost technological exploitation. The molecular approach of solution processing provides unique possibilities to create atom-scale tailored materials even in large scale from metal-organic molecular building blocks, which can be crystallised for purification.

However, although the solution chemical routes have seen a rapid development during the recent decades proving to achieve unique materials of various shapes and complexities there is still need for further development, in particular regarding reproducibility and crystal quality. Here, the complex often multi-step processes, including kinetically controlled reaction chains makes it hard to gain a fundamental understanding allowing for highly controlled processing of high quality, complex composition metal-oxides, not the least when considering the important doped oxide semi-conductors.

This talk gives a short, general description of solution based processing using hetero-metallic alkoxide precursors and inorganic salts complexed with organic groups, and the thermal processing taking the precursor molecules into the ceramic target materials. Advantages and challenges with the two precursor systems are discussed.

Examples of processes yielding complex, nano-structured functional metal-oxides as nano-particle, nano-phase sponges and thin- and ultra-thin films are given. A particular focus is put on the relationship between the choice of precursor and processing parameters, and the final metal-oxide microstructure, atomic structure and properties. This includes the dopant atom oxidation-state, coordination and distribution, which strongly determines the optical and magnetic properties of a given doped oxide. These are important structural details often missing also for other chemical and physical materials preparation techniques which leads to slow progress in important fields such as fossil-free energy conversion, e.g. solar fuel catalysis and magnetic oxide semi-conductors. Metal-oxide systems discussed include Co- Al- and Ln-doped ZnO, $CoFe_2O_4$ (CFO) – (Sr,La)MnO_3 (LSMO) multilayer films.

…..The phase-development taking place upon heating of gels, powders or liquid precursor concentrates to yield the target oxides were studied in detail with a wide range of analytical techniques including: TG-DSC, XRD, XPS, IR-spectroscopy, EXAFS, SEM-EDS, and S/HRTEM-ED/EDS/HAADF/EELS and ePDF. In some cases, DFT calculations were employed to derive plausible complex dopant structures supported by the above experimental techniques.

The examples are chosen to give a general discussion about how the choice of precursors and processing parameters can be used to obtain high quality complex oxides of various micro-structures, as well as target materials with potential for use in sensors, catalysis, solar-cells and fuel generation, photo-active self-cleaning surfaces, optically active materials, and electro- and magnetic thin films.

Brief overview of metallic nanowire based transparent conductive materials

D. Bellet[1,*], L. Bardet[1], A. Khan[1,2], M. Del Mar Rodriguez Robles[1], S. Maurya[1,2], B. Zheng[1], S. Schumacher[1], C. Sanchez Velasquez[1], D. T. Papanastasiou[1], C. Jiménez[1], D. Muñoz-Rojas[1]

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[2]*Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR 5026, F-33600 Pessac, France*

Transparent electrodes (TE) play a pivotal role within numerous devices in optoelectronic or energy areas. This concerns for instance devices such as solar cells, light-emitting devices, touch screens, transparent heaters, low-emissivity films or smart windows. TE should exhibit high optical transmittance and low sheet resistance, as the two prevailing properties. However other characteristics appear also significant depending on applications; this concerns for instance optical haziness or mechanical flexibility. Transparent conductive oxides (TCO) have been studied for several decades, and are the most commonly used TE in industrial devices. Among them, indium tin oxide (ITO) films are the most common TE materials used by industry due to their good optical and electrical properties, while aluminum doped Zn oxide (AZO) or fluor-doped tin oxide (FTO) exhibit also good potential. TCO have been deeply investigated and optimized, however TCO are brittle and could be expensive. The development of next generations of optoelectronic devices needs TE that exhibit good optical and electrical properties, good flexibility and moreover their fabrication has to be compatible with high-throughput fabrication for industrial applications (roll-to-roll for instance) and low cost. Several emerging TE have been investigated with this aim: this includes carbon nanomaterials, conductive polymers and metallic nanostructures.[1,2]

Among the latter, metallic nanowire (MNW) networks have received intensive research interest thanks to their high electrical conductivity, optical transparency in visible and near infrared regions and excellent flexibility performances[3,4]. Such TE consist of a network of randomly oriented and interconnected MNW (so far mainly silver nanowires) deposited on a transparent substrate. While such TE exhibit very good electrical and optical properties, morphological instabilities induced by thermal or electrical stress and high surface roughness constitute the main bottlenecks for further long-term operating performance[5]. Metal oxide layers are shown as a promising protective overcoat around nanowires with encouraging results in terms of stability enhancement as well as flatness improving capability as compared to bare nanowires[6]. The nature of the metal oxides (such as SnO_2, Al_2O_3, TiO_2 and ZnO…) and how they affect concrete device performance is an aspect to be investigated for each application in order to tune and design more efficient device structures[6]. Main research works have dealt with the influence of MNW chemical nature and dimensions, network density, post-deposition treatment on the main properties of MNW networks. As the investigation of MNW based nanocomposites that can exhibit enhanced properties and/or stability has also been the subject of many studies[7].

The aim of this presentation is to give an overview of the main features related to MNW networks intensive research activities, including both fundamental and applicative aspects. The associated assets and drawbacks of MNW networks, as well as the challenges and opportunities, will be presented and discussed.

Associated references:

[1] V. H. Nguyen, D. T. Papanastasiou, J. Resende, L. Bardet, T. Sannicolo, C. Jiménez, D. Muñoz-Rojas, N. D. Nguyen, D. Bellet, *Small* **2022**, 2106006.
[2] X. Lu, Y. Zhang, Z. Zheng, *Adv. Electron. Mater.* **2021**, *7*, 2001121.
[3] T. Sannicolo, M. Lagrange, A. Cabos, C. Celle, J.-P. Simonato, D. Bellet, *Small* **2016**, *12*, 6052.
[4] D. Tan, C. Jiang, Q. Li, S. Bi, J. Song, *J Mater Sci: Mater Electron* **2020**, *31*, 15669.
[5] J. J. Patil, W. H. Chae, A. Trebach, K. Carter, E. Lee, T. Sannicolo, J. C. Grossman, *Adv. Mater.* **2021**, *33*, 2004356.
[6] A. Sekkat, C. Sanchez-Velasquez, L. Bardet, M. Weber, C. Jiménez, D. Bellet, D. Muñoz-Rojas, V. H. Nguyen, *J. Mater. Chem. A* **2024**, *12*, 25600.
[7] L. Bardet, M. Akbari, C. Crivello, L. Rapenne, M. Weber, V. H. Nguyen, C. Jiménez, D. Muñoz-Rojas, A. Denneulin, D. Bellet, *ACS Appl. Nano Mater.* **2023**, *6*, 15234.

Adaptive Chromogenic Material for Smart Windows

Juris Purans[1]
[1] *Institute of Solid State Physics University of Latvia*

The number of buildings featuring glass facades or large windows is steadily increasing, driven by rising living standards and evolving architectural trends. This shift highlights the growing need for energy-efficient building solutions. One promising approach involves the development of adaptive glass coatings with tailored optical properties to (1) reduce heat transfer through windows, and (2) block irritating visible (VIS) and ultraviolet (UV) light. Chromogenic thin films—such as electrochromic, thermochromic, and photochromic materials—are at the forefront of smart window technology.

Within the EU HORIZON project *Smart Windows for Zero Energy Buildings*, innovative single- and multi-layered transition metal oxide (TMO) thin films have been designed and fabricated. These include electrochromic (WO_3 and NiO) and photochromic rare-earth metal oxyhydrides (Y-O-H), utilizing advanced reactive magnetron sputtering and industrially scalable roll-to-roll (R2R) deposition techniques.

Building on pioneering work initiated in the 1980s [1], synchrotron radiation XAFS studies (accompanied by Raman, XRD, and electrochemistry) have been extensively applied to investigate electrochromic materials and devices developed at ISSP LU: cathodic electrochromic oxides such as WO_3, MoO_3, and NiO-WO_3, as well as anodic oxides including NiOx, IrOx, and NiO-IrOx [2,3].

The discovery in the 2010s of photochromic yttrium oxohydrates (YOH) [4] and the family of rare-earth oxohydrates (REOH) represent a groundbreaking class of inorganic mixed-anion compounds with exceptional photochromic properties. We have extended these investigations to multilayer photochromic Y-O-H and electrochromic MoO_3 systems [5], as well as antibacterial TCO coatings such as WO_3/Cu/WO_3 [6], highlighting their potential for multifunctional applications. Additionally, large-area roll-to-roll deposition of YHO and WO_3/Cu/WO_3 has been explored to enable scalable production for smart windows and other optoelectronic devices. This work underscores the potential of advanced chromogenic materials to transform energy-efficient building technologies, offering a significant contribution toward achieving zero-energy goals.

Acknowledgment:

This research was supported by the HORIZON-WIDERA-2022-TALENTS-01-01: ERA Chairs Project “Smart Windows for Zero Energy Buildings” (SWEB), Grant Agreement No. 101087367. The authors also acknowledge the SWEB project and the Thin Films Laboratory team (see [1-6] for their invaluable contributions.

References:

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Organic materials for bioelectronic devices

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Bioelectronics is the emerging interdisciplinary field that integrates biology with electronic systems to revolutionize the way we diagnose and treat disease. Its origins can be traced back to the 18th century, when Luigi Galvani's experiments with detached twitching frog legs revealed the nature of electricity in living organisms. Today, this legacy continues in a plethora of bioelectronic devices which include defibrillators and pacemakers to prevent or correct arrhythmias, cochlear implants to provide the sense of hearing, and glucose monitoring devices to help diabetics manage their disease. However, the coupling between biology and electronics is limited by the materials that can form stable interfaces with the tissue and transduce signals across the biotic/abiotic ensemble. Recently, organic electronic materials have emerged as a promising solution. These materials offer their unique properties, which include mixed ionic/electronic conductivity, mechanical flexibility and enhanced biocompatibility, and which make them ideal for interfacing biological systems.

In this talk, I will provide an overview of the field of bioelectronics and explore its potential to address unmet medical needs. I will present examples of innovative devices designed to bridge the gap between biology and electronics and demonstrate how organic materials open new avenues for studying and treating disease.

High-power impulse magnetron sputtering as a knob for tailoring transparent conductive oxides

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Transparent conductive oxides (TCO) are undoubtedly one of the most important classes of materials today. The challenges of our civilization in the field of energy self-sufficiency and sustainability cannot be solved without them. Since TCOs combine two generally contradictory properties (electrical conductivity with optical transparency), precise control of their composition or structure is necessary.

High-power impulse magnetron sputtering (HiPIMS) is an advanced magnetron sputtering method. Thanks to the pulsed energy supply to the discharge it is possible to achieve very high target power densities (up to a thousand times higher compared with a standard dc magnetron sputtering) and thus to some extent control the energy supplied to the growing layer. This allows, for example, the influence of the crystallinity and other properties of the layers. In addition, different parameters of the plasma discharge under different discharge conditions (voltage pulse length, target power density, etc.) can lead to different transfer of the target material to the substrate. In the case of a compound target, for example, it is possible to change the elemental composition of the layer without having to change the elemental composition of the target.

In this presentation, we show several successful demonstrations of HiPIMS deposition of various TCOs, namely IGZO [1], AZO[2], WO_x [3], $V_{1-x}W_xO_2$ [4] or Cu_2O [5].

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From Crystal Symmetry to Heat Flow: Resolving Anisotropic Transport in Gallium Oxide Phases

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In low-symmetry monoclinic crystals with non-orthogonal axes the anisotropic nature of properties such as elasticity and dielectric response gives rise to unconventional phenomena, including hyperbolic sheer polaritons[1], charge density waves or topological phase transitions not observed in higher symmetry materials[2]. In this work, we present a comprehensive, contactless investigation into the anisotropic phonon-governed properties of the ultra-wide bandgap semiconductor Ga_2O_3, with a focus on both nanoscale phonon dynamics and nanoscale thermal transport phenomena[3]. We employ a suite of complementary, all-optical spectroscopic techniques to map phonon behavior over multiple frequency and length scales. Anisotropic thermoreflectance thermometry provides sub-degree angular resolution of in-plane responses[4], while polarized, angle-resolved Brillouin light scattering (BLS) probes acoustic phonons to extract the anisotropy of phonon phase velocities[5].

Most notably, extreme UV transient grating spectroscopy experiments performed at the FERMI free-electron laser facility enable access to grating spacings as short as 26 nm[6]. This capability is crucial for isolating phonon contributions with varying mean free paths, including those relevant to nanoscale thermal transport that are elusive in conventional setups. Variation of the nanoscale grating spacing and temperature enables high and low frequency band-pass filtering in the THz regime. Furthermore, the transient responses reveal multiple oscillatory modes - attributable to GHz surface acoustic waves which reveal characteristic anisotropy. To complement our experimental findings, we perform ab-initio Green-Kubo calculations[7] and Boltzmann Transport Equation (BTE) simulations to capture non-equilibrium phonon interactions and the interplay between phononic properties and thermal conductivity anisotropy. Our results deepen the understanding of anisotropic thermal transport in transparent conductive metal-oxides and provide guidelines for optimized heat dissipation.

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Tailored liquid-phase chemistry to achieve low-temperature synthesis of $BiVO_4$ for photoelectrochemical water splitting

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In order to reduce global dependence on fossil resources, utilization of renewable energy sources is key. Electrification is accepted as an efficient path forward, but issues arise while matching supply and demand. These issues can be addressed by directly coupling energy harvesting to storage of energy, for example by using hydrogen as a means to store energy. To this purpose, photo water splitting is investigated over the last decades to link energy harvesting to energy storage, directly. Amongst other options, photoelectrochemical (PEC) hydrogen production is considered because of its potentially high energy efficiency due to a high level of (material) integration. Within this field, $BiVO_4$ (BVO) is known to be a material with a good balance between durability, bandgap, absorption and bias requirements; all characteristics which are vital for versatile PEC electrodes[1]. The high level of integration – often named as the hallmark of PEC technology – is limited by material synthesis and preparation methods[2], which may require high temperatures of up to 600°C to yield functional BVO. These temperatures are destructive for typical TCO materials used, e.g. ITO or FTO. In addition, scalability of the material preparation process is vital to increase impact of the BVO and PEC technology in general.

In this study, we opted to lower the synthesis temperature of BVO using wet-chemical methods while using solvents and processes which allow cost-effective and scalable production in the near future. Wet-chemical processing of BVO was established by using aqueous and non-aqueous formulations. A broad range of solvents was considered, combining liquid phase and metal-ion compatible ligands and / or stabilizers that could lead to soluble complexes. Suitable combinations were found and studied by using thermogravimetric analysis (TGA) and powder X-ray diffraction (XRD). Various deposition methods were employed for layer formation from small to large scale, ranging from spincoating and dipcoating to spray deposition, yielding functional devices consisting of several stacked materials. These materials were further studied with thin film XRD, optical spectroscopy (UV-VIS) and linear sweep voltammetry (LSV) using a solar simulator (AM 1.5). The result obtained in this study indicate that tetragonal BVO crystallization onset occurs at 300°C, where Bi_2O_3 may form a secondary phase. Upon increasing the temperature to 400°C, the purity of BVO increases. To increase the photocurrent, an electron transfer layer (WO_3) and BVO doping with Mo(VI) was applied. The photocurrent increased to 1.45 mA/cm^2. This outcome opens possibilities to use TCO's with limited temperature stability and enhance BVO quality by limiting negative solid state diffusion effects such as sodium migration. In addition, larger scale application has been shown as well, potentially increasing the impact of this technology in the near future.

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Industry-Scaled DC Sputtering of $SnZnO_x$: Toward Indium-Free Transparent Electrodes for Solar Cells

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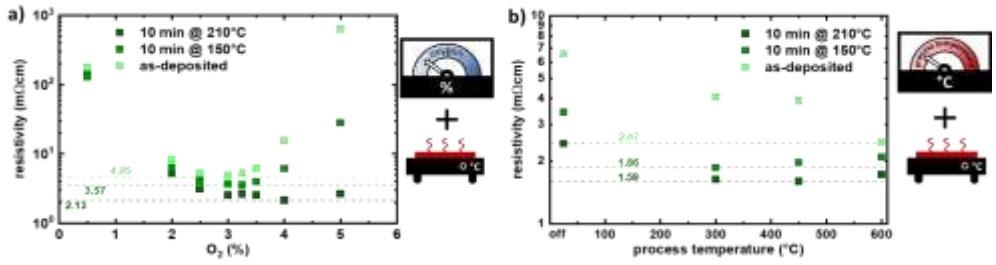
Transparent conductive oxides (TCOs) are used in many optoelectrical devices, such as solar cells or light-emitting diodes. Often, these devices require TCOs to be deposited at low temperatures (e.g., OLEDs, silicon heterojunctions, or perovskite/silicon tandem cells) without compromising their excellent optoelectrical properties, which limits the selection of suitable materials. Therefore, the most widely used TCOs are indium-based. However, indium's scarcity and increasing demand for optoelectronic devices will likely lead to supply challenges and rising costs[1]. Herein, we report on a study of SnO_2-based TCO, namely tin-zinc oxide (ZnO < 8 wt.%), as a promising indium-free alternative. The deposition was done in an in-line DC sputter system from ceramic tube targets. The optoelectrical properties of the tin-zinc oxide (SnZnOx) were optimized by tuning deposition parameters, namely the oxygen concentration in the argon process gas and the radiative substrate heater's temperature, as well as the post-deposition annealing treatment temperature. Fig. 1a) shows the resistivities (ρ) of SnZnOx films measured by 4-point-probe under varying oxygen concentration and the effect of the annealing of the same samples. As can be seen, in the as-deposited state, a minimum ρ of ~4.85 mΩcm was reached for an oxygen concentration of 3 %. The ρ of SnZnOx films with both higher or lower oxygen concentration were higher. At annealing temperatures of 150 °C and 210 °C the minimum ρ was further reduced to 3.57 mΩcm, and 2.13 mΩcm, respectively. Interestingly, the more oxygen was added, the higher the impact of the annealing on the ρ of the films. With that in mind, the effect of applying heat during the sputtering process was also explored (see Fig. 1b)). It was found that when setting the heaters to 600 °C (which yield a substrate temperature of < 200 °C), the ρ of an as-deposited film was about the same, 2.47 mΩcm, as a sample that was deposited without using heaters (heaters off) and annealed at 210 °C. Interestingly, the ρ of films that were deposited while heating during the sputtering process were, independent of the annealing, significantly smaller than films that were deposited without heaters. The lowest ρ achieved in this study was 1.59 mΩcm at 3.5 % oxygen content, 450 °C heater temperature, and annealed at 210 °C. This is still approximately three times higher than a typical ITO or IZO film, which reaches ρ of well below 0.5 mΩcm, and ~ 50 % higher than the ρ of an reactive plasma deposited (RPD) SnOx achieved by Koida et al., but it shows the great potential of that material and of sputtering as a feasible deposition method [2]. Additionally, the indium-free TCOs were characterized by means of Hall-effect, spectrophotometry, and x-ray diffraction. In the next step we will implement these TCOs in solar cells.



Resistivities of $SnZnO_x$ films deposited at a DC power of 2 kW, using an industry-scaled (0.6 m) ceramic tube-target, implemented in the multifunctional cluster tool KOALA

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Triode Plasma Approach to Low-Damage TCO Deposition for Silicon Heterojunction Solar Cells

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Transparent conducting oxides (TCOs) are essential in various optoelectronic applications, including carrier-selective passivating contact solar cells, due to their excellent transparency and electrical conductivity. However, conventional diode-configured sputtering methods often introduce significant sputter damage, which degrades the surface passivation quality of a-Si:H/c-Si silicon heterojunction (SHJ) solar cells. This degradation is primarily caused by the bombardment of highly energetic oxygen ions, resulting in partially irreversible damage even after thermal annealing. In this presentation, we propose a triode plasma sputtering configuration that integrates a negatively biased mesh electrode into the conventional diode system. Measurements showed that sputter damage in SHJ devices can be assessed by observing the evolution of implied open-circuit voltage (iV_{oc}), effective carrier lifetime (τ_{eff}), and low-temperature hydrogen exodiffusion in SHJ precursor structures. Our triode plasma approach suppresses oxygen ion bombardment, reducing τ_{eff} degradation from 96% (diode) to just 7% (triode). We also observed that triode-configured plasma not only reduced sputter damage but also altered the properties of as-deposited ITO films, which serve as indicators of this reduction. The triode configuration not only minimizes oxygen ion damage but also yields ITO films with enhanced carrier mobility, higher refractive indices, and lower extinction coefficients. Furthermore, the reduction in ion bombardment is reflected in a shift in the preferred crystal orientation of the ITO films from the (400) to the (222) plane.

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Revealing the incorporation sites and local structure of nickel and selenium in doped copper iodide thin films

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Copper iodide (CuI) is a promising p-type semiconductor for transparent electronic applications such as solar cells, flat panel displays, and LEDs. The electrical properties of CuI can be tailored by substituting it, for example, with nickel (Ni) or selenium (Se) [1,2], yet the specific incorporation sites and mechanisms of these elements within the CuI matrix are not fully understood. This study presents an investigation of polycrystalline CuI thin films with varying selenium and nickel concentrations, deposited by pulsed laser deposition (PLD) and reactive co-sputtering on glass substrates[3]. CuI:Ni thin films (1–30 at% Ni) and CuI:Se thin films (0.4–3.8 at% Se) were prepared and capped with 150 nm and 200 nm Al_2O_3 layers, respectively, to prevent oxidation. X-ray Absorption Spectroscopy (XAS) was performed at ~10 K at the Cu, Se, and Ni K-edges to investigate the local structure of Ni and Se in the CuI matrix.

For the CuI:Ni thin films, the near edge structure and the extended X-ray absorption fine structure (EXAFS) at the Cu K-edge indicate potential copper oxidation[4]. These effects diminish with increasing Ni concentration. Preliminary results from Ni K-edge EXAFS analysis reveal that Ni is coordinated by both I and O atoms, indicating different bonding environments. This is supported by microstructural studies, which show phase separation and the formation of secondary Ni-containing phases, such as NiI_2 and $NiI_2(H_2O)_6$, especially at high Ni content[3]. These secondary phases complicate the interpretation of the Ni local structure, and further detailed EXAFS analysis at the Ni K-edge is currently underway to clarify these findings.

For the CuI:Se thin films, EXAFS fitting at the Cu K-edge reveals only a slight increase in the Cu–I bond length with increasing Se content, suggesting that Se doping up to 3.8 at% induces only minor changes in the local Cu environment. EXAFS analysis at the Se K-edge shows that Se atoms are predominantly coordinated by Cu, with no evidence of Se–Se bonding. The Se–Cu bond lengths remain nearly constant across doping levels, and structural disorder is low. These findings indicate that at the studied low concentrations, selenium incorporates uniformly, most likely substituting copper on lattice sites without significantly disrupting the CuI structure. Overall, these results highlight the contrasting behavior of the two dopants: while selenium has minimal structural impact at low concentrations, nickel appears to oxidize at low doping levels and potentially forms secondary phases at the higher concentrations.

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Low-resistivity of highly nitrogen-doped p-type Cu_2O thin films prepared by reactive HiPIMS

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One of today's challenging scientific topics is finding a suitable p-type TCO that would at least approach the optoelectronic properties of the n-type counterpart [1]. Finding such p-type material is a necessary condition for the further sustainable technological development of society. The realization of p-n junctions using transparent conductive materials will enable the development of a new generation of invisible electronics, contribute to reducing the energy requirements of various optoelectronic devices or lead to the production of more efficient solar cells. Transparent conductive materials based on Cu_2O appear to be among the most promising. This is mainly due to the abundance of elements used, their non-toxicity and interesting optoelectronic properties. One of the limiting factors in Cu_2O layers is the low mobility of free holes. In our previous work [2], we demonstrated that post-deposition laser annealing can effectively enhance hole mobility.

In our work, we systematically investigated the role of nitrogen incorporated in Cu_2O thin films, mainly on optical and electrical properties, namely optical band gap and electrical resistivity. The Cu_2O:N films were prepared by reactive HiPIMS of Cu circular target (100 mm in diameter) in $Ar+O_2+N_2$ atmosphere. The pulse-averaged target power density (S_{da}) was varied from ≈ 100-1300 Wcm^{-2}, and the fraction of N_2 in ($Ar+N_2$) mass flow was 0–90 %. A decreasing trend for resistivity has been seen with the increasing amount of nitrogen. The prepared p-type Cu_2O:N films with the highest value of a nitrogen fraction of 90% exhibited very low resistivity about $5 \times 10^{-2}\ \Omega cm$ exceeding current state of the art.

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Magnetically Tailored Metal Oxide Thin Films as Efficient Catalysts for Green H_2 and NH_3 Synthesis

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Thin films of semiconductor oxides offer tunable electronic properties and high surface-area interfaces, making them ideal platforms for efficient small molecule activation in green hydrogen and ammonia production. The growing possibilities of engineering nanostructures in various compositions (pure, doped, composites, heterostructures) and forms has intensified the research on the integration of different functional material units in a single architecture to obtain new photo- and electrocatalytic materials. We report here on the influence of external magnetic fields applied parallel or perpendicular to the substrate during plasma enhanced chemical vapor deposition of transition metal oxides. Films grown from transition metal precursors showed pronounced changes in crystallographic textures depending upon whether CVD was performed with or without external magnetic field. Investigations on the water splitting properties of the hematite films in a photoelectrochemical reactor revealed superior photocurrent values of hematite photoanodes deposited in external magnetic field. This talk will demonstrate that applying magnetic fields during growth of thin films can fundamentally reconfigure lattice characteristics. This is manifested in the alteration of their crystallographic structure and the topology of the surface states. This dual modulation precisely tailors their intrinsic and emergent electrochemical properties. The MF-CVD approach establishes a groundbreaking and versatile strategy to transform functional materials at the atomic level.

Activation of thin film growth versus plasma damage – the challenge in sputtering of transparent conductors and active semiconductive coatings

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Optoelectronic devices such as thin film solar cells, flat panel displays and (O)LED stacks require transparent and conductive electrodes, where low pressure synthesis by sputtering is a common technique to manufacture degenerate n-doped wide bandgap oxide films as transparent conductors even on sensitive substrates, e. g. on organic ink in AM-LCD displays, on OLEDs on web or even on Perowskite solar cells. With the breakthrough of AM-OLEDs, even more demanding materials properties must be realized. On the firsthand side, the synthesis of amorphous high mobility active semiconductive oxides must be realized for the channel layer. On secondhand side, it's question of amorphous, dense high-k material to realize the dielectric layers.

For many of these applications, it's crucial to optimize the thin film growth conditions to obtain smooth and dense films with stable properties under load. The necessary activation of thin film growth is done by both, substrate heating and plasma activation, but the ability for substrate heating are very limited when it comes to sensitive organic materials. The plasma activation, e. g. by RF, pulsed magnetron or biased magnetron sputtering, on the other hand, reveals substantial problems in terms of particle damage due to high energetic species, e. g. due to negatively charges oxygen atoms accelerated in the cathode sheath.

Our studies reveal that particle energies exceeding ~20 eV energy at the substrate have the potential to degenerate the film properties. On the other hand, low energetic high ion flux to the substrates has the ability to improve the film properties. In this paper, we review the subject of plasma damage in oxide film sputtering and we emphasize in particular a novel technique, the pulsed reactive hollow cathode gas flow sputtering, which offers plasma densities of ne = 1010 cm-3 at the substrate under conditions where DC magnetrons operate at ne = 108 cm-3. Pulsed operation of the source allows for extraction of fast particles from the plasma, where the energy can be controlled by the reverse voltage of the generator.

The benefits of this approach will be shown for magnetron and hollow cathode gas flow sputtering of selected transparent conductive oxides, oxide semiconductors and dielectric materials.

Reaching beyond Diamond to Sapphire, a 7 eV Semiconductor

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We report Si-doped α-$(Al_xGa_{1-x})_2O_3$ with the sapphire structure and a bandgap exceeding 7 eV synthesized by suboxide MBE (*S*-MBE). In *S*-MBE, pre-oxidized molecular beams of the constituents, i.e., Ga_2O and SiO for the growth of Si-doped α-$(Al_xGa_{1-x})_2O_3$, are supplied. Providing a suboxide molecular beam bypasses the rate-limiting first step of the two-step reaction mechanism involved in the growth of α-Ga_2O_3 by conventional MBE. As a result, growth rates exceeding 1 μm/h for α-$(Al_xGa_{1-x})_2O_3$ by *S*-MBE are readily achieved on $(10\bar{1}0)$ sapphire substrates, resulting in films with high structural perfection and smooth surfaces. To get electrical conductivity in the Si-doped α-$(Al_xGa_{1-x})_2O_3$ layers, we find it necessary to deposit two layers. First a relaxed α-$(Al_xGa_{1-x})_2O_3$ buffer layer is grown at high substrate temperature (T_{sub}) on a $(10\bar{1}0)$ sapphire substrate. This is followed by an Si-doped α-$(Al_xGa_{1-x})_2O_3$ overlayer that is commensurately strained to the underlayer and grown at low T_{sub}. Only overlayers grown at low T_{sub} are found to exhibit conductivity. While conductive films have been achieved at growth rates as high as 4.2 μm/h, typical rates for the doped layers are around 0.6 μm/h. The growth window for conductive Si-doped *a*-Ga_2O_3 (x=0) films is approximately T_{sub} = 425–525 °C; at higher x the growth window for conductive Si-doped α-$(Al_xGa_{1-x})_2O_3$ films narrows to approximately T_{sub} = 470–500 °C. In these bilayer structures we observe room-temperature mobilities as high as 90 $cm^2/(V \cdot s)$ for α-Ga_2O_3. The α-$(Al_xGa_{1-x})_2O_3$ films conduct for x as high as 0.58, corresponding to a bandgap of 7.01 eV. This makes α-$(Al_xGa_{1-x})_2O_3$ the highest bandgap semiconductor known. Conductivities at room temperature greatly exceeding all prior reports on α-$(Al_xGa_{1-x})_2O_3$ films are achieved at high x.

*This work was performed in collaboration with the coauthors listed in the references below.

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Return

Laser growth and processing of materials in the nanotechnology era

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Benchmarking Membrane Electrode Assembly Inks with Transparent Conductive Oxides for Proton-Exchange Membrane Water Electrolysis

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A central challenge in solar hydrogen production is replacing high-performance, stable noble metal catalysts in water electrolyzers and photoelectrocatalytic systems with non-noble metal alternatives. Unlike noble metals, which often require no or minimal support, non-noble metal catalysts are prone to degradation and typically demand suitable chemical environments for prolonged operation due to their dynamic behavior.[1] Identifying stable, conductive, and chemically resistant supports for the oxygen evolution reaction (OER) is thus crucial. TCOs are attractive catalyst support candidates. While doped TCOs offer good conductivity, minimizing ohmic drop in real applications, dopant corrosion can lead to gradual performance loss. Metal oxidation and anodic dissolution further complicate stability, particularly during the OER.[2]

We have successfully employed TCO-coated anode supports, specifically ITO and FTO, in the evaluation of non-noble molecular pre-catalysts.[3-6] These supports offered the experimental flexibility and high reproducibility needed for *operando* and post-catalysis tests, clearly elucidating changes in molecular pre-catalysts and the role of side reactions during the OER at a laboratory scale in 3-electrode or H-cells.

More recently, we began investigating TCOs as ink constituents for membrane electrode assembly (MEA) fabrication in proton-exchange membrane (PEM) single water electrolysis cells. In these setups, TCO particles are mixed with the catalyst, Nafion solution, and other additives in varying ratios, undergoing different treatments to produce catalyst ink spray-coated onto the PEM. Developing such ink compositions is a complex and laborious optimization challenge. Our current work utilizes commercial, uniform FTO-, ITO-, and ATO-coated support electrodes to study the potential-dependent behavior and interaction with ink components like Nafion. Crucially, this research aims to benchmark the adsorption stability, distribution, charge transfer resistance, and overall catalytic performance, including degradation onset potentials, of various Fe- and Ni-containing molecular pre-catalysts before their incorporation into MEA inks.

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Laser processes for Colloidal Conductive Metal Nitrides

N. Pliatsikas

Real time optical observation of multi-filament formation and electrode remodeling in $Ag/SiO_2/Au$ memristors

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We report the direct optical observation of resistive switching mechanisms in $Ag/SiO_2/Au$ memristive devices using in-situ microscopy during electrical characterization. Our findings reveal multiple critical current thresholds that separate standard memristive behaviour (volatile and non-volatile) to permanent electrode remodelling. Unlike conventional filamentary switching, which occurs at nanoscale dimensions[1,2], we demonstrate that increasing compliance currents from 0.5µA to 50mA triggers the formation of multiple micron-sized filamentary structures visible under standard optical microscopy. These structures appear precisely coincident with the high-to-low resistance state transitions. Differential interference contrast microscopy reveals both Ag extrusions and corresponding voids, confirming a substantial material redistribution process. AFM measurements verify these features as physical Ag protrusions extending from the electrode surface. Notably, the controlled formation of multiple parallel filaments and high current handling capability (up to 70mA) suggest applications beyond conventional memristors, including reconfigurable RF circuit elements, high-power switching, and plasmonic devices. The dependence of filament distribution on device geometry provides pathways for engineering application specific conduction patterns. This work bridges the gap between resistive switching mechanisms and microscale material transport phenomena with a rare direct visualization, enabling potential applications in optically accessible memory elements where states can be read both electrically and optically, advancing hybrid electro-optical computing architectures[3] and robust neuromorphic systems for high-power environments.

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Development of a synthesis route for $YScS_3$, a potential sulfide p-type TCM

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Within novel transparent conducting materials (TCMs), developing a high-quality p-type remains elusive. Until recently, oxides have primarily been explored for TCMs, because their chemistry is well understood and they are affordable and relatively easy to synthesise. However, oxide p-types consistently show low conductivity[1]. This has been attributed to the high electronegativity of oxygen 'trapping' holes around the oxide ions, leading to a high hole effective mass. Other chalcogenide anions offer an alternative, having lower electronegativity while retaining similar bonding behaviour. This approach has seen some success, with reports of conductivities up to 1000 S cm^{-1} for sulfide TCMs, compared with approximately 400 S cm^{-1} for oxides[1]. However, these are not yet comparable to n-types, so further research is necessary. One challenge is that non-oxide materials can be difficult to synthesise, impeding their development.

In 2020 Zhang et al.[2] predicted Zn-doped YScS3 as a good p-type TCM, with a low calculated hole effective mass of 0.48 m_0, comparable to the electron effective mass of ITO[3]. $YScS_3$ has previously been synthesised[4], but its properties were not studied. We have developed new methods to synthesise $YScS_3$. Powders have been synthesised by conversion of the oxides under CS_2 gas, from which pure single crystals were grown by chemical vapour transport. Zn-doped powders have been synthesised in a two-step method, with Sc-deficient powders formed under CS_2, followed by incorporation of Zn in a sealed tube. This will enable $YScS_3$ to be assessed as a TCM. Moreover, optimizing the synthesis of $YScS_3$ provides insights for producing other novel sulfide TCMs.

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A REJUVENATION STUDY OF WO_3 AND Re:WO_3: THIN FILMS DEPOSITED ON FTO SUBSTRATE USING ULTRASONIC SPRAY PYROLYSIS

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One of the challenges for electrochromic materials used in smart windows is to ensure the durability and stability of electrochromic device. Studies concerning charge insertion and extraction in electrochromic materials have shown that the degradation of these materials can be associated with ions trapped within the host structure [1].In this work, WO_3 thin films deposited by the spray pyrolysis technique, were under cyclic voltammetry processes until loss of electrochromic properties were observed. Based in previous studies related to the recovery of degraded electrochromic properties of metal oxides carried out by other research groups [2], in samples synthesized by the magnetron sputtering technique, in this work we present results on the rejuvenation of crystalline WO_3 electrochromic films synthesized employing the ultrasonic spray pyrolysis technique. WO_3 and rhenium doped WO_3 thin films were deposited on FTO substrates using the spray pyrolysis deposition technique. A 0.01 M solution of WCl_6 dissolved in dimetil formamide (DMF) was used to prepare the WO_3 thin films.In the case of films doped with rhenium, the proportional amount of doping desired was added from a solution of NH_4ReO_4 in DMF and deposited at a temperature of 500 ° C, with an air pressure of 5kg / cm^2, with a activation time of 300 ms and a time between operations of 1200 ms. Our samples presented thickness running between 600-1100 nm and electrical resistivity of 5-13Ω/□. In order to determine the WO_3 thin films electrochomic properties, cyclic voltammetry experiments were performed using H_2SO_4 as electrolyte with a fixed sweep speed varying the potential in the range of -1600 mV to -1660 mV, using platinum electrodes as counter electrode and reference electrode. Then pristine and 2% Rhenium doped WO_3 films were under 5000 ions injection and extraction voltammetric cycles. The rejuvenation of our WO_3 films was performed in samples that lost 90 % of transparency after 5000 ions insertion and extraction cycles. The noticeable rejuvenation and recovery of electrochromic properties of our materials observed in our WO_3 thin films is reported and discussed in present work.

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Insight into the morphological instability of metallic nanowires under thermal stress

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Silver nanowires (AgNWs) are key components in emerging transparent conductive materials, offering a scalable, flexible, and high-performance alternative to brittle oxide-based conductors. Yet, their long-term stability remains a critical concern. It is well known that, under thermal stress, AgNWs spontaneously fragment into periodic chains of nanospheres, even at temperature more than 600°C below the bulk melting point of silver. This degradation mechanism drastically reduces network conductivity.

This instability has often been described by analogy with the Plateau–Rayleigh instability of liquid jets [1]. However, this fluid-based framework fails to quantitatively match experimental observations in solid-state nanowires [2]. In this work, we revisit the origin of this phenomenon using a solid-state diffusion model initially proposed by McCallum et al. [3], which considers curvature-driven mass transport in a solid "line of thin film" resting on a substrate, an approach that motivated this work.

High-resolution electron microscopy is used to monitor the thermal evolution of nanowires with varying diameters, and statistical analysis of the resulting breakup wavelengths is compared to both Rayleigh's predictions and the solid-state model of McCallum et al.

These findings refine our understanding of how nanowire morphology evolves under heat and provide a theoretical basis for temperature-induced failure in AgNW networks [4]. By identifying the relevant physical mechanism underlying thermal degradation, this work contributes to the design of more stable and reliable transparent conductors for optoelectronic devices operating under demanding conditions.

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Sputter deposited CuO-WO_3 Nanosized Heterojunctions for Gas Detection

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In this study, we explore the synthesis of nanostructured Metal-Oxide Semiconductor (MOS) system of cupric oxide (CuO NPs) and tungsten oxide (WO_3) films, subsequently utilized as conductometric gas sensors[1],[2]. Nanoparticles of CuO were synthesized using a magnetron-based gas aggregation nanoparticle source (GAN) and deposited on and beneath transparent ultra-thin films of (WO_3). During high-temperature stabilization for gas sensing measurements, interfacial reactions between CuO nanoparticles and WO_3 led to the formation of copper tungstate ($CuWO_4$), creating a multi-component heterostructure [3].

The gas sensing performance of the CuO-WO_3 system was evaluated under varied operational conditions. The composite exhibited enhanced sensitivity, selectivity, and stability compared to individual components, attributed to synergistic interactions at the nanoscale. Key metrics such as response/recovery times and humidity tolerance were systematically analyzed, with optimal samples demonstrating rapid response dynamics and robust performance under humid environments. Selectivity studies revealed preferential sensitivity toward acetone, suggesting tunability for practical applications.

Material characterization via SEM confirmed the uniform distribution of CuO nanoparticles (20–50 nm) embedded within the WO_3 matrix. XRD and Raman spectroscopy validated the coexistence of CuO, WO_3, and $CuWO_4$ phases. The improved sensing mechanism is ascribed to the formation of nanosized heterojunctions at CuO/WO_3 and $CuWO_4$/WO_3 interfaces and charge carrier modulation via $CuWO_4$, which amplifies conductivity changes upon gas adsorption[4]. These findings highlight the potential of engineered heterostructures in advancing gas sensor technology, offering a pathway for designing high-performance, multi-functional sensing platforms through controlled nanoscale integration. Further optimization of composition and interfacial engineering could enable tailored responses for environmental monitoring and industrial safety systems.

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Cation Engineering and Quantum Effects in Zinc Tin Oxide Films

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Amorphous zinc tin oxide (a-ZTO) has emerged as a promising candidate among transparent conducting oxides (TCOs) due to its excellent optical transparency, controllable charge carrier concentration, and the use of earth-abundant elements. To optimize its performance for applications in transparent electronics, it is essential to understand the correlation between its local bonding environment and its macroscopic electronic properties. In this work, we investigate the structural and electronic characteristics of a-ZTO thin films fabricated via magnetron sputtering and spray pyrolysis, with a particular focus on how variations in the Zn:Sn cation ratio influence material behaviour.

Using a combination of X-ray absorption techniques—X-ray absorption near-edge structure (XANES) and extended X-ray absorption finestructure (EXAFS)—we demonstrate that although the films are amorphous in long-range order, their short-range structure is dominated by ZnO- and SnO_2-like units. These local motifs are found to significantly influence conduction band hybridization, thereby affecting charge carrier mobility, concentration, and band gap values.

Complementary in situ X-ray photoelectron spectroscopy (XPS) and scanning tunneling spectroscopy (STS) measurements reveal a measurable blue shift of ~0.33 eV in the electronic band gap, attributed to quantum confinement. STS results are compared with optical band gaps obtained from Tauc analysis of UV-Vis spectra. Together, these findings deepen our understanding of the structure–property relationships in a-ZTO and offer insights for the rational design of next-generation transparent electronic materials.

Maximizing Electrical Conductivity in Amorphous Oxide Semiconductors

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Amorphous oxide semiconductors (AOS) with weak metal-oxygen bonding, such as In- or Sn-based oxides, are disordered within the short- and medium-range structure, making every metal-oxygen polyhedron unique in itself and/or its environment. The resulting intricate coordination distribution combined with an increased number of degrees of freedom supports coexistence of extended, weakly localized, and charge trap defects in sub-stoichiometric amorphous oxides and promotes switching between shallow and deeply bound states, invisible to conventional x-ray or electron beam probes and static measurements of carrier concentration and carrier mobility. Lack of microscopic understanding of the origins of oxygen defects with various degree of electron localization, different binding energies, and unique dynamical properties, make the electron transport and optical transmission hard to control experimentally even in commercialized AOS.

In this work, experimentally-validated statistical methodologies that involve ab-initio non-stoichiometric liquid-quench molecular dynamics simulations, advanced time- and temperature-dependent structural analysis, and accurate hybrid-functional calculations are employed to identify, classify, and quantify various oxygen defects in prototype AOS, In_2O_{3-x} and SnO_{2-x}. To derive the materials genome of the complex defect formation in these amorphous oxides, multiple descriptors of the defect's local structure are considered in concert with extended bond reconfiguration that occurs to accommodate the defect in the disordered lattice. The time-resolved behavior sheds light on the defect stability, defect transformations, and defect diffusion. Matching the results with the defect's ability to induce, compensate, or trap electronic charges, helps detangle the role of specific defects in competing mechanisms for carrier generation, charge scattering, instabilities, and optical absorption. Moreover, we further explore (pre)crystallization-mobility dependence in multi-cation AOS to accurately describe the structure-property relationship in these systems within relevant parameter space.

The results of this work provide practical design principles for next-generation transparent (micro) electronics, *e.g.*, ultra-low leakage switching transistors and high-resolution sensors, MEMS, and for neuromorphic computing applications. The results also help explain unusual quantum behavior, namely, superfluid stiffness in superconducting amorphous indium oxide that raises exciting questions about the role of disorder in quantum phase transitions.

Solution-Processed YIZO-Based Synaptic Transistors for Neuromorphic Applications

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Neuromorphic electronics, which emulate the operational principles of neural synapses, represent an emerging computing paradigm emphasising cognitive computing capabilities. This paradigm combines rapid parallel processing with high energy efficiency, significantly advancing beyond traditional von Neumann computing systems.

Essential synapse-like device characteristics such as history-dependent analogue states and non-volatile memory have enabled the realisation of two-terminal memristive structures, phase-change memories, and ferroelectric memories as fundamental building blocks of neuromorphic systems. These devices exhibit key synaptic properties by temporally separating signal transmission and the self-learning process, a critical attribute for cognitive computing. However, this temporal separation remains a limitation inherent to two-terminal devices.

In contrast, synaptic transistors (three-terminal devices) perform both signal transmission and self-learning processes concurrently, providing enhanced synapse emulation. Various device architectures and materials have demonstrated synaptic transistor behaviour, notably floating-gate, electrolyte-gate, ferroelectric-gate, and metal oxide dielectric configurations.

This talk specifically focuses on oxide-based synaptic transistors, a class of materials capable of operating at high frequencies without the need for additional switching elements. These materials offer tunable properties and compatibility with CMOS device fabrication techniques. We present and discuss synaptic properties observed in solution-processed thin-film transistors (TFTs) employing Y_2O_3:Al dielectrics and semiconducting channels based on YIZO. Our findings demonstrate variable synaptic functionality across frequencies ranging from 10 mHz to 90 kHz, supported by detailed performance analysis through the paired pulse facilitation index and frequency response. Additionally, the underlying conduction mechanisms enabling synaptic behaviour are examined and discussed.

Stretchable conducting polymers and devices for biosensing applications

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The low elastic modulus of polymers matches that of soft biological tissues and draws increasing interest towards soft and even stretchable health-monitoring devices. However, for these applications, the electronic and mechanical properties of conducting polymers and devices still need to be improved.

Furthermore, organic electrochemical transistors (OECTs) currently attract vast interest for biosensing applications due to their mixed electronic and ionic conduction, which makes them ideal transducers of biological signals. Moreover, due to their low operating voltages (<1V), these devices are of special interest for sensing applications in close contact to the human body and especially for sensing applications in aqueous environments with liquid analytes.

The first part of my talk will focus on our work on biosensors based on planar OECTs, which are able to e.g. detect the SARS-CoV-2 spike protein down to 10-17 molar concentrations in aqueous PBS, artificial saliva, and human serum solutions with good specificity[1].

In the second part of this talk, I will summarize our efforts on stretchable electronics including a fast reliable and easy transfer-printing method for the deposition of conductive polymer films on stretchable, biodegradable substrates.[2] Taking advantage of this method and infusing the substrates with small-molecule plasticizers that also diffuse into PEDOT:PSS films improves the electrical performance as well as the mechanical properties and enables a unique platform for fundamental insights into the behavior of stretchable electronic materials and devices.[3] Finally, I will present our work towards intrinsically stretchable OECTs.

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Advances in electron microscopy for atomic-scale insights to engineer functional oxide thin films

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Many functional oxide materials can be sensitively tuned by careful control of the atomic lattice structure via epitaxial strain: macroscopic properties exhibit exquisite dependence on local parameters such as bond lengths, angles, and distortions. With recent and ongoing advances to improve spatial resolution and access various *in situ* conditions such as variable temperatures or electrical bias, scanning transmission electron microscopy (STEM) is a powerful tool to directly visualize and quantify relevant structure parameters with local sensitivity to inform future engineering of functional oxide films.

The layered Ruddlesden-Popper oxide Ca_2RuO_4, for example, exhibits a first-order isosymmetric insulator-to-metal transition (IMT) at elevated temperatures. Strain engineering through careful choice of substrate dramatically shift the transition temperature to either higher or lower temperatures, even suppressing it entirely in either direction (i.e., stabilizing purely metallic or insulating behaviour). At intermediate strains, mesoscopic structural analysis by x-ray phase reconstruction demonstrated the coexistence of metallic and insulating structural phases below the reduced IMT temperature[1]. Here, we employ variable-temperature cryo-STEM to track the nanoscale configuration and evolution of these divergent phases, spanning hundreds of nanometers with atomic resolution. Our results provide new insights about the relevant elastic and lattice energies and their competition in epitaxial films.

In some compounds, epitaxial strain can mimic the effects of other extreme conditions such as high pressure. Following its initial discovery under high hydrostatic pressure, the recent stabilization of superconductivity in compressively strained bilayer nickelate $La_3Ni_2O_7$ thin films opened the door to exquisite investigation of atomic structure and bonding environments thought to drive superconductivity. Leveraging the highest accessible spatial resolution and light-element sensitivity enabled by state-of-the-art multislice electron ptychography, we survey a series of bilayer nickelate thin films spanning a full series of tensile and compressive strain, revealing a strain-dependent evolution of octahedral symmetry. We combine these experimental with strain-decomposed DFT calculations to investigate correlations between the observed atomic structure and superconductivity.[2]

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Repairable, Recyclable, and Stretchable Electronic Materials

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Materials capable of regenerating after damage have attracted considerable interest since ancient times. For example, self-healing concretes resistant to earthquakes, aging, weathering, and seawater were used in ancient Rome and continue to be the subject of modern research.

While a variety of mechanically self-healing materials have been developed, self-healing conductors remain relatively scarce. Nevertheless, they are garnering significant attention for applications in electronic skin, wearable and stretchable sensors, actuators, transistors, energy harvesting systems, and energy storage devices such as batteries and supercapacitors.[1] These self-healing and recyclable conductive materials offer the potential to reduce electronic waste by enabling the repair and reuse of damaged components, thereby extending the lifespan of electronic devices. They are particularly relevant for wearable and biomedical electronics, which are frequently exposed to mechanical stress that can damage their components.

Conducting polymers possess several properties that make them well-suited for bioelectronics and stretchable electronics, including mixed ionic-electronic conductivity (resulting in low interfacial impedance), chemical tunability, solution processability (including compatibility with printing techniques), and biomechanical compatibility with living tissues. However, their generally poor mechanical robustness limits their intrinsic self-healing capabilities.

To address this challenge, our group has developed a series of self-healing and stretchable conductors by blending aqueous suspensions of the conducting polymer poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) with mechanically reinforcing materials such as polyvinyl alcohol (PVA), polyethylene glycol (PEG), polyurethanes, and tannic acid.[2-9]

In this presentation, I will highlight different types of self-healing behaviors and relate them to the corresponding electrical and mechanical properties of the materials. Applications of these self-healing gels and films as epidermal electrodes, electronic tattoos, and other flexible devices will also be discussed.

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Return

Reactive High Power Impulse Magnetron sputtering of oxide thin films

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Thin films of metal oxides are widely used in many applications. In general, there is a great interest in deposition techniques that enable phase control of oxide thin films. However, synthesis of crystalline films may be challenging when the growth temperature is limited, for instance on temperature sensitive polymer substrates. TiO_2 is one example of a material where specific crystallinity is frequently required.

Physical vapour deposition methods such as magnetron sputtering can reduce the growth temperature by employing energetic species. The growth of crystalline TiO_2 thin films by physical vapor deposition techniques typically requires a deposition temperature well above 200°C. Therefore, this contribution deals with reactive magnetron sputter deposition of TiO_2 thin films with ion assistance using reactive high power impulse magnetron sputtering (HiPIMS). Specifically, energy input during the film growth is analyzed and different contributions are discussed.

It is shown that the geometry of the deposition system is an important factor. With a long target-substrate distance, the total energy flux is too low and the deposited films remain X-ray amorphous irrespective of the ion energy unless substrate heating is applied. Despite that, films prepared by an optimized HiPIMS process exhibit up to 3 times higher photocatalytic activity evaluated by photodegradation of stearic acid, as compared to reference pulsed DC films prepared using the same setup. Furthermore, by tuning the oxygen partial pressure and deposition rate, the internal disorder in the deposited thin films can be increased, making them suitable for crystallization during post-deposition annealing.

When the target-to-substrate distance is reduced, the total energy flux is increased. As a result, the film crystallinity is greatly improved. Growth of anatase as well as rutile can be achieved by changing the total deposition pressure. Even here, the HiPIMS process facilitates crystallization of the films as compared to pulsed DC. The deposition, however, results in a pronounced unintentional heating of the substrate and the ion energy is only a smaller part of the total energy input.

In summary, the HiPIMS deposited films clearly outperforms the ones prepared by pulsed DC. Although the exact growth conditions depend on the deposition geometry and specifics of the deposition setup, some general trends can support the process development.

Two-Layer ITO Metallization in Transparent Electronics

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Introduction

Enabling invisible electronics requires that both transistors and interconnects are transparent in the visible spectrum [1]. Interconnects made of ITO offer >80% transparency in the visible range and a resistivity of ~100 μΩcm [2]. Currently, ITO is used as large-area electrodes, e.g., in solar cells, and typically patterned by wet etching. For metal pitch <10 μm, typically found in integrated circuits, dry etching is required. This study presents several key processes for implementing a two-layer ITO metallization scheme within a CMOS platform, with a focus on dry etching of ITO. These processes provide a way of fabricating transparent circuits.

Experiments & Results

ITO was deposited on thermally oxidized 100 mm silicon wafers with dc magnetron sputtering. Forming gas anneal (FGA) of ITO at 450 °C yielded sheet resistance of ~5 Ω/sq (400 nm). ITO is patterned with I-line stepper lithography. An ICP-RIE process with $CH_4/Cl_2/H_2$ chemistry and SiO_2 hard mask was developed, enabling well-defined ITO layers with a 4 μm metal pitch (Tab. 1). The two-layer ITO metallization was evaluated with contact chain structures. I-V measurements across 120 chips demonstrated average contact resistance of ~85 Ω (Fig. 1). The compatibility of TiW/Al or TiN/Al to ITO was evaluated for the fabrication of measurement pads to provide external connections. While the measured resistance between TiW/Al and ITO was low (~3-5 Ω), metal delamination was observed in SEM after FGA (Fig. 2). TiN/Al on ITO was intact after FGA, albeit with higher resistance (~6-8 Ω).

Conclusions

A process to define 2 μm half-pitch ITO interconnects using dry etching has been established. Two-level metallization was evaluated by contact chains. The compatibility of TiW/Al and TiN/Al to ITO layer was investigated.

Table 1. ICP-RIE details of ITO etch

Etch Parameters	*Values*	*Units*
Cl_2 flow rate	9	sccm
H_2 flow rate	5.5	sccm
CH_4 flow rate	7.5	sccm
RF Bias Power	90	W
ICP Power	1000	W
Substrate Heating	60	°C
He Cooling	5	sccm

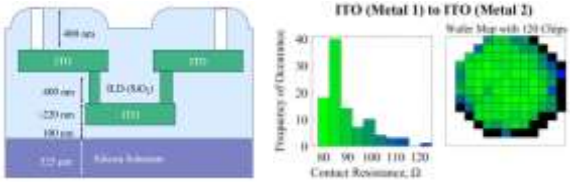

Figure 1. (a) Schematic illustration of ITO to ITO contact experiment. (b) ITO to ITO contact resistance for 120 chips (R_{AVG} = 85 Ω)

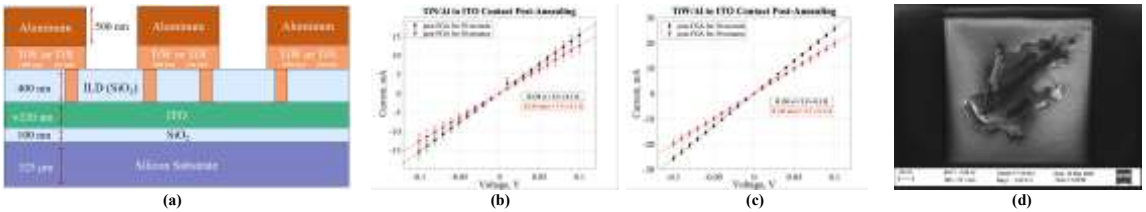

Figure 2. (a) Schematic illustration of TiW/Al or TiN/Al to ITO wafers. I-V results of (b) TiN/Al to ITO contact (c) TiW/Al to ITO contact. (d) Metal delamination of TiW/Al in SEM, the metal film burst from probing.

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Acknowlegments

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High sensitivity H_2 gas sensor gas sensor utilizing large on/off ratio of amorphous In-Ga-Zn-O thin film transistor

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Amorphous oxide semiconductors, (AOSs) such as amorphous In-Ga-Zn-O (*a*-IGZO), are widely used as channel materials in thin film transistors (TFTs) for flat-panel displays [1]. Applications of AOS TFTs are extended beyond displays e.g. to gas sensors. *a*-IGZO TFTs can attain large on/off ratios more than 10 orders of magnitude, so the *a*-IGZO TFT gas sensors are expected to achieve ultra-high sensitivity. *a*-IGZO TFT gas sensors have been applied to detection of NO_2 [2] and volatile organic molecules [3] so far. However, only *a*-IGZO thin film has been used for H_2 gas detection [4], and there have been a few reports using *a*-IGZO TFTs. In this study, we fabricated *a*-IGZO TFTs with good switching characteristics at high temperatures where H_2 gas sensor operates and evaluated the gas sensor performances.

We measured *a*-IGZO TFT performance at 250ºC in air and a mixing gas of H_2 and air. The H_2 concentration of the mixing gas was fixed at 100 ppm. First, we measured an initial I-V curve in air. Then we introduces the H_2 gas and measured I-V curves cyclically for 5 times at one-minute intervals. After the measurements in H_2, we stopped H_2 flow and measured I-V curves for 20 times. Fig. (a) shows transfer curves of *a*-IGZO TFTs in air without and with H_2 flow. After the H_2 introduction, the turn-on voltage (V_{on}) shifts to the negative V_G. This shift would be caused by H_2 adsorption on the *a*-IGZO surface, which increases the carrier density and the conductivity of *a*-IGZO [4]. Fig. (b) shows the V_G dependece of H_2 gas sensitivity calculated from the ratio of I_D at each V_G in air without and with H_2 flow. The gas sensitivity reached a maximum value of $>10^6$, indicating that a high sensitivity H_2 gas sensor can be realized by applying good switching of *a*-IGZO TFTs. Fig(c) shows the time variation of V_{on}. The V_{on} shifts in response to the flow change of H_2 flow, confirming that the change in V_{on} is related to H_2 adsorption and desorption.

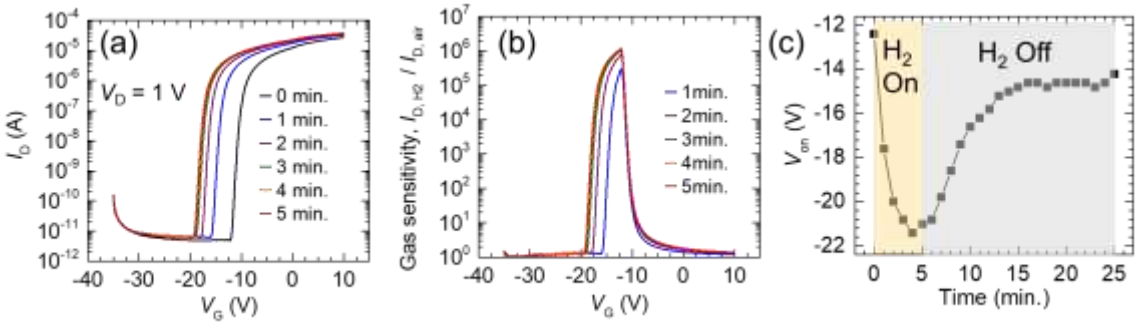

Fig. 1(a) Changes of *a*-IGZO TFT transfer curve by flowing H_2 gas. (b) V_G dependence of H_2 gas sensitivity calculated from the ratio of I_D in air and H_2. (c) Time dependence of V_{on} by On/Off switching of H_2. Yellow and gray regions indicate H_2 on and off, respectively.

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Optical anisotropy of pristine and reduced V_2O_5(010)

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The vanadium-oxygen system consists of four single valence phases as well as a range of mixed valance phases. Many of the phases exhibit a semiconductor-to-metal transition linked to the strongly correlated nature of the vanadium 3d electrons. VO_2 sees application in electronics and uncooled bolometers due to its semiconductor-to-metal transition close to room temperature and V_2O_5 is intensively researched for gas sensing and supercapacitor technologies. V_2O_3 has received interested as a strongly electron correlated semi-metal with p-type conductivity and increased visible optical transparency due to electron correlation shifting the screened plasma energy [1,2]. The reduction of single valance phases is complex resulting in the coexistence of multiple phases that can be close in stoichiometry but exhibit drastically different electronic and optical properties. This is a challenge but can also be utilized in resistive switching, for example [3].

In this work, the optical anisotropy of pristine and reduced single crystalline (010) orientated V_2O_5 is presented. Reflectance anisotropy spectroscopy (RAS) measures the difference in reflection along two orthogonal surface directions and provides a non-destructive probe that can be employed in real-time to monitor changes in thin films. Pristine orthorhombic (010) orientated V_2O_5 exhibits strong reflectance anisotropy with significant features beyond the optical bandgap of 2.5eV. The spectra is well described by the resolved optical constants extracted by ellipsometry. Vacuum annealing has been performed at four different temperatures and X-ray Diffraction and RAS have been conducted after each anneal. Depending on the anneal temperature, different phases are introduced into the V_2O_5 crystal including V_4O_9, V_6O_{13} and VO_2. Spectral features of each of these phases are identified. V_6O_{13} is understood in terms of the axially resolved optical constants from the literature, while isotropic VO_2 modifies the total reflection once it undergoes it's semiconductor-to-metal phase transition at 340 K. This understanding of the optical response of the ideal single crystal facilitates applying RAS to monitor the growth and changes of V_2O_5 thin films in-real time.

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Two-dimensional electron (2DEG) and hole (2DHG) gases onto β-Ga_2O_3

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A new generation of UWBG semiconductors will open new territories for higher power rated power electronics and solar-blind deeper ultraviolet optoelectronics. Gallium oxide - Ga_2O_3 (4.5-4.9 eV), has recently emerged pushing the limits set by more conventional WBG (~3 eV) materials such as SiC & GaN as well as for transparent conducting oxides (TCO) like In_2O_3, ZnO and SnO_2 to name a few.

While there are several *n*-type transparent semiconductor oxides (TSO) for optoelectronic applications their required *p*-type counterpart oxides are known to be more challenging. We have demonstrated that Ga_2O_3 is also the intrinsic (or native) *p*-type TSO. [1]

In 2019, we first reported [2] a two-dimensional electron gas (2DEG) onto beta-Ga_2O_3, a solid that is a pure insulator in its bulk but has a metallic conductive termination presenting a two-dimensional conductive channel at its surface. β-Ga_2O_3 thin films exhibited degenerate semiconductor conduction with a room temperature $n = 8\times10^{18}$ cm^{-3} electron concentrations and $\mu = 19$ cm^2/Vs Hall electron mobility. Under the Thomas-Fermi approximation, the sheet charge concentration of the 2DEG is $n_s \sim 2\times10^{14}$ cm^{-2}. This 2DEG was found to be resistant to high dose proton irradiation (2 MeV, $5 \times 10^{15} cm^{-2}$ dose) and was largely invariant (metallic) over the phenomenal temperature range of 2 K -850 K. In 2023, we first reported [3] a two-dimensional hole gas (2DHG) onto beta-Ga_2O_3. Although two-dimensional electron gases have been realized in a number of semiconductor surfaces, examples of two-dimensional hole gases (2DHG) - the counterpart to 2DEG - are still very limited. In this work, we report what appears to be an exceptional *p*-type 2DHG surface on a Si-doped monoclinic (010) β-Ga_2O_3 epitaxial films which are *n*-type in the bulk. The majority of the free carries at the surface have been determined to be holes with a sheet concentration of $p \sim 8.7\times10^{13}$ cm^{-2} and a puzzlingly high mobility value of $\mu_h \sim 80$ $cm^2/(V\cdot s)$ at room *T*.

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Hyper-gap transparent conductor

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An elusive conductor with perfect optical transparency holds revolutionary potential for fields such as optoelectronics and nanophotonics. This hypothetical metal possesses an unprecedented spectral gap[1,2], dubbed the "hyper-gap" in its absorption spectrum, separating the intra-band and inter-band absorptions, in which the optical losses could completely vanish — a property currently achievable only within the bandgap of insulators. However, realizing such a hyper-gap metal demands an exotic electronic structure, where the conducting bands have a bandwidth narrower than their energy separations from the remaining electronic states. Despite decades of searching[3], no evidence has yet surfaced on where this material might be found or if it is even possible. Here, we present the first observation of this long-sought-after hyper-gap in a family of organic metals, the Fabre charge-transfer salts[4], through first-principal predictions coupled with both electrical and optical measurements. A remarkable transparent window, spanning from visible red to near-infrared wavelengths, is identified in bulk single crystals that remain transmissive over thirty microns thick. The corresponding absorption coefficient is the lowest recorded among all known stoichiometric metals, rivaling that of commercial thin films of transparent conductive oxides. This discovery[5] introduces a new path, beyond traditional doping strategies in insulators, to combine electronic conduction and optical transparency in intrinsic solids.

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Transparent and conductive codoped-ZnO thin films (IGZO, IAZO, AGZO) deposited by ultrasonic chemical spray technique

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Indium doped zinc oxide (IZO) thin films were deposited onto soda-lime glass substrates by the ultrasonic chemical spray (USP) technique. The influence of different Zn precursors (zinc acetate, AcZn, zinc sulfate, SZn, and zinc chloride, CZn), used in the preparation of the starting solutions, on the structural, optimal, morphological and electrical characteristics was analyzed. Starting solutions were prepared with a molar concentration of 0.2M and an atomic concentration of In of 3 at%. The deposition conditions were kept constant, with a substrate temperature of 450 °C and a deposition time of 12 min. From the structural analysis, a preferential orientation along the (101) plane was observed for all IZO films. The optical transmission oscillated in the range of 61-81 %, confirming the transparency of all deposited films. The bandgap values, E_g, around 3.5 eV, showed slight variations with the different types of Zn precursor employed. The films were designed for being employed as Transparent Conductive Oxide (TCO) films, in this respect, the best figure of merit or quality factor for TCO applications were obtained in the IZO films doped with 3 at% of In in the starting solution, with a value of 2.49×10^{-3} $(\Omega/\square)^{-1}$, calculated from an optical transmission of 81 % and a sheet resistance of 50 Ω/□. According to the results obtained, IZO thin films deposited by USP technique are potentially applicable in the field of optoelectronics, mainly as transparent electrode.

Keywords: Zinc oxide, thin films, ultrasonic chemical spray, TCO.

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Hydrogen in indium oxide and gallium oxide

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Indium oxide, with a band gap of 2.7 eV, is widely used as a transparent conducting oxide. Gallium oxide, with a band gap of 4.8 eV, is also conductive and remains transparent into the UV, and $(Al_xGa_{1-x})_2O_3$ alloys have even larger band gaps. Hydrogen is often introduced during growth or processing of the material; in fact, in the widely used technique of metal-organic chemical vapor deposition (MOCVD) hydrogen is present in the metal-organic precursors and often used as a carrier gas. It is therefore important to assess the impact of hydrogen on the properties of these materials. We address these issues using first-principles calculations based on density functional theory. In both In_2O_3[1] and Ga_2O_3[2] hydrogen acts as a shallow donor, i.e., it contributes to *n*-type conductivity, but its behavior changes in $(Al_xGa_{1-x})_2O_3$ alloys.[3] Hydrogen can also interact with other impurities or defects in the material.

We have also studied diffusion. In monoclinic β-Ga_2O_3, the most stable phase, hydrogen diffusion is highly anisotropic. For protons, the migration barrier is as low as 0.28 eV along the [010] direction.[3] In In_2O_3, with the bixbyite structure, local hopping of the proton, corresponding to a realignment of the O-H bond, can also occur with a low activation energy of 0.24 eV; however, this process does not lead to long-range diffusion.[4] The long-range migration path of H^+ in In_2O_3 can be decomposed into rotations of the proton around oxygen and jumps between two oxygen atoms, with a higher overall activation energy of 0.94 eV. We compare our results with recent experiments.

Work performed in collaboration with M. L. D. Franckel, J. L. Lyons, S. Mu, M. E. Turiansky, J. B. Varley, D. Waldhör, M. Wang, and D. Wickramaratne.

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Electrochromic materials for visible and near infrared light modulation

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Electrochromic materials can reversibly change their optical properties by varying the external electrical stimuli. Since the first experimental demonstration of electrochromic phenomenon in tungsten oxide, electrochromic technology has been extensively developed. Currently, electrochromism based devices can be found in windows of energy efficient buildings, smart phones, goggles, information displays, anti-glare rear-view mirrors, etc. In inorganic electrochromic materials, transition metal oxides are most studied, and oxide thin films can change colors and transmittance of the near-infrared between a transparent and a colored state upon small ion intercalation. In an electrochromic material or device, an ideal scenario is that visible and near-infrared light can be independently regulated, that is bright mode (both VIS and NIR are highly transparent), cold mode (transparent for VIS but not for NIR), warm mode (transparent for NIR but not for VIS) and dark mode (both VIS and NIR are blocked). However, electrochromic devices typically suffer from single-mode control, i.e., simultaneously varying the visible and near-infrared light. Electrochromic effect combined with surface localized plasma resonance (LSPR) were recently found to be able to sequentially modulate near-infrared and visible light. In this talk, we report our recent progress on dual-band modulation, with a special focus on achieving a transition from bright mode to warm and dark mode, as well as bright mode to cool and dark mode. We believe our findings show substantial fundamental insight into electrochromism in cathodic oxides, and provide a new starting point for designing electrochromic devices with superior performance.

Novel chemical vapor deposition process of ZnO and Ga_2O_3 films by nonequilibrium atmospheric pressure N_2/O_2 Plasma

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We have successfully generated a nitrogen plasma near atmospheric pressure with a high electron temperature (>4000 K) and a low gas temperature (<400 K) using dielectric barrier discharge. By employing this non-equilibrium nitrogen plasma, in which the emission corresponding to the N_2 second positive system was predominantly observed, self-limited nitridation of Si at a thickness of approximately 1.8 nm was achieved at room temperature. The leakage current of the resulting nitride film was found to be more than two orders of magnitude lower than that of films nitrided using RF plasma, where atomic nitrogen active species are predominantly observed [1]. By introducing only 1ppb O_2 gas, oxidation is recognized. We have studied the effect of active species on the growth of oxide films such as ZnO and Ga_2O_3 in nitrogen nonequilibrium plasma generated near atmospheric pressure using home-made chemical vapor deposition systems. Optical emission spectroscopy was performed to evaluate the electronically excited species present in the plasma. In the spectra, the N_2 second positive system (N_2 2_{PS}) and the NO-γ system (NO-γ) were predominantly observed. The NO-γ emission was detected only at an $O_2/(O_2 + N_2)$ flow rate ratio ranging from 0 to 1%. Figure 1 shows the optical emission intensities of N_2 2_{PS} and NO-γ as a function of the $O_2/(O_2 + N_2)$ flow rate ratio. The intensity of NO-γ decreased drastically upon the introduction of the Zn source material [$Zn(OD)_2$], particularly at $O_2/(O_2 + N_2)$ ratios of 0.04–0.2%, suggesting that NO radicals play an important role in the decomposition and/or oxidation of $Zn(OD)_2$. Figure 2 presents the XRD profiles of ZnO films deposited at various $O_2/(O_2 + N_2)$ ratios, ranging from O_2-rich to N_2-rich gas compositions. With decreasing $O_2/(O_2 + N_2)$ ratio, the degree of (0001) preferred orientation in ZnO films was markedly enhanced. These results indicate that N_2 plasma with a small amount of O_2 (<1%) provides superior crystallographic quality compared to O_2-rich plasma. We further investigated the role of active species in the growth of oxide films such as ZnO [2] and Ga_2O_3 [3] using our in-house chemical vapor deposition systems with nitrogen non-equilibrium plasma generated near atmospheric pressure. Highly resistive ZnO epitaxial films were successfully fabricated even at a substrate temperature as low as 200 °C. The residual donor concentration was measured to be below 1×10^{13} cm^{-3}, which is highly beneficial for achieving p-type ZnO and for piezoelectric applications. The surface reaction mechanisms involved in the growth of oxide films such as ZnO and Ga_2O_3 are also discussed, with particular emphasis on the reduction of residual donor concentration and the potential for N_2 doping.

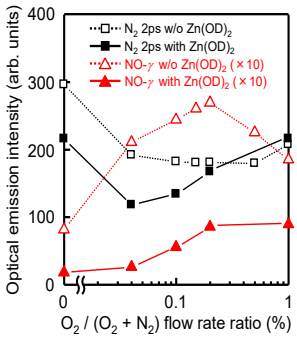

Fig. 1 O_2 / (O_2 + N_2) flow rate ratio dependence of the OE intensity of N_2 2ps 337 nm (square) and NO-γ 234 nm (triangle). The open and close symbols correspond to the absence and presence of $Zn(OD)_2$ in the mixed gases, respectively.

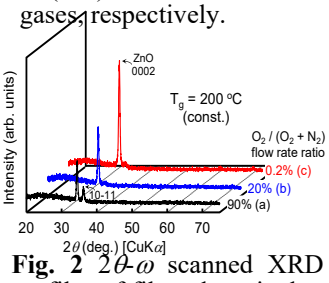

Fig. 2 2θ-ω scanned XRD profiles of films deposited at O_2 / (O_2 + N_2) flow rate ratio of 90% (a), 20% (b) and

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Creation of Material Libraries of Wide and Ultra-Wide Bandgap Conductive Oxides by Combinatorial Pulsed Laser Deposition

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The discovery of new functional materials by exploring the phase space of multinary alloys is greatly accelerated by high-throughput experimental and computational screening methods In the realm of experimental research, high-throughput screening necessitates the utilization of sample sets that exhibit a systematic variation in material properties. These properties may include, but are not limited to, chemical composition, layer thickness, and other parameters. These can, among other methods, be realized by combinatorial pulsed laser deposition (C-PLD) enabling to create spatially addressable material libraries to be analyzed with spatially resolving physical property screening methods for high-throughput characterization [1]. The current status of C-PLD will be discussed, along with recent methodological developments.
We will illustrate the implementation of segmented PLD targets in the creation of lateral and vertical continuous composition spread material libraries (CCS-ML) for wide and ultra-wide bandgap group III sesquioxides or transition metal sesquioxides [2]. Group III sesquioxides have emerged as promising materials for applications in next-generation high-power electronic devices [3]. We address the physical properties of various polymorphs of $(Al,Ga,In)_2O_3$ as a function of cation composition.

Additionally, the physical properties of ternary α-$(Me,Ga)_2O_3$ TCOs are presented. Spatially addressable CCS-MLs of $(Cr_xGa_{1-x})_2O_3$, $(Ti_xGa_{1-x})_2O_3$, and $(V_xGa_{1-x})_2O_3$ were synthesized by C-PLD over a broad compositional range with high chemical resolution and experimentally investigated by high-throughput mapping using a variety of analytical methods including X-ray diffraction, energy-dispersive X-ray spectroscopy, UV-VIS transmission and spectroscopic ellipsometry measurements. For $(Cr_xGa_{1-x})_2O_3$ and $(V_xGa_{1-x})_2O_3$, phase-pure growth in the rhombohedral crystal structure was demonstrated over the entire composition range. For the $(Ti_xGa_{1-x})_2O_3$ CCS-ML, the α-phase was stabilized up to x=25%. A substantial red shift of the absorption edge with increasing x was found for all investigated MLs. These findings demonstrate the feasibility of the α-$(Me,Ga)_2O_3$ material systems for bandgap engineering over an exceptionally large energy range without phase-separation
A FAIR data management solution for thin film deposition and characterization data is finally presented, with a focus on the digitization of PLD process data and metadata.

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Return

Transparent electrodes and semiconductor materials for electrocatalysis applications

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Electrochemical catalysis is an important part of research in the modern world due to its various applications. Electrocatalysis is an important part of research for application in the development of sensors for use in environmental chemistry and biomedical research, development of capacitors, batteries, energy conversion and conservation, waste water treatment. The development of nanotechnology has significantly contributed to the accelerated development of these areas. A very important place in each of these fields of research is occupied by transparent materials and semiconductor nanomaterials. Electrodes based on transparent nanomaterials are an indispensable part of the development of electrochemical sensors[1]. Indium tin oxide (ITO) electrode forms an important basis for the construction of biosensors based on electrocatalysis and their application in biomedical research. In addition to this application, the electrocatalytic degradation of chemicals of emerging concern (CEC) and persistent and mobile organic chemicals (PMOCs) based on these electrodes is very common today. In addition to ITO, carbon nanostructures, other metal oxides, MXenes, polymer materials and nanocomposites also play a significant role in this field. Semiconductor nanomaterials possess unique optical, electrical, thermal and catalytic properties. Therefore, they have attracted great interest in the construction of electrochemical (bio)sensors and the development of technologies for water purification by electrocatalysis[2]. The catalytic properties of semiconductor nanomaterials can reduce the overvoltage of some important reactions in electrochemical catalysis, or provide reversibility for redox reactions that are irreversible on traditional electrodes, which can sometimes further improve electrochemical reactions. Their application in the field of electrocatalysis is today indispensable for applications in biomedicine and environmental chemistry.

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Micro/nano-structures of transparent oxides by laser processing for optoelectronics and smart surfaces

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The need for advanced materials and systems with new functionalities has motivated the development of micro/nanostructures on solid surfaces, which are necessary for the fabrication of functional devices for novel applications. In this talk, we will discuss the development of functional micro/nanostructures, based on transparent oxides combined with laser-processed surfaces.

Combining silicon micro/nanostructures with thin semiconducting ZnO films results in electronic heterojunctions with increased surface area for improved optoelectronic performance, especially for broadband photodetectors with enhanced photoresponse[1]. Furthermore, isotype heterojunctions of n^+-ZnO/n-Si result in wavelength-selective, high-speed photodetectors with self-powered operation, which can be further engineered by careful selection of the electronic properties of the constituting materials[2,3]. “Smart” surfaces of controllable extreme wetting states are obtained by combining photoresponsive metal oxides with laser-processed micro/nanostructured substrates, which can reach complete water repellence without chemical modification[4]. Thin TiO_2 films, immobilized on microstructured surfaces, show increased photocatalytic activity for the degradation of water pollutants and the development of water cleaning technologies[5]. Laser scribing of transparent, conductive oxide films, to be used as electrodes in thin-film photovoltaic systems will be discussed.

Acknowledgement: This work was carried out within the framework of the Action 'Flagship Research Projects in challenging interdisciplinary sectors with practical applications in Greek Industry', implemented through the National Recovery and Resilience Plan Greece 2.0 and funded by the European Union - NextGenerationEU (Acronym:3GPV-4INDUSTRY, project code: TAEDR-0537347).

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The Plasma Plume Deflection and Target Surface Roughness During Pulsed Laser Deposition of Functional Oxides

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Pulsed laser deposition (PLD) is a highly flexible, fast and reproducible physical vapor deposition technique that uses a pulsed laser to ablate a target material, producing an excited laser-induced plasma. The ablated material condenses onto a substrate. PLD allows for direct control of growth parameters such as laser pulse frequency, laser fluence, pressure and ambient gas mixture. Although simple to set-up, the ablation process is difficult to model because of its non-equilibrium nature due to the high pulse energy incident within a short laser pulse duration (typically 20 ns for excimer lasers)[1].
Ablation of any target material requires optimization of the process parameters.
Some targets used in PLD develop a rough surface structure after prolonged use, which causes the plasma plume to permanently deflect toward the incident laser beam during the ablation process. Typically, the plume deflection increases until a stable surface morphology is reached[2].
In this work, we present a correlation of the plasma plume deflection during the deposition process with the target surface roughness and morphology after the deposition from different ceramic metal oxide targets. The target surface roughness and topography are measured by laser scanning microscopy. The plasma plume deflection is evaluated from images captured by a camera. The deflection angle is determined utilizing a Python script that uses image moments to calculate the angle of the plasma plume.

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Heuristic approach to the fundamental optical constants of silver nanowire networks: experiments and theory

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Silver nanowire (AgNW) networks are emerging as a leading class of Transparent Conducting Materials (TCMs), offering a unique combination of high optical transparency, excellent electrical conductivity, mechanical flexibility, and scalable, cost-effective production routes. This association of properties makes them key building blocks for a wide range of devices such as photovoltaic cells, OLEDs, transparent heaters, sensors or smart windows[1]. The conductivity of AgNW networks arises from a percolation mechanism through nanowire junctions, while their transparency results from gaps between the nanowires, illustrating an intrinsic interplay between these properties. Understanding the optical properties of AgNW networks, often described by their refractive indices (n, k), is critical for advancing their integration into multilayer systems and devices. Furthermore, refractive indices provide fundamental insight into the material's optical behavior and enable accurate simulations of complex multilayer designs using the Transfer Matrix Method[2].

This study combines Mie's scattering theory and van de Hulst's mixing model to theoretically determine the refractive indices of AgNW networks without relying on fitting parameters. For the first time, refractive indices across the visible and near-infrared spectrum are calculated and validated upon experimental results. Transmittance spectra, derived from numerical solutions of Fresnel's equations, show strong agreement with measurements, particularly for nanowires with larger diameters and at shorter wavelengths, with a relative error below 10% at $\lambda = 550$ nm. Crucially, the findings of the present research also highlight for the first time in optical measurements the predominantly metallic optical behavior of AgNW networks deposited on glass substrates.

By accurately modeling the optical properties of AgNW networks, this work facilitates their integration into multilayer optical systems, supporting the development of innovative devices such as displays, sensors, and energy-efficient smart windows. Additionally, this research paves the way for a more advanced theoretical understanding of the optical properties of silver nanowire networks at the fundamental level.

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Flexible, printed absorbers for shielding against microwave radiation

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Absorbers in microwave region of the electromagnetic spectrum are of great importance, due to their application as protective coatings against this radiation. Moreover, Perfect Metamaterials Absorbers (PMAs) have attracted much research attention during the last decade as they are able to fully absorb the microwave radiation. The PMAs are based mainly on periodic metallic structures with both specific periodicity and geometry.

In the present work, the properties of conductive inks, as well as of the substrates were investigated, in order to fabricate PMAs based on printed metallic periodic structures. More specific, nanoinks based on Ag or other metals were examined as far as their morphology, viscosity, resistance etc. concern, while flexible substrates such as kapton and textiles were characterized and tested for their ability to print metallic structures on them. Finally, different geometries and sizes were tested to be printed on the substrates, according to simulations that have been done.

Moreover, the metallic periodic structures fabricated by 3D printing technique on flexible substrates as well as on textiles, were investigated as perfect absorbers for electromagnetic waves in the microwave region of 9 GHz to 14 GHz. Specifically, various topologies were designed, simulated, and developed to control surface impedance and achieve electromagnetic absorption at microwave region. The level of transmission and reflection of the developed samples was measured with appropriate waveguides. From these, the absorption was calculated and found to be enhanced for these printed periodic metallic structures between 9 and 10.5 GHz, indicating a possible perfect absorber in the microwave region of EM radiation.

Acknowledgements

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QM/MM Investigations of Defects in MgO and Their Use as a Model System for High-T_c Superconductivity

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The defect chemistry of magnesium oxide has been extensively studied for many years, with a myriad of applications in catalysis, optoelectronics and many other fields. Both vacancies and substitutionals have been shown to be effective in providing MgO with additional useful properties. Our work employs modern hybrid quantum mechanical – molecular mechanical (QM/MM) techniques, using the ChemShell code[1], to both reassess previously investigated defects and probe others that have been less researched.

Whereas a number of different transition metal ions have been investigated and widely applied as substitutionals in MgO, for example Ni and Co in catalytic systems, research into copper dopants in MgO is more sparse. Currently, the work on such systems is largely focused on nanoparticles, some uses in catalysis or the Jahn-Teller distortion induced by the dopant[2]. Our work focuses instead on the localisation and possible trapping of charge carriers within a $(CuO_6)^{10-}$ unit. Whereas oxygen bound polarons have been observed with a number of doped metal oxides[3], currently, there is no evidence for the influence that copper has, in this regard. Hybrid-DFT within QM/MM has been utilised to track the migration of such holes, with further electromagnetic resonance (EPR) calculations allowing for direct comparison to experimental work. Our work will be used to guide future investigations of hole states and bipolaron formation in superconducting cuprate materials.

Additionally, the optical excitations of F-centres within MgO have been investigated and compared to previous theory of their excited states. It has been well reported that excited states of electrons within oxygen vacancies in MgO are hydrogenic in character with distortions from the crystal field environment[4,5]. Through use of time-dependent DFT (TDDFT) within a QM/MM scheme, these characteristics are reinvestigated.

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Extrinsic Doping Mechanism in Sb_2O_5 as a Promising n-type Transparent Conducting Oxide

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Transparent conducting oxides possess a unique combination of optical transparency and electrical conductivity, making them indispensable in optoelectronic applications. [1] However, the heavy dependence on a small number of established transparent conducting oxides (In_2O_3, SnO_2, ZnO and Ga_2O_3) places limitations on the number and types of devices they can support. Additionally, the high cost due to the scarcity of rare elements raises concerns about their long-term sustainability and large-scale production. [2] Discovering more wide band gap oxides that can be doped to display metallic-like conductivity is therefore necessary.

In this work, we use the PBE0 hybrid functional to investigate the defect chemistry of the binary Sb(V) system, Sb_2O_5. [3] We observe a large optical band gap over 3.6 eV, enabling transparency. The calculated Sb_2O_5 electronic structure shows a dispersive conduction band minimum with low electron effective masses, indicating the potential for high electron mobility. *ShakeNBreak* was used to generate different distortions for finding the groundstate structure, and *Doped* was used to manage all the defect calculations and analysis.[4–6] A rare 4-electron negative-U behaviour was found in the Sb vacancy with an oxygen trimer and split-vacancy configuration formed. Although the intrinsic point defect study shows that Sb_2O_5 does not display metallic-like conductivity, with extrinsic doping of Fluorine (F), Tungsten (W) and Molybdenum (Mo), Sb_2O_5 displays degenerate n-type transparent conducting behaviour. Our band alignment calculations demonstrate that Sb_2O_5 has a larger electron affinity than the established transparent conductors, which can facilitate electron extraction for organic solar cell applications. The findings of this under-explored Sb(V) binary system demonstrate the feasibility and potential for Sb(V)-based materials to be promising transparent conducting oxides.

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Full Subgap Defect Density of States in p- and n-type Metal Oxide Transistors

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Recent developments in the Ultrabroadband Photoconductive Density of States (UP-DoS) method enable the acquisition of full subgap DoS on metal oxide thin-film transistors (TFTs), including $InGaZnO_x$, SnO and Cu_2O channel materials.[1,2] To achieve full valence-to-conduction band edge coverage, we continuously scan the incident laser photon energy from $h\nu$ = 0.1 to 3.6 eV, yielding an integrated trap density, $N_{tot}(h\nu)$, that increases stepwise as each subsequent subgap defect state is ionized. The identity of each defect peak is assigned by comparing the derivative UP-DoS spectra, $dN_{tot}/dh\nu$, to both DFT+U simulations and experimental defect recombination lifetimes.[1,2]

For p-type channel TFTs, UP-DoS spectra of SnO and Cu_2O reveal metal vacancy peaks near the valence band maximum that determine the TFT equilibrium hole concentration and Fermi level energy. Due to its measured small bandgap of 0.7 eV, unipolar p-type transistor behavior in SnO is achieved only when the defect DoS near the conduction band minimum, attributed to oxygen interstitials, is sufficiently large to suppress n-type conduction. For Cu_2O TFTs, UP-DoS reveals the presence of a minority phase of CuO existing at a heavily oxidized semiconductor-dielectric interface. This oxidized minority phase explains the large discrepancy between the measured Hall mobility (μ_{Hall} = 20 $cm^2V^{-1}s^{-1}$) and field effect mobility (μ_{FE} = 0.2 $cm^2V^{-1}s^{-1}$) for Cu_2O thin-films.[1]

In contrast to p-type materials, n-type amorphous $InGaZnO_x$ is dominated by oxygen vacancies with different neighboring metal coordinations. Near the conduction band edge, UP-DoS reveals the presence of a broad Gaussian electron trap state centered at 0.4 eV. Using a 10K atom DFT+U simulation, this defect state is further assigned as a (In In In Ga) coordinated oxygen vacancy. For 15 different TFT processing conditions, UP-DoS measures the trap density of this In-rich electron trap state to show an inverse correlation with both TFT mobility and subthreshold swing. This correlation is validated using a first-principles DoS mobility model that shows the tail-state conductivity requires the inclusion of this broad shallow donor peak to reasonably simulate a-$InGaZnO_x$ TFT transfer curves.

Finally, we reconfigure our UP-DoS microscopy method to use high-power femtosecond lasers that selectively ionize specific defects while also annealing the amorphous $InGaZnO_x$ lattice. The end result suggests a fundamental transformation of the active-channel material that boosts field-effect mobility >10x, with minimal impact on TFT reliability.

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Oxidation-resistant Cu-based nanowires transparent electrodes activated by an exothermic reaction

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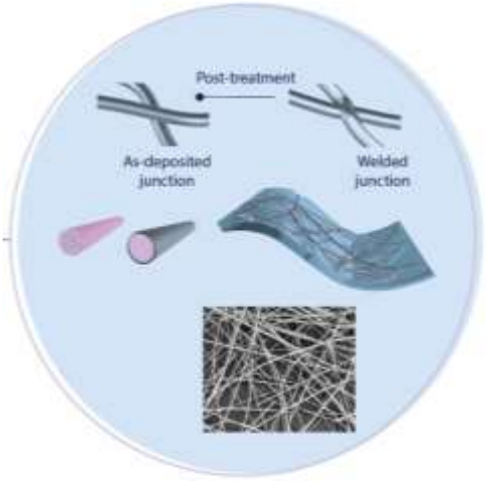
Metallic nanowire percolating networks are one of the promising alternatives to conventional transparent conducting electrodes. Among the conductive metals, copper appears as a relevant alternative to develop electrodes in a more sustainable and economical way (abundance of the supplies, geo-political risks regarding the supplies, environmental impact, and cost).[1] However, Cu nanowires suffer from high instability in air, and one of the ways to increase stability as well as to boost properties related to transparent electrodes is to combine the Cu with another metal, resulting in bimetallic nanowires. Even though the field of fabrication of nanoalloys has been advancing at a rapid pace in the last two decades, binary nanowires are difficult to produce due to a wide range of parameters that must be aligned in regard to metals that are being combined. We are currently experimenting how the allowing of Cu-based nanowires with nickel can be exploited for the development of metal nanowire networks with high oxidation resistance. We report a novel synthesis and a new way of optimizing performance of a CuNi transparent electrode through enhancing interconnectivity of NWs, based on a reducing treatment at room conditions. [2]



Schematic of most common approaches for preparing bimetallic CuM NW-based transparent electrodes

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Electrical Properties of Heterostructure Metal - Polyarylene Ether Ketone Copolymer - TCO

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The report presents the study of the unique properties of non-conjugated transparent polymers from the class of aromatic polyether - polyarylene ether ketones, - to form low resistance electrical contact metal/polymer/transparent conductive oxide (TCO). The conductivity mechanisms in thin polymer films in the heterostructure metal/polymer/TCO have been investigated experimentally. Particular attention has been paid to the electronic structure of polymers and mechanisms of a highly conductive state (HCS) formation.

A number of polyarylene ether ketones copolymers (co-PAEK) with a concentration of phthalide or fluorene cardo groups of 5, 10, 15, 20 and 25% with a close molecular weight were synthesized. The thermo mechanical and electrical properties of copolymers have been studied depending on the content of cardo groups. An increase in the concentration of cardo groups leads to an increase in the glass transition temperature of the copolymer.

TCOs based on doped indium oxides (ITO (In_2O_3:Sn); IFO (In_2O_3:F)) with a thickness of 100±10 nm were deposited on silicon substrate by ultrasonic spray pyrolysis under various atmospheric conditions (Ar or O_2 carrier gas). The samples under study were sandwich structures with a co-PAEK layer applied to the TCO using the spin-coating method, followed by spraying a thin metal electrode made of copper or tin onto the polymer layer.

The parameters of charge carriers in the metal/co-PAEK/IFO and metal/co-PAEK/ITO structures were assessed depending on the concentration of cardo groups in co-PAEK; the atmosphere of TCO growth (Ar or O_2); the type of metal of the upper electrode (Sn or Cu). The electronic parameters of the obtained structures were estimated within the injection model of charge carrier transport limited by the space charge region. The model is well suited for describing the results obtained from the current-voltage characteristics of structures. It was found that the best electronic parameters (charge carrier mobility, carrier concentration) for all the studied copolymers in the metal/co-PAEK/TCO structure were provided by using an ITO film obtained in O_2 atmosphere, which in turn can be associated with the energy structure of the co-PAEK/TCO contact. The dependence of the electronic transport properties of the metal/polymer/TCO system on the thickness of the co-PAEK polymer film was established. In the films with a thickness less than the critical one (d_{cr}), an injection mechanism of charge carrier transfer was detected. It was found that d_{cr}, at which the transition to the highly conductive state (HCS) is observed, is higher for structures with ITO layer grown in an oxygen atmosphere. In particular, it was found that for ITO $d_{cr} \approx 1$ μm, and for IFO $d_{cr} \approx 650$ nm. It was also found that when using Cu as the upper electrode, the probability of transition to the HCS for thicker films is higher than when using Sn.

The use of thin co-PAEK films in metal/polymer/TCO heterojunction makes it possible to create ohmic contacts to TCO, taking into account the good adhesive and optical properties of co-PAEK [1].

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From Sensing to Energy: Metal Oxide Nanostructures for Green Technologies

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Metal oxides are versatile functional materials widely used in sustainable technologies due to their chemical stability, tunable electronic properties, and ease of integration into miniaturized systems. In the field of chemical sensing, they serve as highly sensitive and selective materials capable of detecting a wide range of gases and biomolecules, which is essential for real-time monitoring in lab-on-a-chip devices and point-of-care medical diagnostics. These applications benefit from the miniaturization, low power consumption, and fast response times enabled by metal oxide-based sensors.

Beyond sensing, metal oxides—such as NiO, ZnO, and CeO_2-based composites—play a critical role in the development of next-generation energy conversion systems like Solid Oxide Fuel Cells (SOFCs). Their function as catalysts and electrode materials supports efficient electrochemical reactions, enabling clean energy production from hydrogen or bio-derived fuels.

Integrating these materials into multifunctional platforms bridges the gap between sensing and energy, paving the way for self-powered diagnostic tools and compact, eco-friendly devices. From a sustainability standpoint, metal oxides offer high availability, recyclability, and compatibility with low-temperature fabrication methods, making them ideal candidates for scalable, green technologies that align with circular economy goals and carbon neutrality strategies.

We will explore the synthesis, characterization, and performance evaluation of chemical sensors and Solid Oxide Fuel Cells (SOFCs) using nanostructured materials. These samples were characterized using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), and Raman spectroscopy. Electrochemical performance, including I–V characteristics and Electrochemical Impedance Spectroscopy (EIS), was evaluated at different temperatures and gas flow conditions.

Acknowledgements

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Materials Design of High Carrier Transport Oxide Films for Various Applications

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We have developed highly transparent conductive oxide (TCO) films based on *n*-type-doped zinc oxide (ZnO) and indium oxide (In_2O_3) with thicknesses (*t*) ranging from a few nanometers to micrometers [1]. Our main concern is achieving high carrier transport (e.g., 145 $cm^2/(Vs)$) at high carrier concentrations (N) ranging from 2×10^{20} to 2×10^{21} cm^{-3}, independent of *t*. The N and *t* values depend heavily on the application. Transparent conductive electrodes, for example, require *t* values ranging from 100 to 150 nm for solar cells [2] and liquid crystal displays (LCDs) [3,4]; electromagnetic shielding requires *t* values greater than 1 μm; gas sensors [5] require *t* values of 50 nm; γ-radiation resistance [6] requires *t* values of 200 nm; and antibacterial applications require *t* values of 50 nm. Recently, we achieved high Hall mobility in polycrystalline W-doped In_2O_3 (IWO) with *t* below 10 nm [7]. We have successfully fabricated continuous, 2-nm-thick amorphous IWO films on glass substrates [1]. In this talk, we will discuss how to achieve TCO films with high carrier transport and explain the physics of the free electron system in IWO films, which differs from that of most metals, and discuss dominant factors governing carrier transport.

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Switching the Transparency of Semiconductor Thin Films

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When a semiconductor material is irradiated by an intense laser with excitation energy larger than its band gap, a large number of valence electrons can be excited into its conduction band. These excited electrons rapidly relax, and then transiently occupy at the bottom of the conduction band. Such transient occupation, named transient Pauli blocking effect [1, 2], reduces the material's ability to absorb light, potentially enabling the switching from an opaque state to a transparent one on ultrafast timescales. This physics provides a foundation for designing ultrafast optical switching devices. Even more remarkably, when the laser is modulated at ultrahigh speeds, the effect can be dynamically controlled, unlocking new possibilities for advanced optical technologies [1].

In this talk, I will present recent progress in ultrafast optical switching in semiconductor films, with a particular focus on multivalley materials [1]. By irradiating the multivalley material Ge with an intense pulsed laser, ultrafast optical switching between transparency and opacity across a wide wavelength range is achieved. Femtosecond time-resolved transient transmission measurements revealed that this ultrafast optical switching occurs in both the Γ and *L* valleys, enabled by intravalley and intervalley scattering processes. Moreover, I also will discuss the shift in plasmon resonance wavelength in transparent conducting materials induced by intense laser irradiation, which offers an additional pathway for developing optical switching devices [3]. These works are expected to open new doors for possible applications in optical multiband communications, optical computing, and beyond.

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Nanomaterials for Semi-Transparent Photovoltaics and Transparent Wood

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We have developed silicon nanocrystal quantum dots[1] and noble metal nanocluster[2] based luminescent solar concentrator (LSC) devices for semi-transparent photovoltaics. Both types of nanoparticles were optimized through core and ligand engineering to achieve high quantum yield and large Stokes shift necessary for this application. A specific polymer matrix (thiol-ene) was applied to stabilize these inorganic luminescent fluorophores[3]. An improvement of light conversion efficiency in the polymer shell (quantum yield > 70%) was found in both types of nanoparticles and attributed to the reaction with active thiol radicals[4].

The LSC device is configurated as a triplex with a polymer film containing nanoparticles sandwiched between two glass sheets. Such components are intended to be used as glazing units for building-integrated photovoltaics. They feature low-haze (< 5%), high visible light transparency (>50%) and large area (30x30 cm^2). Color control can be realized through selective Mie scatterers, where color neutral devices were demonstrated[5]. Integration with smart windows and other utilization strategies will be discussed[6].

As another manifestation of a functional transparent composite, we developed transparent wood with strong mechanical properties and variable haze[7]. After delignification of the wood scaffold a refractive index matching polymer was filled in the lumen space to create an optically homogeneous material. We studied basic optical properties of this new composite, such as transparency and haze, as well as light propagation mechanism using time-resolved techniques[8, 9]. Prospects of using this renewable material for glazing and other applications will be reviewed as recent advanced led to the realization of thick (up to 15 mm) components[10].

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Colloidal Metal Oxides for Printed Electronics

S. Kassavetis

Challenges and perspectives in r-GeO_2 heteroepitaxy

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The ultra-wide bandgap semiconductor rutile germanium oxide (E_g = 4.6 eV) has the potential to rapidly become the new big actor in the field of power electronics.[1] In comparison with the widely investigated β-Ga_2O_3, a major potential advantage of r-GeO_2 is the predicted possibility to obtain ambipolar doping for *pn* homo-junctions device architectures.
Experimentally, it has been already demonstrated its bulk growth with controllable n-type conductivity (Sb).[2] While this opens up for the future evolution of homoepitaxy, at present bulk r-GeO_2 substrates are not commercially available; therefore, the development of this material system must rely on heteroepitaxy. Its epitaxial growth faces two major challenges: (1) the two-step growth kinetics involving the preliminary formation of the volatile GeO suboxide (limiting its growth rate)[3] and (2) the strong competition between the amorphous material and the rutile phase stabilization.[4] In this work we cover such aspects by investigating r-GeO_2 epitaxial layers deposited by MOVPE on different orientations of isostructural r-TiO_2 substrates. By combining experimental (e.g., (S)TEM, SEM, XRD, AFM, EBSD) and theoretical data we will focus on strain, faceting and growth rate in defining the overall structural quality of the deposited epilayers.

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Protection of Transparent Electrodes based on metallic nanowires by nitrides deposited by Plasma-Enhanced ALD

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Transparent electrodes (TEs) are critical components of many devices in daily life, such as displays, wearable electronics, solar cells, sensors, light-emitting diodes, and many more [1]. They consist of a transparent conductive material (TCM) deposited on a transparent substrate; the main requirement is to exhibit a high optical transmittance and a low sheet resistance. Other essential features like stability, flexibility, uniformity, and cost-effectiveness must be considered. The most studied and used TCM in the last four decades is indium tin oxide (ITO), an n-type semiconductor with 80 % transparency in the visible range and low electrical resistivity ($\sim 10^{-4}$ Ω·m) [2], nevertheless, its ceramic nature and scarcity in the Earth's crust have driven an ongoing race to develop alternative ITO-free TEs for the next generation of flexible electronic devices. In response to this scenario, silver nanowires (AgNWs) assembled within a percolation network are a promising contestant, not only because their physical performance is nearly comparable to ITO but also due to their high mechanical flexibility and compatibility with cost-effective solution-based techniques. However, their performance and integration into devices are limited by their morphological instability caused by the high surface effects [3].

In previous work, we investigated the possibility of coating such Ag nanowires with a robust and stable AlN diffusion barrier by Plasma-Enhanced ALD (PEALD) at 250 °C [4] to prevent the reaction of silver atoms with the environment and their surface diffusion. The current work intends to continue the research at a lower deposition temperature (200°C) and higher growth per cycle (GPC) for a cost-effective approach. The results show that an optimal coating thickness of 3 nm of AlN can resist thermal stress up to 400 °C and electrical stress of 11 V, while the bare nanowires present an irreversible morphological change after 300 °C and 6 V respectively. Regarding the adhesion to the substrate, the bare ones can be easily removed with a force of only 10 mN, in comparison the coated ones remain in the glass substrate even after an applied force of 6 N. Additionally, no optical transmittance loss was exhibited, due to the high optical bandgap of AlN (6.42 Ev), a remarkable asset of this approach.

Nitride-coated silver nanowire networks are TEs that can be integrated into transparent heaters or low-emissivity coatings.

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Direct observation of the density of in-gap states of In_2O_3:H thin films and the origin of instability of thin film transistors

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Nowadays, displays are essential devices in the information society. Their performance largely depends on the properties of the thin-film transistors (TFTs) in the displays. In recent years, the advancement of display technologies such as OLED and μLED has required the demand for TFTs with high field-effect mobility (μ_{FE} ~100 cm^2 V^{-1} s^{-1}). *n*-type transparent oxide semiconductors (TOSs) are commonly used as channel layers in TFTs, and hydrogen-doped indium oxide (In_2O_3:H) has attracted significant attention due to its high μ_{FE} (~100 cm^2 V^{-1} s^{-1}) [1].

However, the electron transport properties of In_2O_3:H are highly sensitive to the deposition and post-annealing conditions. Furthermore, the TFT characteristics are easily degraded under applying electric field and/or UV irradiation stress. The possible origin of such instability is the small electronic states in the bandgap, known as in-gap states. Despite their importance, in-gap states are extremely difficult to measure because their density is extremely low. Hard X-ray photoelectron spectroscopy (HAXPES) has been utilized to probe the in-gap states in the bulk directly. Previously, we demonstrated that high-energy excitation sources in HAXPES can induce sample damage in amorphous $InGaZnO_4$ which is commercially used as a channel layer of TFTs [2]. In this study, we investigate the density of in-gap states of In_2O_3:H thin film by high-sensitivity ultraviolet photoelectron spectroscopy (HS-UPS) using low-energy photons. Low-energy photons minimize sample damage and achieve a long probing depth. We reveal the origin of the instability of TFTs based on the in-gap states observed directly.

In_2O_3:H films were fabricated by pulsed laser deposition at room temperature [3] and post-annealed in air at 300 °C for one hour. Figure 1 shows the HS-UPS spectrum in the gap region as a function of binding energy. The valence band maximum is set at the binding energy of 0 eV. The arrows show the Fermi level (E_F). The excitation source was Xe I ($h\nu$ = 8.4 eV). The HS-UPS measurements clarified the line shape of the density of in-gap states over nearly four orders of magnitude. After performing He I HS-UPS ($h\nu$ = 21.2 eV) and XPS ($h\nu$ = 1253 eV), we observed the generation of photo-induced in-gap states near the E_F and the shift of the E_F. These results indicate that Xe I HS-UPS is more suitable for probing the in-gap states of non-damaged In_2O_3:H. We will also discuss the origin of the photo-induced in-gap states and the relationship between in-gap states and instability of TFTs at the meeting.

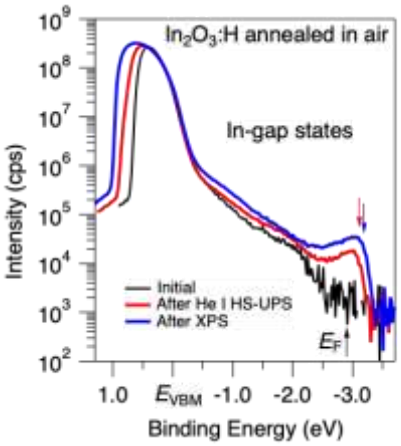

Figure 1 High-sensitivity ultraviolet photoemission spectra in the band gap region. The excitation source is Xe I ($h\nu$ = 8.4 eV).

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New evaluation method on various gas barrier performances using functional oxide films (1); O_2 or H_2O barrier properties

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Keywords: gas barrier films, zinc tin oxide, silicon nitride, transparent conductive oxide (TCO)

Recently, the development of electronic devices on flexible substrates such as polyethylene terephthalate (PET) has been challenged by their poor intrinsic gas barrier properties compared to glass or silicon substrates. As device components are susceptible to degradation caused by atmospheric oxygen or water vapor gas, achieving low water vapor transmission rate (WVTR) and oxygen transmission rate (OTR) are important to ensure device stability and reliability. Among various candidates, amorphous zinc tin oxide (a-ZTO) and amorphous silicon nitride (a-SiNx) films have emerged as promising materials due to their excellent gas barrier performance.[1-3] In this study, a-ZTO[1)] or a-SiNx[2), 3)] thin films with thicknesses ranging from 20 to 200 nm were deposited on glass substrates by RF sputtering using a ZTO (Zn:Sn=2:1) or Si targets, respectively. For the gas barrier evaluation, these a-ZTO and a-SiNx films were deposited onto glass substrates pre-deposited with various transparent conductive oxide (TCO) layers, such as amorphous indium zinc oxide (a-IZO)[4),5)] or ITO films. The as-deposited films and post-annealed films in air were evaluated in carrier density (*n*) of the TCO layers by Hall effect measurements in order for the quantitative estimation on how many oxigen vacacies were disappeared by the annealing oxidation, reflecting the amount of oxygen transmitted [3)]. Figures 1 (a)-(c) and (d)-(f) show the electrical properties of ITO and IZO thin films coated with the gas barrier layers, respectively, where the as-deposited films and the post-annealed films are indicated by ● and ▼, respectively. For ITO films [1], coating with a-SiNx (≥20 nm) prevented a decrease in carrier density after annealing at 400 °C in air, indicating excellent barrier performance. In contrast, a-ZTO films (even at 150 nm) or additional 100 nm SiNx layers on ZTO/ITO showed the decrease in carrier density, suggesting oxygen diffusion from ZTO into the ITO layer in Fig. 1-(b) and (c) because ofn the high annealing temperature of 400 °C. In the case of IZO films, the use of a-SiNx (≥20 nm) and a-ZTO (≥20 nm) films as the over layers effectively suppressed carrier reduction after annealing temperature at 250°C. With thicker ZTO films (≥150 nm) or additional 100 nm SiNx film depositions, the decrease in carrier density was negligible, confirming their oxygen barrier effects. On the evaluation on H_2O vapor barrier properies Al doped ZnO (AZO) films were adopted as the TCO, that will be reported in detail in the conference.

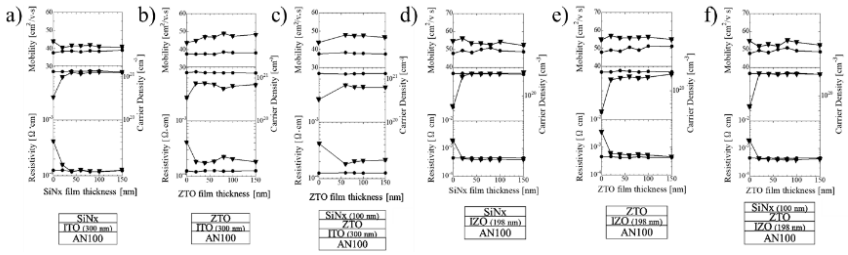

Fig. 1. Electric properties of SiN_x ZTO and SiN_x/ZTO films were deposited on ITO film (a) – (c) and IZO film (d) – (f)

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Electrospun fiber coatings as new transparent conductive coatings

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Transparent conductive coatings (TCC) are used as transparent electrodes for displays, sensors, photovoltaics, transparent heaters, antennas, etc. Mainly, ITO (tin-doped indium oxide) layers are used as TCC, but other materials are also being investigated to replace ITO, such as layers with silver nanowires or silver nanoparticles, graphene, printed metal grids, etc.
Great efforts are being made to obtain flexible and cost-effective transparent conductive coatings that can be produced in a large area.
To obtain flexible and cost-effective transparent conductive coatings with low sheet resistance and high transmission, that can also be produced cost-effectively over a large area, a new technology has been used to produce TCC: the electrospinning process.

Two production routes were investigated:
In the first route, polymer fibers containing silver nanoparticles as nuclei were spun on polymer foil. An electroless silver coating was then applied to obtain conductive fibers. After an additional copper plating, which was performed electroless or galvanically, highly conductive coatings with a sheet resistance of 5 Ω/sq, a total transmittance of about 90 % and a low haze of 2 % or less could be obtained.
In the second route, fibers with a higher metal content were spun on foil, which were already conductive after heat treatment at approx. 100 °C. By subsequent electroless copper plating, sheet resistances of 4 Ω/sq, a total transmission of about 90 % and a low haze of about 2 % were achieved. The second route is advantageous for upscaling to produce large area coatings.
The fiber coatings have a very high aspect ratio: The fibers have a thickness between 1 µm and 3 µm and a length of several cm. The fiber coatings are flexible and stretchable and suitable for flexible devices with a wide range of substrates.

By variation of the spinning parameter and the spinning ink, the thickness and the density of fibers can be adjusted and thus also the resistance and the optical properties.
Various demonstrators, such as a transparent heater and a proximity sensor, have been produced using such electrospun fibers and the results will be presented.
The use of the fibers as a transparent heater was tested with a thermal imaging camera. By heating the electrospun fiber coating with a low power density of about 12 mW/cm^2, the temperature of the sample was homogeneously increased from room temperature (21 °C) to about 31 °C. This could be used for de-icing of automotive windows or blades of wind power plants. In addition, a proximity sensor was fabricated to demonstrate the properties of the electrospun fibers.
Possible applications for electrospun fiber coatings are transparent electrodes for flexible displays, sensors, photovoltaics, wearables, antennas, skin patches, antistatic coatings, transparent heaters, etc.
By using a roll-to-roll machine with an electrospinning unit, the fabrication of large area electrospun coatings was shown, which is currently under development to enable industrial applications.

Surface activation of $BiVO_4$ for improved performance in alkaline photoelectrochemical water splitting

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Among various options to decarbonize society, hydrogen is foreseen to play a key role. Hydrogen serves both as a renewable energy carrier and as feedstock for chemical processes beyond electrification. However, green hydrogen production remains limited, driving the development of new technologies to bring the production costs down substantially. Various promising technologies have been studied to date, including photoelectrochemical (PEC) hydrogen production. The use of $BiVO_4$ (BVO) as PEC anode is widely spread in research, where a mix of beneficial properties related to bandgap, light absorption, bias requirements and flexible use at higher pH has been ascribed to this material.[1] However, its surface activity for the oxygen evolution reactions (OER) is limited. Previous studies reported introduction of an electrocatalyst to enhance the reactivity or reduce surface recombination of electron-hole pairs, such as cobalt phosphate.[2] In view of scalability and cost-effectiveness, alkaline conditions are preferred to reduce PEC system costs. In this study, we introduce bimetallic NiFeOOH electrocatalysts on top of BVO and functionalize the BVO surface with a borate treatment to significantly improve kinetics in the OER and suppress surface charge recombination in the BVO layer.

Thin NiFeOOH catalyst layers were deposited on BVO photoanodes (FTO/WO_3/BVO layer stack, prepared by spincoating) via light-assisted electrodeposition (LA-ECD) and precipitation deposition, with (electro)deposition parameters optimized for both bare BVO and BVO-based heterostructures. Borate functionalization was achieved by facile immersion. Photoelectrochemical performance was assessed under alkaline conditions using a solar simulator (AM1.5) and linear sweep voltammetry (LSV). Optical and structural properties were characterized by UV-Vis and X-ray diffraction (XRD), respectively. To elucidate the role of surface treatments in enhancing the solar-driven OER, electrochemical impedance spectroscopy (EIS) was employed to probe charge transfer resistances and capacitances.

Among the techniques and surface treatments investigated, LA-ECD of NiFeOOH yielded the highest performance with up to a 53% increase of photocurrent (to max. 1.3 mA cm^{-2}) compared to pristine BVO under alkaline conditions. EIS characterization indicates both improved kinetics as well as higher electrochemical surface area for the electrodeposited substrates as contributors for the performance increase. The thin electrocatalyst layer appears transparent in the UV-Vis region and is compatible with front- and back-illumination of BVO. Electrochemical analysis revealed that local potentials required during the ECD process may exceed the stability window of BVO under given conditions, leading to damage in the material. Although the facile borate treatment avoids this issue, the performance enhancement was slightly lower, with a 36% increase in photocurrent. The demonstrated surface activation strategies for BVO offer scalable pathways to enhance PEC performance, contributing to the viability of solar hydrogen in decarbonizing society.

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Uncovering the element-specific interatomic distances throughout the Cu(Br,I) alloy system

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Copper(I) iodide (CuI) is both a transparent and p-type semiconductor with various applications, e.g. in diodes, solar cells, blue and UV LEDs and thin film transistors. [1][2] Next to various other forms of doping and alloying, anion substitution with bromide can be used to tune the free hole concentration in functional layers, enabling optimized performance of active devices.[3]

To understand the change of material properties with different alloying compositions, it is vital to investigate not only the crystal structure, but the displacement of the atoms in their local environment within the crystal lattice. In consequence, X-ray absorption spectroscopy was used at the Cu, Br and I K-edges to determine the fine structure of $CuBr_{1-x}I_x$ samples. The samples investigated had anion compositions x varying from 0 to 1 and were realized by solid state synthesis of crystalline powders or by pulsed laser deposition.[4]

The absorption spectra at the Cu K-edge - both in the near-edge and extended region - prove the formation of copper oxides, primarily in the powder samples. The thin films had been capped with an Al_2O_3 layer in situ, as an approach to prevent further post-deposition oxidation. The analysis of the extended fine structure at the I and Br K-edges reveals a nonlinear change of the average Cu-Br and Cu-I bond lengths with composition x with consistent results for powder and thin film samples. This bond length dependence is different from that observed for group III-V and group II-VI zincblende alloys,[5] which show a linear dependence on the composition. Comparison to the bond length change in $RbBr_{1-x}I_x$,[6] crystallising in the rock salt structure, shows similarities that may identify this bond length bowing as a characteristic feature of group I-VII alloys.

Unlike the first nearest neighbour bond lengths, the distances between second and third nearest neighbouring atoms in the $CuBr_{1-x}I_x$ samples are consistent with previous findings for other zincblende alloys. The respective interatomic distances vary linearly with composition. Furthermore, the distances between third nearest neighbours coincide for both types of absorbing atom and follow the virtual crystal approximation. This indicates that the lattice distortions seen on a local scale due to alloy-induced lattice mismatch average out at distances larger than the second nearest neighbour shell.

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Metallic Thin Films: Back to the Future

Clark Bright

Many applications for the mid infrared (IR) waveband (3 um – 5 um) and far IR waveband (8 um – 12 um) require the use of a transparent conductive coating (TCC). Typically, there are three choices for the TCC: doped metal oxides, i.e., transparent conductive oxides (TCO), e.g., indium oxide or zinc oxide; very thin metallic films, e.g., silver, gold and silver-gold alloys; or grid or mesh patterned opaque EC coatings. A review of some quite old previous results (Ref 1 – 3), and a limited literature review of previous and current results were analyzed and compared with the requirements of some typical applications in these two wavebands. While physics doesn't change, our understanding of these laws does and technology advances. Our better understanding, means we can meet more demanding application requirements. In a recent paper (2024), I discussed transparent conductive oxides (TCO) and the impact of the carrier concentration N on the mobility u, and therefore, on the plasma wavelength and the spectral transmittance bandwidth. Lowering N, allows transmittance further into the near infrared. However, eventually, N will become so low that the TCO is no longer degenerate, and it becomes a semiconductor rather than a true ("metallic") conductor. This makes using a TCO problematic in the mid IR waveband and very compromised in the far IR waveband. A better choice for a TCC for these two IR wavebands may be very thin metallic films. A second paper in 2024 discussed achieving high transmittance with very thin metallic films, which were inhibited from having an island type structure and becoming electrically discontinuous. With these techniques, very thin metallic films can be an effective TCC with good IR transmittance. Measured results and some calculated results for these films are compared with "current" application requirements.

Beyond the pixel: oxide TFTs shaping smart, sustainable systems

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Thin-film transistors (TFTs) have been essential to the display industry, enabling active-matrix backplanes for individual pixel addressing. However, their unique advantages—such as ultra-low cost, mechanical flexibility, and compatibility with large-area fabrication—have also driven major advancements in flexible system-on-chip (SoC) integration over the past decade. Building on our group's extensive experience at CENIMAT|i3N in low-temperature oxide TFTs, this presentation explores three distinct application domains where low-voltage operation and/or low power consumption were primary design constraints:

- Pixel circuits for electroluminescent displays, targeting µLEDs and spin-coated quantum-dot (ELQD) technologies. These circuits were optimized for a 35 µm pixel pitch in high-resolution displays, with sub-3 V data voltages enabling microampere-range currents and fine gray level control in miniaturized light-emitting elements.
- Ionizing radiation detectors, with fast response and high sensitivity to x-rays. Since the initial demonstrations of oxide TFTs as dosimeters by University of Bologna and NOVA FCT [1], more recently we optimized a bi-layer gate dielectric structure by atomic layer deposition enabling unprecedented sensitivity of (63±2) V/Gy, an order of magnitude larger than previously reported values [2].
- Energy management circuits for autonomous sensing platforms. These include an ultra-low-power wake-up timer (27 nW) [3] and voltage regulation blocks capable of supplying three independent power rails from solar energy sources. Key strategies included the use of low-dropout regulators and circuit topologies that exploit transistor leakage currents to generate ultra-low-frequency timing signals.

In addition, an innovative and universal approach for integrating these flexible circuits with other components—whether on rigid or flexible substrates—will be presented. This method uses conductive adhesives with printed interconnects to link flexible circuit pads to external components, overcoming the limitations of wire bonding and direct printing techniques.

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Precision Engineering of Functional NanoOxides at Industrial Scale: from Lab Scale Research to the TRL ladder

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Metal-Oxides (MeOx) offer a fertile landscape in modern nanotechnology spanning fundamental-research topics to commercial-commodities. Current breakthrough in understanding of their physico-chemical properties that determine the desired functions of MeOx's at the nanoscale, reveal that lattice-"nanoproperties" (quantum-size-effects, nanostrain, suface/bulk-defects, chemo-doping, spin-doping) are the key-parameters to control. In this endeavor, the transition from lab-scale to industrial-scale requires a mounting dexterity in synthesis methods that allow "precision-engineering" not just synthesis of the desired material phase.composition.
Herein we discuss current advances in Flame-Spray-Pyrolysis (a-FSP) technologies[1,2] as a scalable technology that allows bridging the Lab-to-Industrial production of functional nanomaterials. We position precision-engineering by FSP-technologies at the Technology-Readiness-Level (TRL) ladder, as defined by NASA and the E.U. We highlight specific examples where precision-engineering of Transparent Metal Oxides (e.g. ZrO_2[3], Tandalum-Oxides[4], SnO_2[5]) by FSP allows their transformation to functional nanoplatfroms, with emphasis on energy technologies and sensing.
Within the TRL-frame of regulations, key-challenges in transforming the Lab-Scale finding to Industrial-Technology are highlighted from two perspectives: control of the desired properties and cost-efficiency.

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Sputtering Technologies for the Deposition of Transparent Conductive Oxides on Large Areas

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For the deposition of transparent conductive materials (TCOs), different properties are required depending on the application. A low absorption combined with sufficient electrical conductivity is crucial. Other important properties may include temperature stability as well as humidity and heat stability.

This presentation will demonstrate the production of TCOs using magnetron sputtering, as this technology is widely used in the industry and can be scaled up for large areas. A significant advantage of sputtering technology is that different generator types (DC, MF, RF, HIPIMS) can significantly influence the plasma and energy distribution at the substrate, which in turn has a major impact on film formation and its properties.

Furthermore, additional parameters such pressure and substrate temperature, as well as the composition of the target during production, affect the later film properties. Examples of developments in various TCO materials and their applications in products will be presented.

Computational prediction of $Cd_2Sb_2O_7$ as a candidate TCO

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Transparent conducting oxides (TCOs) are central to the field of modern optoelectronics, displaying a unique combination of high electrical conductivity and optical transparency, with applications in touch screens, photovoltaics, LCD and OLED displays, and more. [1] The industry standard for TCOs is Sn-doped In_2O_3 (ITO), which displays optical transmission greater than 90%, with low resistivity and high carrier mobility. However, indium is expensive and has low earth-abundance. Alternative materials that offer comparable or superior properties using different elements are in high demand. [2,3]

Recently, Sb(V) oxides have emerged as promising candidates. [4,5] Sb(V) possesses the $(n-1)d^{10}ns^0\ np^0$ electron configuration common to many TCO cations, including In(III) in In2O3, leading to a highly disperse conduction band and a large band gap.[5] The Sb(V) oxides also display three-dimensional connectivity of SbO_6 octahedra, creating electron pathways that enable high conductivity. $ZnSb_2O_6$ [4] was computationally predicted and experimentally realised as a TCO, and Sb_2O_5 [5] is predicted to be suitable as well, motivating further exploration of this family of materials.

$Cd_2Sb_2O_7$ contains Sb(V) and was flagged in a high-throughput study as having a relatively large band gap and low electron effective mass, suggesting possible transparency and conductivity. [6] However, there has been no investigation into the material's defect chemistry. For these reasons it was decided to investigate $Cd_2Sb_2O_7$ more thoroughly. The optoelectronic and structural properties of $Cd_2Sb_2O_7$ were calculated using the hybrid PBE0 functional along with its intrinsic and dopant defect chemistry. Its charge transport was calculated using a combination of ab initio and semi-empirical DFT based methods.

Our results suggest an optical band gap in the transparent range, a high intrinsic electron carrier concentration due to antisite defects, giving high intrinsic mobility and conductivity, and a large doping window, enabling n-type doping to further enhance conductivity. This provides further evidence for the potential of Sb(V) oxides as TCOs.

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Fast solution of inverse problems on IGZO transistor characterization via tandem neural network

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Operation characteristics of In-Ga-Zn-O thin-film transistors (TFTs) are influenced by semiconductor properties of their channel layers such as defect distributions and electron transport properties, which are altered largely by process conditions [1]. Accordingly, it is important to analyze these semiconductor properties for feedback to the process conditions to improve TFT performances. TCAD device simulators are useful tools for simulating TFT characteristics from input of semiconductor properties and device structures (forward problem). In contrast, there was no approach to solve the inverse problem that calculates semiconductor properties directly from TFT characteristics; therefore, non-linear optimization using TCAD simulations is employed but it needs large numbers of trial-and-error calculations and is expensive in time. Such inverse problem process is expected to speed up by machine learning (ML) approaches. It is, however, challenging due to the multivaluedness in the relation between semiconductor properties and TFT characteristics; different semiconductor properties may give nearly the same TFT operation characteristics.

This study develops a neural network (NN) model to solve multivalued inverse problems and applies it to the fast analysis of semiconductor parameters from transistor characteristics. Conventional inverse NNs have been utilized for such problems by simply swapping descriptors and objective variables; however, they struggle to predict semiconductor parameters that exhibit ranges exceeding several orders of magnitude. We employ a tandem NN architecture that connects a pre-trained forward NN and an inverse NN, where the total loss function includes both the prediction errors of semiconductor parameters and the reconstruction errors of transistor characteristics, each weighted appropriately. As a result, we successfully performed inverse analysis to estimate physically plausible semiconductor parameters that accurately reproduce transistor characteristics. Our results enable real-time and autonomous analysis and feedback control of semiconductor and device fabrication processes, helping accelerate the development of new semiconductor materials and devices.

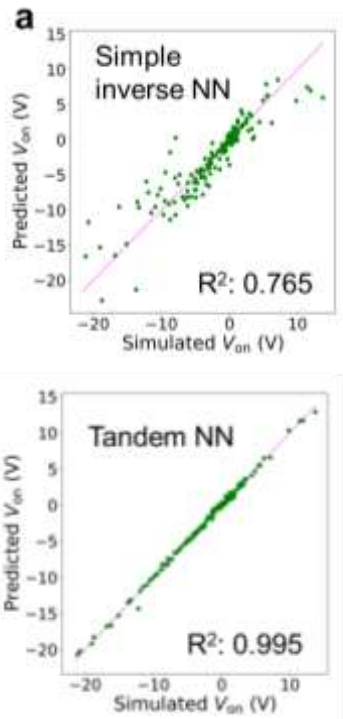

Figure: Parity plot showing reproduction accuracies of TFT parameter, Von, from obtained semiconductor parameters with simple inverse NN and Tandem NN

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Structural properties of Ga_2O_3 thin films grown via dc-pulsed magnetron sputtering using a liquid gallium target

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Our research has been dedicated to investigating the potential of dc-pulsed magnetron sputtering for the preparation of gallium oxide (Ga_2O_3) as a semiconductor material suitable for high-power and high-frequency applications. Ga_2O_3 is notable for its ultra-wide bandgap of approximately 4.8 eV, high electron saturation velocity, and its ability to withstand a high breakdown electric field of about 8 MV/cm. While epitaxial techniques for growing high-quality β-Ga_2O_3 films have advanced considerably, they still suffer from low deposition rates, which limit scalability.

Our primary objective was to enhance the crystal quality of Ga_2O_3 films produced by dc-pulsed magnetron sputtering - a method known for its high deposition rate but typically challenged by the formation of well-ordered crystalline structures. An advantage of this method lies in the ability to tune oxidation conditions during growth via discharge parameters, which have a significant impact on the resulting film properties.

We focused on reactive magnetron sputtering of Ga_2O_3 films from a liquid gallium metal target. The resulting film quality and characteristics were strongly influenced by several key factors, particularly the substrate temperature and the choice of substrate material—quartz, silicon, and sapphire. Our study aimed to understand how these variables affect film structure and to optimize deposition conditions for practical applications.

We successfully deposited crystalline Ga_2O_3 films exhibiting a strong preferential orientation. Our experiments revealed that increasing the substrate temperature promoted crystallization, but also unexpectedly diminished the strength of the preferred orientation. To explore this further, we studied the effect of varying the pulse length in the dc-pulsed sputtering process and analyzed how it shaped the resulting film structure. These experiments were conducted across different substrates, showing that the choice of substrate plays a critical role in determining the final microstructure of the Ga_2O_3 films.

Transparent conductive Cu diffusion barriers: A 2-dimensional combinatorial screening study on the In-Zn-O system

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Metallization costs can account for a significant proportion of the total processing cost of optoelectronic devices – for silicon solar cells up to 20-30%[1]. This high cost combined with supply-chain concerns motivate the substitution of costly contact materials such as silver by more abundant and less expensive metals like copper. However, the utilization of Cu gives rise to the issue of its high mobility, which potentially compromises device performance due to copper ingress into the Si wafer. Consequently, a diffusion barrier is required between the Cu contact and the active material. The employment of a transparent electrode that is capable of performing this additional function would result in a reduction of both processing time and costs.
Since amorphous thin films are reported to possess superior diffusion barrier performance compared to polycrystalline thin films[2], amorphous In-Zn-O (a-IZO) is a promising candidate for such a multifunctional transparent conductive Cu diffusion barrier.

In this study, we perform an accelerated co-optimization of electrical conductivity, optical transmission in the UV-Vis-NIR range and Cu diffusion barrier performance of the In-Zn-O material system. To accelerate this process, we combine high-throughput synthesis of materials libraries by combinatorial magnetron co-sputtering and high-throughput characterization procedures of XRF, XRD, Four-Point-Probe electrical conductivity measurements and UV-vis-NIR photospectroscopy. Due to the strong influence of even subtle changes in the oxygen content of the IZO films on the electrical and optical properties, materials libraries were deposited with 2-dimensional composition gradients covering the cation concentration (i.e. In/Zn) as well as the oxygen content.
The application of this approach enables the assessment of compositional limits of applicability as transparent conductive materials on a single material library. The electrical conductivity varies over several orders of magnitude with a maximum of $2.4 \cdot 10^3$ S/cm in the center of the library for a room temperature deposition. Simultaneously, the low oxygen content region of the library exhibits a substantial increase in absorptance up to 26%, averaged between 350 and 1100 nm, indicating a compositional limit of the applicability as transparent electrode. To screen the Cu diffusion barrier performance, thin materials libraries (23 ± 1 and 8 ± 1 nm) are reproduced on silicon wafers, covered with 100 nm Cu and heated in vacuum. The formation of Cu silicides for different cation and anion compositions is monitored by XRD and compared to the response of Cu films deposited directly on Si wafers without an IZO barrier. The diffusion behavior in selected samples is further investigated by means of XPS and ToF-SIMS measurements.

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Exploring the Sb (V) oxides: transport and defect properties of ASb_2O_6 (A = Mg, Ca, Sr, Ba, Cd)

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Transparent conducting oxides (TCOs) possess a unique combination of optical transparency and electrical conductivity, making them essential for numerous optoelectronic applications including electron transport layers in solar cells [1-3]. However, the number of oxides that are both transparent to visible light and exhibit the metallic-like conductivity required for such applications is limited to a few well-established systems. Recently, $ZnSb_2O_6$ and Sb_2O_5 have been proposed as promising Sb(V)-based oxides [4,5,6], demonstrating transparent conducting behavior, unusually deep band edges, and interesting band alignment for optoelectronic applications. Building on the promising results of these two systems, we extended our exploration to ASb_2O_6 compounds (A = Mg, Ca, Sr, Ba, Cd) in search of alternative candidates for practical TCO applications. Our findings indicate that $CdSb_2O_6$ and $MgSb_2O_6$ exhibit excellent transport and optical properties, positioning them as strong contenders for the future of TCOs. The defect chemistry of these two oxides was also investigated, providing valuable insights into their behavior for working applications. Finally, our work reveals a strong correlation between the atomic packing factor (a measure of how efficiently atoms are packed in a crystal structure) and carrier mobility, offering a potential approach for rapid screening of promising candidates within this class of materials.

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New evaluation methods on various gas barrier performances using functional oxide films (2); Hydrogen gas barrier properties.

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1. Background

Hydrogen energy is considered to be the promising energy source due to its environmental benefits and relatively simple production processes. Whereas, several challenges, such as leakage and hydrogen embrittlement, must be addressed. Therefore, the development of hydrogen gas barrier performance to prevent hydrogen transmission should be quite important. In this study, Pd-capped amorphous WO_3 films were used to evaluate the hydrogen gas barriers performance quantitatively for the various films using gasochromic behaviour of WO_3.

2. Experimental Procedures

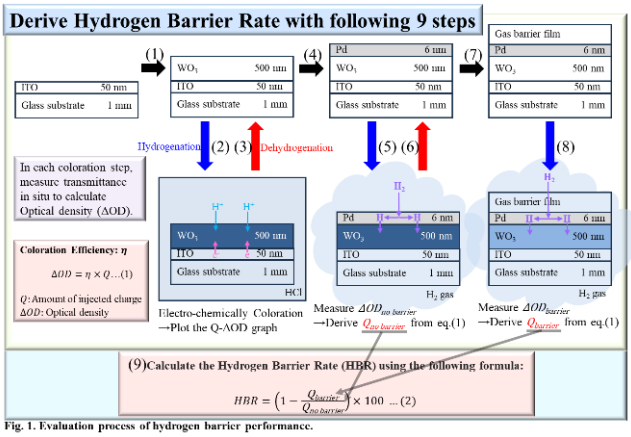

Fig. 1. Evaluation process of hydrogen barrier performance.

The schematic illustrations for this hydrogen barrier rate (HBR) analyses are shown in Fig. 1. All the films in this study were deposited using reactive sputtering. Gas barrier films (GBF) of amorphous SiO_2, Al_2O_3, and SiN_x with various thicknesses were deposited on the Pd-capped a-WO_3 films. The hydrogen transmission flux (HTF) defined as the slope of the plot of hydrogen amount per unit area and time (/cm^{2}sec) was also estimated.

3. Results

Figure. 2 shows the transmittance spectra before and after hydrogen exposure for both GBF-coated and uncoated samples. As for the example, the results on the SiO_2 films as GBF with various thicknesses are presented. HBR for three different gas barrier materials are shown in Fig. 3. The thicker films clearly exhibited higher HBR. The order of barrier performance was SiN_x > Al_2O_3 > SiO_2. The plot of hydrogen amount per unit area versus time, used to derive the HTF, is shown in Figure. 4, and the HTF values for each barrier film are summarized in Figure. 5.

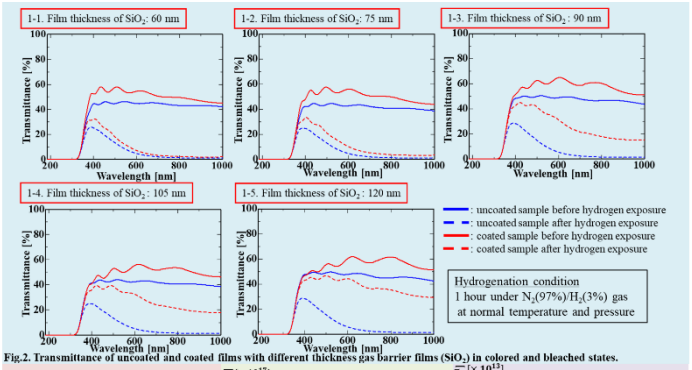

Fig.2. Transmittance of uncoated and coated films with different thickness gas barrier films (SiO_2) in colored and bleached states.

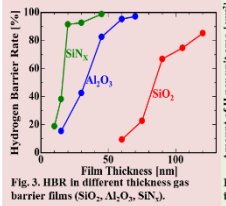

Fig. 3. HBR in different thickness gas barrier films (SiO_2, Al_2O_3, SiN_x).

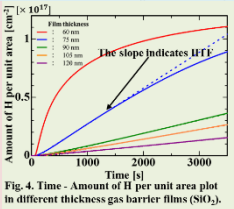

Fig. 4. Time - Amount of H per unit area plot in different thickness gas barrier films (SiO_2).

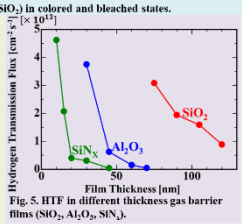

Fig. 5. HTF in different thickness gas barrier films (SiO_2, Al_2O_3, SiN_x).

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Deep Acceptor Polarons in a-TeO_2 and Hydrogen-induced Instabilities in IGZO

John. Robertson[1,2], Hailing. Guo[1,3], Yuzheng Guo[3], and Ruyue Cao[1,4]

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The talk is in two parts. There is a lack of p-doped amorphous semiconductors with moderate deposition temperature for back-end of line (BEOL) semiconductor processing. Undoped β-TeO_2 is a high mobility p-type semiconductor[1]. However, there has been no experimental proof that p-type doping leads to conductive acceptor states, as E_F of undoped a-TeO_2 lies near midgap[2]. Recent GGA studies on As_{Te} sites found shallow p-type states[3], but the unit cell was too small. Larger 216-atom cells using hybrid HSE functionals presented here find deep states, Fig. 1. The acceptors form deep, non-doping configurations with angular polaronic distortions (Fig. 2) with broken As-O bonds. This is more complex than simpler vacancy defects[4], Fig 2. The band edge energies fall outside the limits for doping[3,4]. The distortions arise because the network has a low mean coordination of 2.4, the floppy limit for such lattices[5].

We also study hydrogen-induced instabilities in the n-type InGaZn oxide semiconductor, of major technological interest for BEOL processing. Some Metal-H and oxygen-H configure-ations proposed in Bang[6] are evaluated using GGA+U and HSE calculations, Fig. 3.

1. A Zavabeti, et al, Nature Electronics **4** 277 (2021)
2. J Shi, .. K H L Zhang, App Phys Lett **122** 101901 (2022)
3. J Robertson et al, App Phys Lett **124** 212 101 (2024)
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6. J Bang, S Matsuishi, H Hosono, APL 110 232105 (2017)

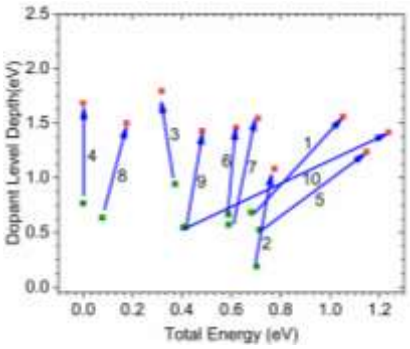

Fig. 1. GGA, green dots. HSE, red dots for various p-dopant sites.

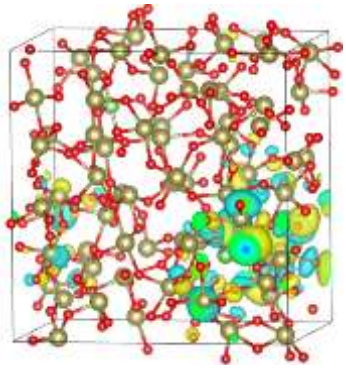

Fig. 2 Atomic structure and localised acceptor state of As_{Te}.

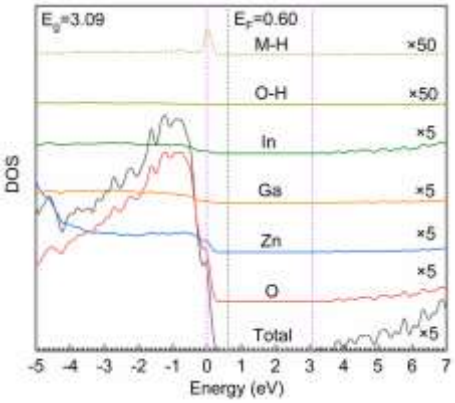

Fig. 3 Partial density of states of M-H and M-OH configurations in amorphous IGZO.

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First-principles study of carbon-doped Cu_2O and lead-free A_2ZrX_6 defect perovskites for optoelectronic applications

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The development of new wide-bandgap semiconductors is critical for advancing transparent and optoelectronic device technologies. In this work, we report density functional theory (DFT) studies on two classes of wide-bandgap materials with enhanced potential for optoelectronic applications: (i) carbon-doped cuprous oxide (Cu_2O), and (ii) lead-free halide defect perovskites, A_2ZrX_6, where A is an organic cation and X is a halogen.

Cu_2O is intrinsically a p-type semiconductor due to the presence of Cu vacancies. In this study, we examine the effects of carbon doping, considering substitutional doping at the oxygen and copper sites, as well as interstitial incorporation, using PBE and PBE+U approaches. Our results indicate an enhancement of the p-type character when carbon substitutes for an oxygen atom. In contrast, substitution of a copper atom by carbon or interstitial incorporation of carbon leads to shallow donor defect states near the conduction band minimum (CBM), thereby introducing compensating n-type conductivity.

We also report results on the structural and electronic properties of lead-free, halide, “defect” perovskites of the form A_2ZrX_6. These systems hold significant potential for many optoelectronic applications due to their stability and tunable properties. Utilizing PBE and HSE06 functionals, we systematically investigate the impact of A-site cation and X-site halogen substitutions on the structural and electronic properties. Specifically, we consider A = ammonium (NH_4^+), methylammonium ($CH_3NH_3^+$), dimethylammonium ($(CH_3)_2NH_2^+$), trimethylammonium ($(CH_3)_3NH^+$), formamidinium ($CH(NH_2)_2^+$), trimethylsulfonium ($(CH_3)_3S^+$) or phosphonium (PH_4^+); and X = Cl^-, Br^-, or I^-. Our calculations reveal that both A-site and X-site substitutions significantly affect the band gap and the lattice parameters. Increasing the size of the A-site cation generally enlarges the unit cell, while halogen electronegativity directly correlates with the band gap, yielding the lowest values for iodine-containing systems and methylammonium cation in the A-site. We predict a wide range of band gaps (from ~4.79 eV for $(PH_4)_2ZrCl_6$ down to ~2.11 eV for MA_2ZrI_6, using HSE06).

Our first-principles predictions for C-doped Cu_2O and Zr-based defect perovskites highlight their potential as next-generation semiconductors with tunable optoelectronic properties.

Acknowledgment: This work was carried out within the framework of the Action 'Flagship Research Projects in challenging interdisciplinary sectors with practical applications in Greek Industry', implemented through the National Recovery and Resilience Plan Greece 2.0 and funded by the European Union - NextGenerationEU (Acronym: 3GPV-4INDUSTRY, project code: TAEDR-0537347).

Spray pyrolysis of ternary oxides – the case of Cu_xCrO_2 and a-$ZnSnO_3$

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Spray pyrolysis is a popular method for the low-cost synthesis of oxides and other compounds in thin film form. Here we discuss several limitations and pitfalls of the method when working with ternary and quaternary compounds. Specifically, we outline how precursor solubility, thermal decomposition, but also desorption of intermediate species from the sample surface govern the spray pyrolysis growth process.

We present optical real time measurements of sample growth for ternary transparent conducting oxides (TCO; p-type Cu_xCrO_2 and n-type a-$ZnSnO_3$) illustrating stark difference between the growth rate of binary oxides and ternary oxides using the same precursors and growth conditions.

We illustrate how the several steps of spray pyrolysis affect the stoichiometry transfer from the solution to the thin film and how the choice of instrument geometry and nozzle type affect the electrical and optical properties of the TCOs. For the ZTO system we present how changes in the spray setup and nozzle type can significantly improve the film properties when using low-cost chloride precursors which were previously found unsuitable in an air blast nozzle system. When used in conjunction with medical grade ultrasonic nozzles these precursors can provide good films.

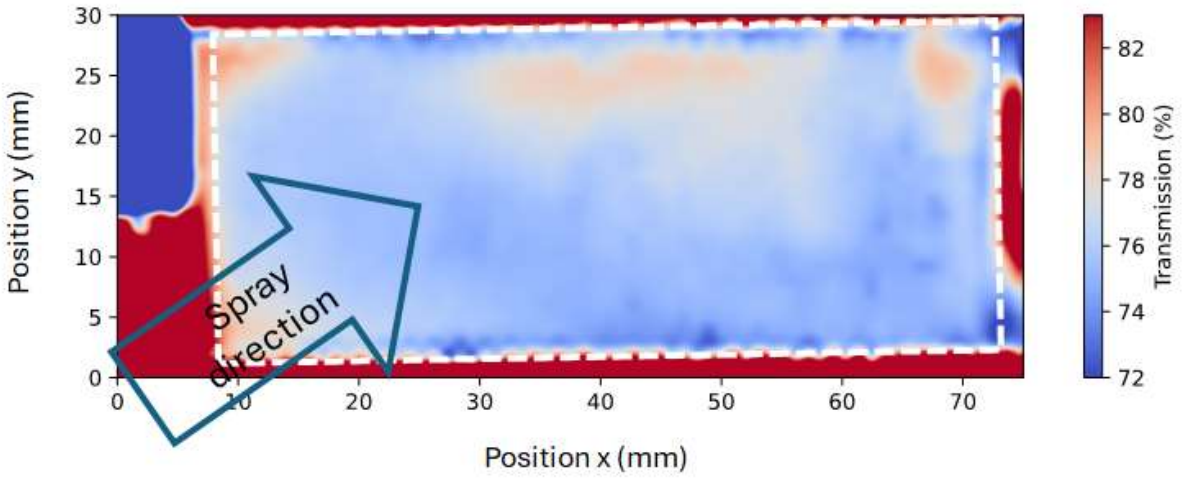

Figure 1: Example UV-VIS spectrophotometry map (1mm sampling) showing the average transmission in the photon energy range of 1.5 to 3.0eV for a ZTO sample on glass grown with a single ultrasonic nebulizer and chloride precursors ($SnCl_2$, $ZnCl_2$). Small transmission variations arise from thickness variations and differences in surface roughness (leading to differences in scattering). The dashed line indicates the usable sample area unaffected by gas flow disturbances and shadowing by holding clamps.

Photocatalytic Materials for a Greener Tomorrow

D. Katerinopoulou[1], A. Stoumpidi[1], I. Kitsou[2], A. Zourou[3], A. Karagianni[3], K.V. Kordatos[3], A. Tsetsekou[2], V. Binas[4], G. Kiriakidis[1]

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The growing demand for a cleaner and more sustainable environment has driven the development and adoption of green technologies across many aspects of daily life. In particular, the need for purified air [1] and water [2]—further emphasized by the recent pandemic —has brought photocatalytic (P/C) materials to the forefront [3]. This presentation will elaborate on the general applications of photocatalytic materials and their advantages in mitigating environmental issues. Moreover, the study will be focused on the synthetic route as well as the characterization of novel core-shell structures in terms of morphological, structural and photocatalytic activation. The formation of the core-shell begins with TiO_2 as the core material following the decoration, shell formation, with carbon dots (CDs) and/or silver (Ag) nanoparticles through chemical modification. The well-defined core-shell structures were confirmed via transmission electron microscopy (TEM) images and the crystalline structure was defined from X-ray diffraction (XRD) analysis. All prepared nanomaterials have been evaluated regarding their photocatalytic activity in both liquid and gaseous pollutants. Specifically, the study for the degradation of methylene blue (MB) dye was investigated under direct solar irradiation, whereas the degradation of nitrogen oxides (NOx) was tested under ultraviolet and visible light irradiation, in accordance with standard ISO procedures.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101058422 (SUPREME).

[1] Yuanchen Wei, et al., TiO2-Based Photocatalytic Building Material for Air Purification in Sustainable and Low-Carbon Cities: A Review **(**2023**),** Catalysts, 13, 1466.

[2] Moreno-Vargas, et al., Photocatalysis as an Alternative for the Remediation of Wastewater: A Scientometric Review.” (2024) ChemEngineering, 8, 95.

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Mechanism of Epitaxial Growth of Rutile-type GeO_2 by PLD

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Ultra-wide band gap oxide semiconductors, with band gap energies (E_g) exceeding those of GaN and SiC, have been extensively studied for next-generation power electronics and deep ultraviolet optoelectronics applications. Although β-Ga_2O_3 (E_g = 4.8–4.9 eV) has been the primary focus, it has a critical limitation in the difficulty of achieving p-type doping. In contrast, rutile-type GeO_2 (r-GeO_2) with E_g = 4.68 eV has been emerged as a promising material owing to its potential controllability of both p- and n-type conduction, which is predicted theoretically by first-principles calculations[1]. The extraordinarily short O–O distances in the r-GeO_2 crystal structure enhance O 2*p* – O 2*p* antibonding interactions, raising the energy level of the valence band maximum and making hole doping feasible[2]. Although the number of reports on epitaxial growth of r-GeO_2 films has been increasing[3,4], synthesis of high-quality epitaxial films remains challenging due to competing polymorphs, such as α-quartz and amorphous phases. These phases hinder effective doping with aliovalent ions.

In this study, we systematically investigate effects of deposition conditions, especially focusing on oxygen pressure (P_{O2}) and growth temperature (T_g), on growth of GeO_2 films by pulsed laser deposition (PLD). We successfully controlled the growth phase of GeO_2.

Figure shows the growth phase diagram of GeO_2 films grown by PLD as a function of T_g and P_{O2}. Epitaxial films of r-GeO_2 are obtained at T_g = 500 – 600°C under low $P_{O2} \leq 10^{-1}$ Pa, while the α-quartz phase does not appear under any growth conditions. However amorphous phase coexists under higher $P_{O2} \geq 10^{-2}$ Pa at T_g = 500°C, and only amorphous phase is formed under lower $T_g \leq$ 400°C and higher $P_{O2} \geq 1$ Pa. On the other hand, severe re-evaporation of the film occurs with increasing T_g and decreasing P_{O2}, and finally no film growth is observed at 700°C. These results indicate that low P_{O2} is inevitable to obtain pure r-GeO_2 film; however, re-evaporation of the GeO_2 film becomes serious at the same time. These competing phenomena not only complicate phase stabilization but also hinder precise control of chemical composition particularly when dopant ions are introduced. We will discuss it in more detail at the conference.

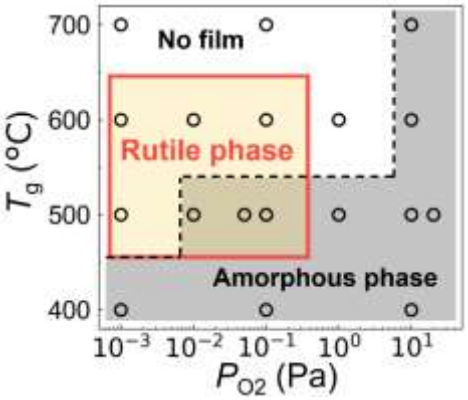

Figure. Growth Phase diagram of GeO_2 film deposited by PLD at different T_g and P_{O2}.

[1] S. Chae, et al., *Appl Phys Lett*, **114**, 102104, (2019). [2] C. Niedermeier et al. *J.Phys.Chem*., **124**, 25721, (2020). [3] S. Chae, et al., *Appl Phys Lett*, **117**, 072105, (2020). [4] H. Takane, et al., *Appl Phys Lett*, **119**, 062104, (2021).

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Ambient-Stable p-Type Transparent CuI Thin-Film Transistors via Room-Temperature Pulsed Laser Deposition

Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1].

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As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidates in the field of transparent electronics.[1] However, the strong compensation effect and air contamination lead to uncontrollable electrical properties.[2,3] As one of the most crucial transparent devices, CuI thin-film transistors (TFTs) face the critical challenge of balancing high performance and environmental stability. Herein, we propose a room-temperature pulsed laser deposition (PLD) process for ambient-stable, high-performance p-type CuI TFTs and circuits. By introducing a buffer layer between γ-CuI film and substrates, the CuI layer exhibits extremely low surface roughness (RMS < 1 nm), and the film thickness can be precisely controlled lower than 5 nm by the number of laser pulses. The free hole carrier concentration can be tuned from 10^{14} cm^{-3} to 10^{19} cm^{-3} and mobility can reach 25 $cm^2 V^{-1} s^{-1}$ comparable to that of bulk CuI by controlling the compensation effect from iodine deficiency.[4,5] In addition, a 200-nm-thick amorphous Al_2O_3 capping layer was deposited *in situ* on the thin CuI film. The concentration of free hole carriers in the covered film decreased by several orders of magnitude and remained stable in the air, enabling long-term device operation under ambient conditions. The optimized TFTs exhibit a field-effect mobility of over 0.5 cm^2 V^{-1} s^{-1} and a high on/off current ratio of ~10^4 with good operational stability and reproducibility. This study provides a promising pathway toward ambient-stable transparent p-type field-effect transistors for complementary electronics in combination with n-type metal-oxide devices.

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Poster Presentation

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3	Improving Hydrogen Sensor Dynamics with Platinum-Decorated CuSCN **A. Sfakianou, E. Skliri, E. Gagaoudakis, C.-P. Tsichlis, Y. Deligiannakis, V. Binas**
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18	Tuning Wettability and Electrochemical Properties of Graphene Thin Films via PECVD Process Parameter Control **N. Kavousanos, M. Apostolopoulou, E. Spanakis, K. Katsara, G. Kenanakis, I. Chronopoulos, S. N. Yannopoulos, D. Vernardou**

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Memristive Devices with Vanadium Oxide: The Effects of Electrode Selection on the Oxygen Migration Mechanism.

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Vanadium oxides have potential applications in memory devices, due to the four oxidation states of vanadium, giving rise to vanadium oxides with varying conductivity depending on their oxidation states. Additionally, VO_2 exhibits a metal-semiconductor transition from the room temperature monoclinic semiconducting state to rutile metallic state at approximately 68˚C. Generally, memristive devices consist of a trilayer metal-insulator-metal structure[1]. They are believed to have a filamentary mechanism, where conducting filaments of metal ions or oxygen vacancy defects are formed through the oxide layer, reducing the device resistance. However, filament formation is a stochastic process, and this contributes to device reliability and reproducibility issues. In the case of phase change materials, the conductivity change occurs over a larger area as the phase change proceeds. Using an oxide system with variable oxidation state, such as vanadium oxide, presents the opportunity to alter the oxide stoichiometry and conductivity via oxygen migration at the metal-oxide interface. This oxygen exchange occurs across the interface area and is dependent on the oxygen affinity of the metal electrode, and the oxide formation energy for the oxide layer[2].

In this work we examine the use of vanadium oxide as the active layer, while varying the electrode metal. The oxide layer has been deposited using reactive magnetron sputtering with oxygen. A range of metals will be investigated as the electrode, to investigate the influence of electrode oxygen affinity on the oxygen migration mechanism. Metals with high oxygen affinity such as Ta and Ti will be compared with low oxygen affinity metals such as gold. This will be investigated for various vanadium oxides, V_2O_3, VO_2 and V_2O_5, as these are metallic, insulating and highly insulating at room temperature, respectively. The investigation of vanadium oxides for interface-type resistive switching presents opportunities to improve the performance of memristive devices, by reducing the randomness of their operation mechanism. This principle may be extended to other oxide systems, to produce a range of more reliable memristive switches.

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Thermal emissivity of silver nanowire networks: a characterization tool for instability studies

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Transparent Conducting Materials (TCMs) are essential components in technologies such as touch screens, solar cells and smart windows. Indium Tin Oxide is the most commonly used TCM, despite its brittleness and the limited availability of indium. Silver nanowire (AgNW) networks have emerged as a promising alternative, offering comparable optoelectronic performance with lower material consumption and production costs. However, AgNW networks are thermally unstable near 300 °C, where nanowire spheroidization leads to the loss of network connectivity[1] and thus overall performance, hindering their integration in complex devices that require process steps at high temperature. In large-area devices, even localized degradation can compromise overall performance, highlighting the need for efficient techniques to identify and characterize locally damaged regions. Current assessments typically depend on time-consuming characterization by Electron Microscopy). In this work, using spray-coated AgNW networks on glass substrates, we demonstrate that thermal emissivity is a sensitive indicator of network integrity, and that its time-dependent evolution reflects ongoing structural degradation.

This work paves the way for large scale applications of AgNW networks by providing a cost-effective tool to assess network's overall integrity. Using thermal imaging at the millimeter-scale, we show that defective regions can be rapidly and accurately mapped across samples. We further investigate how network parameters - such as nanowire diameter and density - influence the emissivity response, providing deeper insight into failure mechanisms. In particular, we find an explicit dependance of the degradation dynamics with the nanowire diameter. This approach offers a scalable, cost-effective method for assessing the structural integrity of AgNW networks, paving the way for their reliable use in large-scale applications.

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Improving Hydrogen Sensor Dynamics with Platinum-Decorated CuSCN

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Gas sensors are devices essential in multiple applications for detecting gas concentrations that human senses cannot perceive. In recent years, hydrogen detection has become particularly important due to its use as a clean and renewable energy source. The need for hydrogen detection stems from the fact that it is odorless, colorless, and highly flammable in the range of 4-75% in air. Therefore, hydrogen sensing is critical for accident prevention and for ensuring the safety and efficiency of energy systems. For these reasons, there is a high demand for reliable, fast, and low-cost hydrogen sensors.
CuSCN is a p-type semiconductor with excellent electronic and mechanical properties and has already been studied as a hydrogen sensor, showing promising results[1]. More specifically, the CuSCN sensor displayed great stability and a very low limit of detection of 200 ppm at room temperature and with a low input voltage of just 0.1V. However, its response times were quite long, ranging from 80 to 600 seconds.
This work aims to improve the response times of the sensor by photodepositing Pt nanoparticles on CuSCN. The photodeposition of Pt nanoparticles was carried out at different weight percentages (0.1%, 0.25%, 0.5% and 0.75% w/w). Structural, optical, and morphological characterization of the prepared samples confirmed the uniform distribution of Pt nanoparticles and preservation of CuSCN's rhombohedral structure. With the deposition of Pt nanoparticles, a significant improvement in response time was observed, up to 90% faster, reaching 16 seconds at 200 ppm for the 0.5% Pt-CuSCN sensor compared to the initial 180 seconds of the CuSCN-based sensor. This improvement is attributed to the increase in the surface area of active sites available for the hydrogen interaction provided by platinum.

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Carbon dots as co-catalysts on TiO_2 for enhancing photocatalytic degradation of methylparaben

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The availability of quality water is a major problem in modern societies due to the continuous release of chemicals to the environment. Among them, organic pollutants, such as pharmaceuticals and personal care products (PCPs), are especially concerning because of their high stability and long-lasting nature [1]. In recent years, heterogeneous photocatalysis on semiconductor catalysts has been in the focus of extensive research as a promising technology for degradation of a wide range of organic pollutants in water. TiO_2 is one of the most investigated photocatalysts, owing to its high photocatalytic performance, strong chemical stability and low cost. However, due to its wide band-gap energy (3.2 eV), it can only be activated by UV irradiation, which accounts only for a small fraction of the electromagnetic spectrum. Among different strategies, loading a carbon-based cocatalyst on the surface of TiO_2 is an alternative and effective method to improve the photocatalytic efficiency of TiO_2. Recently, carbon quantum dots (CQDs) have gained an increasing potential for photocatalytic applications due to their exceptional electron transfer properties, suitable band gap and low-cost synthesis [2], [3].

In this work, aiming at enhancing the photocatalytic performance of TiO_2, we report the synthesis of carbon quantum dots/titanium dioxide (CQDs/TiO_2) composites and the evaluation of their photocatalytic activity in the degradation of an organic pollutant from aqueous media. Firstly, CQDs were synthesized by a microwave-assisted procedure, which then successfully combined with three different types of commercial TiO_2 to prepare CQDs/TiO_2 heterostructures via a hydrothermal method. The obtained materials were characterized by a variety of techniques, including XRD analysis, FESEM/EDS, FT-IR and UV/Vis spectroscopy. The CQDs/TiO_2 heterostructures were tested for the photocatalytic degradation of an aqueous solution of methylparaben, which is a harmful pollutant found in PCPs, under the influence of simulated solar light [4]. A more complete investigation of the photocatalytic efficiency of the synthesized materials is in progress.

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Influence of Cation Ratio and Oxygen Deposition Pressure on Optical and Electrical Properties of Amorphous Copper Tin Oxide Thin Films

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Transparent amorphous oxide semiconductors (TAOS) have become increasingly important in modern electronics due to their combination of optical transparency, high electron mobility, and compatibility with low-temperature, large-area processing. Among emerging TAOS materials, copper tin oxide (CTO) offers promise due to its tunable optoelectronic properties and potential for both n-type and p-type conductivity[1]. However, optimizing its performance requires systematic control over a wide range of parameters, including composition and deposition conditions. In this work, we apply two distinct combinatorial pulsed laser deposition techniques[2,3] to fabricate CTO thin films at room temperature in varying oxygen pressures. This high-throughput approach enables efficient exploration of the compositional and process-dependent property landscapes.

The resulting X-ray amorphous CTO films were investigated structurally, optically, and electrically as a function of copper content and oxygen deposition pressure[4]. We demonstrate the ability to tailor the absorption edge in the range of 1.2–3.2 eV, achieve charge carrier concentrations from 10^{14} to 10^{20} cm^{-3}, and modulate their mobility between 2–11 $cm^2 V^{-1} s^{-1}$. An extended percolation-based random band edge model was applied to temperature-dependent conductivity and Hall effect measurements for different deposition pressures. The degree of structural disorder, quantified by a disorder parameter obtained by fits of the model, was found to be sensitive to oxygen deposition pressure, playing a crucial role in determining the material's optical and electrical behavior. While limited p-type conduction was observed at high Cu content, only n-type CTO exhibited properties suitable for transparent electronics, including high mobility and a bandgap exceeding 3 eV.

These results underscore the benefits of combinatorial fabrication for rapidly identifying optimal synthesis conditions and advancing TAOS materials development. Our findings establish n-type CTO as a promising candidate for integration into transparent and flexible electronic devices.

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Investigation of Bipolar pulsed reactive hollow cathode gas flows sputtering for room temperature deposition of Indium-Zinc-Oxide TCOs and ASOs

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Hollow cathode gas flow sputtering (GFS) is a unique and highly potent technique for depositing metal and reactively sputtered oxide, nitride and oxi-nitride thin films. [Szyszka25] Its key advantage for reactive sputtering lies in maintaining the target in a pure metallic mode. This mode of operation is a crucial advantage for reactive processes. A high inert gas flow, typically argon, through the hollow cathode prevents the reactive gas provided in the substrate vicinity from entering the cathode, thereby effectively suppressing target poisoning. The effective suppression of target poisoning leads to an exceedingly stable and reproducible deposition process, as the target material remains in its metallic state. This not only enables high deposition rates, as later shown for NiO_x, but also allows for precise control over the amount of reactive gas incorporated into the growing film, since the reaction predominantly occurs on the substrate surface rather than on the target.

Due to the hollow design of the cathode and the relatively high working pressure of several 10 Pa, plasma densities in the order of $10^{12} - 10^{14}$ cm^{-3} are achieved without magnetrons, even in the substrate vicinity. At these high pressures, sputtered species and plasma particles are largely thermalized before reaching the substrate. Off-axis sputtering further reduces plasma-induced damage to the thin film, providing an excellent basis for thin film deposition. Utilizing this technique, our group recently achieved deposition rates above 24 μmh^{-1} for NiO_x from a metallic target [Seibertz23], which were later investigated for application in perovskite solar cells [Kumar23].

However, while GFS provides high plasma densities, the high working pressures leading to largely thermalized species can be a bottleneck for achieving high-quality, dense thin films. To overcome this and effectively harness the plasma's extraordinary density for improved layer properties at room temperature without intentional heating or substrate bias (which is unsuitable for coatings on glass), we investigated bipolar pulsing of the hollow target. A rapid increase in the plasma potential is expected to draw higher-energy Ar^+ ions from the plasma onto the floating substrate, thereby improving layer properties. To fully characterize the influence of pulsing parameters, a comprehensive parameter map involving three frequencies, three reverse voltages, and three duty cycles was investigated. Structural and electrical properties of thin Indium-Zinc-Oxide films were analysed by X-ray reflectometry, atomic force microscopy, and Hall measurements, respectively. Finally, a small oxygen series was run to change IZO from TCO to ASO properties. Unoptimized thin films, deposited at room temperature, already revealed a low resistivity of $2x10^{-3}$ Ωcm, with charge carrier concentrations in the order of 10^{19} cm^{-3}. The density of 6,5gcm^{-3} indicates a zinc rich film.

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DC sputtered Al, Al-Si doped ZnO thin films for hydrogen and methane detection

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Abstract: Methane and hydrogen are both odourless, colourless and flammable gases that find worldwide use as fuels for electricity and heating generation, at the automotive industry and various industrial applications. These gases can be explosive if their concentration reach 5-15% and 4-75%, respectively, in an enclosed area and they cannot be perceived by human senses. Thus, there is urgent need to develop low cost, fast responding and reliable methane and hydrogen gas sensors to monitor their concentration during production, storage, transportation, use procedures and possible leakages. To achieve that, a wide range of materials have been used as gas sensing elements, including metal oxide semiconductors, carbon-based material, conducting polymers and other 2D materials.

This work focuses on grow of Aluminum doped and Aluminum-Silicon co-doped ZnO thin films using the DC magnetron sputtering technique. Their structural morphological and optical properties were studied utilizing characterization techniques such as X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), as well as Energy Dispersive Spectroscopy (EDS) and UV-VIS spectroscopy to determine the stoichiometry and their optical energy band gap, respectively. The effect of thickness, sputtering current as well as the operation temperature on the gas sensing performance against methane or hydrogen were investigated, achieving maximum response up to 130%, response-recovery times between 2-4 minutes (hydrogen case) and maximum response up to 740%, response-recovery times between 1-4 minutes (methane case).

Photocatalytic Water Splitting for Hydrogen Production via ZnO/ZnS Heterostructures

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Photocatalytic water splitting using sunlight and water, both naturally abundant resources, has gained significant attention as a sustainable method for hydrogen production. Hydrogen itself is emerging as a promising clean energy source that may contribute to addressing the growing energy crisis, as modern society continues to rely heavily on non-renewable and environmentally harmful energy sources. In this study, a two-step synthesis process was employed for the synthesis of ZnO and ZnO/ZnS semiconductor heterostructures, involving chemical precipitation and photolysis. The synthesized materials in the form of powder were characterized in terms of their structural, morphological, and optical properties using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDS), and diffuse reflectance UV–vis spectroscopy (DRS), respectively. The photocatalytic activity of the materials was evaluated through hydrogen evolution experiments under simulated solar irradiation, in order to compare their efficiency in water splitting. The results revealed a significant increase in hydrogen production following the formation of the ZnO/ZnS heterostructure. This enhancement is primarily attributed to more effective separation and transport of the photogenerated charge carriers, which led to reduced recombination and increased probability of carrier participation in redox reactions on the catalyst surface. The overall findings suggest that the formation of ZnO/ZnS heterostructures via a simple synthesis route can enhance photocatalytic performance, offering a promising direction for the development of efficient materials for solar-driven hydrogen production.

H_2 and CH_4 gas sensors based on DC sputtered In:ZnO thin films

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Semiconducting metal oxides have emerged as highly promising materials in gas sensing applications, attracting considerable scientific interest due to their exceptional capability to detect a wide range of gases at relatively moderate temperatures. It is well established that the sensing performance of both pristine and doped metal oxide gas sensors is predominantly influenced by their morphological aspect ratio and the density of structural defects presented within the material. In this work, the gas sensing properties of thin ZnO films[1] doped with Indium (In) against hydrogen (H_2) and methane (CH_4) gases, were investigated. The gas sensors were fabricated by DC magnetron sputtering technique. To examine the effect of sputtering parameter on the gas sensing performance, sputtering current as well as oxygen content in plasma during deposition were varied. X-ray diffraction patterns of the synthesized films reveal preferential orientation along the (002) plane. The In:ZnO samples reveal a wurtzite hexagonal crystal structure. The morphological properties of thin films were investigated using scanning electron microscopy energy dispersive spectroscopy analysis showcases a homogeneous doping of 5% In. The roughness of the In:ZnO was studied by using atomic force microscopy. The optical properties conducted using UV-Vis spectroscopy indicated 90% transparency, and an optical energy bandgap ranging between 3,45 and 3,53 eV.

Their gas sensing response was evaluated in the presence of hydrogen (H_2) and methane (CH_4) gases[2] at different concentrations (1000-50ppm) and (100%-1%), respectively. The operation temperature was ranged from 25°C (room temperature) to 400°C. The results demonstrate response and recovery times that fall within the fast to moderate range, indicating that the sensors are suitable for applications requiring timely detection, such as environmental monitoring, industrial safety and air quality assessment. This performance ensures reliable operation in scenarios where rapid gas detection is important.

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Microwave-assisted hydrothermal synthesis of spinel AMn_2O_4 (A: Mn, Ni, Zn or Cu) for supercapacitor applications

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Microwave-assisted synthesis of nanomaterials offers several advantages, including short reaction time, energy efficiency, uniform and selective distribution of energy, control over size, temperature and experimental parameters, making this synthesis route more environmentally friendly and efficient than conventional processes. Furthermore, hydrothermal synthesis is a simple, low cost and highly sensitive method to various conditions that allows the growth of unique morphologies in nanoscale with high uniformity and purity. The above advantages can be embraced to applications that strongly depend upon morphology, crystallinity and crystal structure, like energy storage devices such as supercapacitors[1],[2]. Among common materials, namely carbon-based, metal oxides and conductive polymers, Hausmannite (Mn_3O_4) possesses high theoretical capacitance (1370 F/g), wide potential window, variable oxidization states, and cost efficiency. Contrary to these advantages, low electrical conductivity restricts its wide application. Consequently, different approaches have been utilized to enhance the electrochemical performance of Mn_3O_4. Doping with transition metal ions like Ni, Cr, Sn, Co, Cu, etc is one of the frequently used strategies[3],[4].

This work focuses on the growth of spinel manganese oxides (AB_2O_4, A: Mn, Ni, Zn or Cu and B: Mn) via a hydrothermal microwave-assisted method and in particular, in the study of the effect of morphology, crystallinity and conductivity on their electrochemical behavior when tested as supercapacitor electrodes. The structural and morphological properties were characterized by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) as well as Energy Dispersive Spectroscopy (EDS), respectively. The electrochemical performance of the electrodes was studied by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and galvanostatic charge discharge (GCD) curves.

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Size Reduction and Confinement in p-type Transparent Conducting Oxides

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The development of performing p-type transparent conducting oxides (TCOs) remains a significant challenge in the field of optoelectronics. There is currently no material that simultaneously offers sufficient optical transparency and adequate electrical conductivity, both of which are essential characteristics in high performing optoelectronic devices.

In this work we investigate p-type TCOs, grown by a low-cost chemical vapour deposition (CVD) method - spray pyrolysis (SP). SP is a cost-effective method to produce thin films at relatively low temperatures. Our custom-built spray pyrolysis system consists of an atmospheric gas chamber, which allows us to control the gaseous state of the environment using a simple gas inlet valve, ultrasonic medical nebulisers for spraying and mass flow controllers to tune O_2 partial pressures. With this specific system we are able to achieve thickness control in the nm range and large scale film homogeneity.

Due to this growth precision, we can investigate the effect of size confinement on the optical properties of p-type oxides in the 5-50nm thickness range. As p-type TCOs are often used in form of very thin films as hole injection/extraction layers, the expected changes in band gap but also inter band transitions are important to understand the materials performance in devices. We specifically investigate thin films of cuprous oxide (Cu_2O) and vanadium oxide (V_2O_3). The selection of these materials is based on using well understood (in bulk form) binary materials with one having a high hole mobility (Cu_2O), while the other having a high carrier concentration as a correlated metal (V_2O_3). In bulk form Cu_2O has relatively low transparency, due to a bandgap of around 2.1eV. This work demonstrates that if used in ultrathin layers the optical tuning of Cu_2O through size confinement is possible, which lends itself to a broader bandgap, and hence, increased transparency in very thin Cu_2O films.

This work focuses primarily on the optimization of film growth parameters to achieve precise control over stoichiometry, thickness, and uniformity, factors that critically influence material performance. Furthermore, the effect of size confinement and the tuning of optical properties of Cu_2O and V_2O_3 is demonstrated.

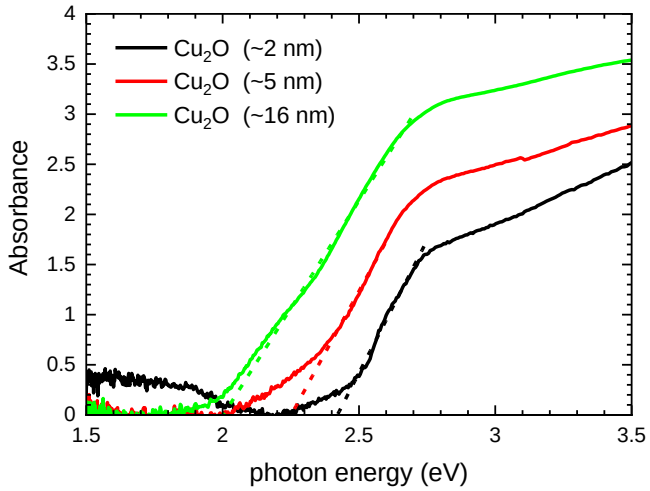

Fig 1: Shift in the optical absorption edge and improved transparency seen in Cu_2O once grown in ultrathin films. Quantifying this behavior is important once p-type TCOs are used in ultrathin form as hole injection layers or in future nanolaminates.

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Electrical failure in microscale silver nanowire networks under voltage pulses

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Silver nanowire (AgNW) networks are widely considered as a key class of transparent conductive materials for next-generation flexible and stretchable electronics. Their compatibility with solution-based processing, combined with excellent optical and electrical performance, makes them suitable for large-area, low-cost device integration. However, due to their geometry, AgNW are inherently susceptible to electrical instabilities [1,2]. In particular, their small cross-sections can lead to significantly high current densities, raising concerns about failure mechanisms such as electromigration, localized Joule heating, or junction degradation under electrical stress.

In this work, we investigate electrical transport in micrometer-sized AgNW networks, ranging from 20 to 30 µm in width, comprising only a few nanowires per conductive path. These microscale networks serve as model systems to study failure mechanisms under pulsed voltage stress. By applying a sequence of voltage pulses of increasing amplitude up to breakdown, generally up to 1 V, we observe the evolution of the network resistance and identify the locations of electrical failure, typically linked to the most stressed junctions or nanowire segments.

To rationalize these observations, each experimental network is mapped to an equivalent electrical circuit, accounting for segment resistances, junction resistances and contact resistances with electrodes. Numerical simulations based on this digital twin circuit allow us to compute local current densities and predict failure-prone zones. The comparison between experimental failure locations and simulated stress maps enables iterative refinement of key parameters, improving the predictive power of the model. In particular, this comparison allows us to extract parameters such as the resistance of AgNW junctions, the critical current density at which failure occurs, and characteristic features of the resulting break morphology.

While the present work focuses on small-scale networks, this methodology lays the groundwork for simulating larger, more realistic AgNW systems involving tens of thousands of nanowires. Such predictive tools are essential for optimizing the design and reliability of transparent conductive architectures, particularly in emerging transparent and flexible device platforms.

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Ferroelectric Thin-Film Transistors via Solution Processing: A Route to Scalable Non-Volatile Memories

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Ferroelectric materials have emerged as promising candidates for data storage applications. As non-volatile memory elements, ferroelectric field-effect transistors (FeFETs) offer several advantages, including high-density integration, low power consumption, non-destructive readout, and scalability. Although various FeFET architectures have been investigated over the past decades, the semiconductor industry has largely focused on one-capacitor-type ferroelectric memories. This preference is primarily due to challenges associated with perovskite-type ferroelectric materials and the integration of silicon-based semiconducting channels in ferroelectric-gate field-effect transistors.

Nevertheless, ferroelectric random-access memory (FeRAM) provides an unmatched combination of low write energy, high speed, and non-volatility, making it a compelling candidate for next-generation non-volatile memory.

From a fabrication standpoint, most reported ferroelectric thin films rely on vacuum-based deposition methods, which are costly and may not be suitable for large-area applications. In this work, we report on solution-processed metal oxide-based FeFETs for ferroelectric memory applications, using bismuth ferrite ($BiFeO_3$), a well-known ferroelectric material. We explore an alternative device architecture involving the deposition of the ferroelectric layer prior to the dielectric, alongside the use of a tungsten-doped indium oxide (In_2O_3:W) semiconducting channel.

This study focuses on, a)the use of soluble precursors that decompose at low temperatures to form highly crystalline ferroelectric films with stable ferroelectric properties, b) the selection of a suitable high-k dielectric that offers both a high dielectric constant and minimal lattice mismatch with the ferroelectric layer, and c) the structure of the ferroelectric film itself, particularly the role of stoichiometry and its influence on bulk defects and interface characteristics.

Ultimately, this work demonstrates the deposition of $BiFeO_3$ films with promising properties, including a coercive field (E_c) of −0.35 MV/cm and +0.32 MV/cm, remnant polarisation of 39 μC/cm², and saturated polarisation of 43 μC/cm². The resulting 1T ferroelectric transistors exhibit strong performance, with high "write 1"/"write 0" current ratios, a memory window of approximately 3.4 V, and significantly reduced leakage currents on the order of 0.1 nA.

Bias Stress Stability in In_2O_3 TFTs Using Optimised Yttria-Stabilised Zirconia Dielectrics

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This work investigates the bias stress stability of metal-oxide thin-film transistors (TFTs) employing a solution-processed yttria-stabilised zirconia (YSZ) dielectric.
YSZ films with varying levels of yttrium doping were prepared by combining zirconium(III) 2,4-pentanedionate with dispersed Y_2O_3 nanoparticles (average particle size: 25 - 40 nm). For the TFTs, indium oxide (In_2O_3) semiconducting channels were deposited onto glass/ITO/YSZ substrates at 400 °C, followed by the thermal evaporation of aluminium source and drain contacts under high vacuum.

Devices fabricated with an optimised YSZ composition (5 mol% yttrium doping) exhibited excellent performance metrics, including negligible hysteresis, low operating voltage (5 V), high electron mobility (>35 $cm^2 V^{-1} s^{-1}$), an on/off current ratio on the order of 10^7, and a low interfacial trap state density (<10^{12} cm^{-2}).

Bias stress tests under ambient conditions - conducted over a total duration of 100,000 seconds - demonstrated outstanding stability for TFTs with the optimised YSZ dielectric. Specifically, the devices exhibited minimal shifts in turn-on voltage (<1%) and subthreshold swing (<1.3%), with electron mobility remaining effectively unchanged under both negative and positive bias stress.

ZnS-based Thin-Film Transistors with Complementary Characteristics for CMOS Applications

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Transparent conducting materials (TCMs), particularly metal oxides, play a vital role in the performance of numerous electronic devices such as solar cells, LEDs, and transparent thin-film transistors (TFTs). While n-type TCMs have been successfully developed and widely adopted in commercial applications, the development of p-type TCMs remains challenging. This difficulty arises from their intrinsically low valence band edge, which hinders effective p-type doping due to doping limit rules and compensation mechanisms.

Zinc sulphide (ZnS), a II-VI semiconductor with a wide direct bandgap of 3.6 eV (in the cubic zincblende phase) and an exciton binding energy of 39 meV at room temperature, is a promising candidate due to its low cost, environmental friendliness, and favourable mechanical properties, including high fracture strength and hardness. Doped and co-doped ZnS with transition and inner transition metals - such as Fe, Co, Ni, Ag, Cu, Mn, Eu, and Sm - has attracted significant attention, mainly for its strong photoluminescence characteristics. These doped derivatives enable full-colour emission across the UV–visible spectrum, presenting exciting opportunities for optoelectronic applications.

A particularly notable feature of ZnS is its capacity to exhibit both n-type and p-type conductivity through appropriate doping strategies—an aspect that forms the core of this study.

Here, we investigate solution-processed ZnS and ZnS:Cu thin films, fabricated under ambient conditions at a substrate temperature of 350 °C, and assess their integration into thin-film transistor architectures. Specifically, we examine the effects of copper doping concentration on the optical and electrical properties of ZnS:Cu, identifying conditions that enable stable p-type conductivity.

Finally, we demonstrate complementary MOS (CMOS) behaviour using ZnS:Cu and ZnS as p-type and n-type semiconducting channels, respectively. The resulting devices exhibit balanced characteristics, including field-effect mobilities of approximately 12 $cm^2/V \cdot s$, symmetric saturation currents, threshold voltages, subthreshold swings as low as 160 mV/dec, and voltage transfer characteristics with gains of around 50, highlighting the potential of ZnS-based materials for CMOS-compatible transparent electronics.

Optimised High-k Composite Dielectrics Enabling Enhanced ZnO TFT Performance

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The emergence of high-*k* metal oxide gate dielectrics as alternatives to SiO_2 has shown great promise for CMOS technologies over the past several years. These materials have demonstrated significant improvements in transistor performance, particularly in reducing power consumption. Various high-k metal oxides have been extensively studied using a range of processing methods. Among the most researched are ZrO_2, HfO_2, and TiO_2, due to their high dielectric constants.

ZrO_2 and HfO_2 exhibit similar properties, including good crystallinity at moderate processing temperatures, a dielectric constant around 25, and a wide bandgap (~5.8 eV). TiO_2, while offering an even higher dielectric constant (60–80) and also crystallising at moderate temperatures, suffers from a relatively narrow bandgap (~3.5 eV), which limits its applicability in CMOS integration. This limitation can be addressed through the use of composite dielectrics that combine high-k materials with both wide and narrow bandgaps.

In this work, we report on the deposition and characterisation of two composite gate dielectrics - hafnium titanate ($Hf_{1-x}Ti_xO_y$) and zirconium silicate ($Zr_{1-x}Si_xO_y$) - and their implementation in ZnO-based thin-film transistors (TFTs). The films were solution-processed at moderate temperatures (<500 °C) in ambient air and were thoroughly analysed using a range of structural, optical, and electrical characterisation techniques, as well as field-effect measurements.

Stoichiometric $Hf_{1-x}Ti_xO_y$ thin films were found to be amorphous, with a smooth surface roughness of approximately 1 nm. The films exhibited a bandgap of ~4.4 eV, a dielectric constant of ~14, and low leakage currents (~10^{-10} A/cm² at 1 MV/cm). When used as gate dielectrics in ZnO-based TFTs, they enabled low-voltage operation (~3 V), a high current modulation ratio (~10^8), a threshold voltage of 0.2 V, subthreshold swing of 0.17 V/dec, and a saturation mobility of 10 cm²/V·s.

Similarly, $Zr_{1-x}Si_xO_y$ thin films were also amorphous, with ultra-smooth surfaces (<1 nm roughness), a wide bandgap (~6.2 eV), a dielectric constant of ~12, and very low leakage currents (~10^{-11} A/cm² at 1 MV/cm). ZnO-based TFTs incorporating $Zr_{1-x}Si_xO_y$ gate dielectrics demonstrated low-voltage operation (4 V), a current modulation ratio of ~10^7, a threshold voltage of 0.1 V, a subthreshold swing of 280 mV/dec, negligible hysteresis, and a high saturation mobility of 57 cm²/V·s.

Solution-Processed MgO Thin Films for Oxide TFTs: Structural and Electrical Optimisation

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This study investigates the deposition and comprehensive characterisation of spray-coated magnesium oxide (MgO) thin films, evaluating their potential as gate dielectrics in thin-film transistors (TFTs) employing tungsten-doped indium oxide (In_2O_3:W) as the semiconducting channel. The MgO films were fabricated via spray pyrolysis under ambient conditions, a low-cost and scalable method well suited for large-area electronics. A range of substrate temperatures was explored to assess its influence on film properties and device performance.

Structural, optical, and electrical characterisation was carried out using a suite of analytical techniques, including UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), grazing incidence X-ray diffraction (GIXRD), atomic force microscopy (AFM), impedance spectroscopy, current - voltage (I-V), and field-effect measurements. The MgO films demonstrated excellent optical transparency, maintaining transmittance between 90% and 96% in the visible spectrum. Increasing the substrate temperature led to a reduction in Urbach energy, indicating improved film order and reduced sub-bandgap defect states. GIXRD confirmed the presence of a well-crystallised cubic MgO phase, and AFM analysis showed smooth surface morphology, with root mean square (RMS) roughness values ranging from 1.5 nm to 4.92 nm, depending on the deposition temperature.

Dielectric performance was also strongly influenced by substrate temperature. The extracted dielectric constant (k) values ranged from 8.8 to 12, while leakage current densities measured at 1 MV/cm were as low as 10^{-8} A/cm², decreasing with increased substrate temperature, pointing to improved film density and reduced defect density.

When implemented as gate dielectrics in bottom-gate, top-contact In_2O_3:W-based TFTs, the MgO films enabled excellent device performance. Key parameters included high field-effect electron mobility of 44 $cm^2/V{\cdot}s$, a large on/off current ratio of 10^7, a threshold voltage of 1.1 V, and a sharp subthreshold swing of 210 mV/dec. Additionally, the interface trap density was calculated to be as low as 1.2×10^{12} cm^{-2}, and the devices operated reliably at a low voltage of 5 V.

These findings demonstrate that spray-coated MgO films offer a promising route to low-cost, high-performance gate dielectrics for next-generation oxide electronics, combining excellent electrical properties, transparency, and scalability.

Phase-Engineered WO_3 Hydrogen Sensors: Impact of HCl-Assisted Precipitation on Structure, Sensitivity, and Low-Power Operation

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Hydrogen (H_2) leak detection is critical for the safe deployment of a hydrogen-based energy infrastructure, requiring sensors that are sensitive, selective, and energy-efficient. In our work, tungsten trioxide (WO_3) powder was synthesized via a precipitation method in which the concentration of hydrochloric acid (HCl) was systematically varied to tune the resulting phase composition and morphology, in order to investigate the effect on the hydrogen gas sensing performance. Phase identification by X-ray diffraction (XRD) and microstructural analysis by scanning electron microscopy (SEM) confirmed the formation of monoclinic, hexagonal, or mixed-phase (hexagonal–monoclinic) WO_3 depending on HCl concentration.

Gas sensors were fabricated by drop-casting WO_3 dispersions onto commercial glass substrates with platinum interdigitated electrodes and they were tested under identical conditions. Dynamic sensing performance toward hydrogen was evaluated between 50 and 400 °C for concentrations ranging from 50 to 1000 ppm in synthetic air. Key parameters, including sensitivity, response and recovery times, repeatability, and detection limit, were systematically investigated. Sensors comprising hexagonal or mixed-phase WO_3 exhibited superior sensitivity at low operating temperatures (~100 °C), while monoclinic-phase devices showed faster response at elevated temperatures. All sensors demonstrated an approximately linear relationship between response and H_2 concentration, enabling straightforward calibration. Notably, stable detection was achieved even under low input voltage (0.1 V), highlighting the suitability of phase-engineered WO_3 for low-power consumption hydrogen gas sensing applications.

Skin-inspired stretchable biogel enables high-performance moisture-electric generation and AI-enhanced closed-loop hydration regulation

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Abstract

Moisture-induced energy harvesters have shown promise for portable power supply[1] and self-powered on-skin sensing in non-invasive health monitoring[2]. However, current materials suffer from trade-offs between electrical and mechanical properties, limiting their energy output and operational stability under physiological conditions. Here, we report a skin-inspired stretchable biogel with bidirectional dual-ion transport highways and a dynamic interpenetrating network that mimics the ion-regulating function of sweat glands and the mechano-adaptive architecture of the dermis.

The biogel combines bidirectional dual-ion transport channels with a dynamic interpenetrating network, enhancing ionic mobility, mechanical adaptability, and structural integrity. Key properties include ultra-high stretchability (750% strain), skin-like Young's modulus (45 kPa), and high ionic conductivity (2.0 S/m at 25°C). Leveraging these, the MEG maintains stable performance over 50 days, delivering 1.3 V open-circuit voltage, 1.1 mA cm^{-2} short-circuit current density, and 114 μW cm^{-2} power density at 60% RH—tripling state-of-the-art systems. The biogel also features strong interfacial adhesion, thermal reversibility, biodegradability, and excellent cytocompatibility, ensuring biosafety and sustainability. Scalable fabrication enables large-area (4000 cm^2) 15 × 15 device arrays, with 120 units powering mobile phones outdoors. Integrated with deep learning skin patches, it achieves 94% accuracy in real-time exercise hydration monitoring via a BiLSTM network, supporting wireless prediction and advancing personalized health management.

Mechanistic studies show that charged functional groups ($–OSO_3^-$/$–COO^-$/$–NH_3^+$) form biomimetic dual-ion channels, enhancing ordered ion migration and suppressing adverse diffusion via a "triple synergistic mechanism" of electrostatic enrichment, directional transport, and disordered diffusion inhibition. Molecular dynamics simulations and in situ spectroscopy (FTIR, Raman) confirm these mechanisms reduce charge recombination, boosting energy output. This work resolves the critical trade-off between mechanical performance and energy efficiency, offering a versatile platform for flexible bioelectronics, sustainable energy harvesting, and AI-driven health monitoring.

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Science Advances in revision

A systematic growth optimisation procedure for spray pyrolysis grown zinc tin oxide

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Spray Pyrolysis is a cost-effective chemical vapour phase deposition employing liquid precursor solutions. It can be used to manufacture ultrathin uniform 2D structures, including oxide thin films. Here we demonstrate a systematic growth optimisation of zinc tin oxide (ZTO) using simple, inexpensive chloride precursors. We employ a custom-built Spray Pyrolysis chamber, with a medical grade spray system and the exploration into the key variables at play and their ideal values for growing ZTO.
Our main avenue of inquiry has been in the variables that affect growth: Precursor molarity and ratio, gas composition, gas flow, and growth temperature. As the growth chemistry in SP can be complex, we employ a Box-Behnken design optimisation procedure where key variables are changed in a grid like matrix with randomised run order to minimise the impact of other, unintended influences.
By analysing the films thickness and homogeneity, sheet resistance, carrier concentration and mobility, as well as UV-VIS transmission we can extract optimal growth conditions for different applications from the single systematic optimisation run. Growth conditions for the best mobility for transparent thin film transistors or lowest sheet resistance for transparent contacts will greatly differ.
The optimisation method helps to understand the complex spray pyrolysis growth process and while results are influenced by the specific chamber design, as well a selection of precursor salts and solvent, the Box-Behnken method has been shown to be a useful tool to identify optimal conditions.

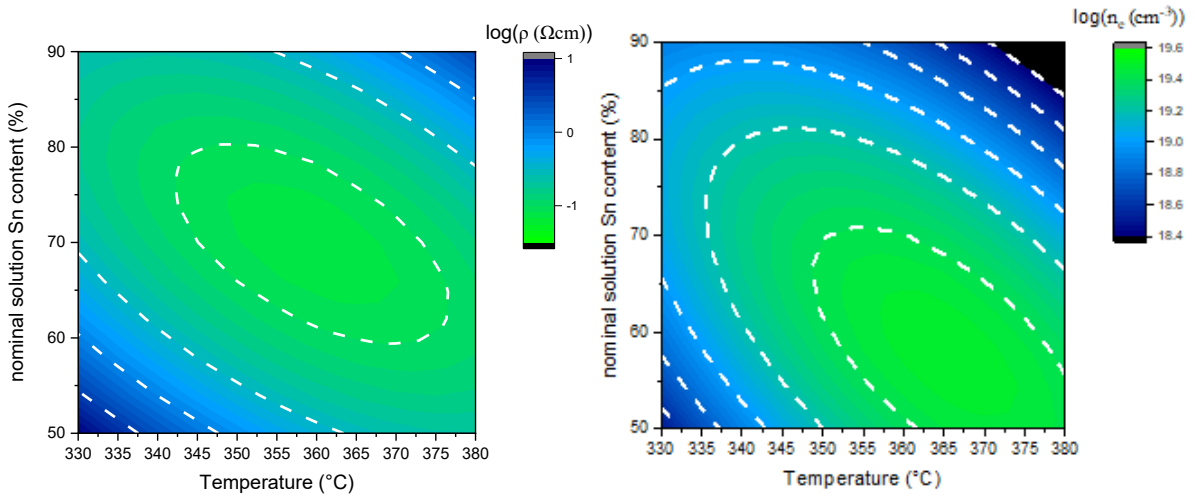

Figure 1: Example result of an ANOVA (Analysis of Variance) fit on a set of ZTO films grown in a Box-Behnken design varying the growth temperature, the Zn/Sn ratio in the solution and the total precursor molarity. The specific results visualise the variation of film properties via quadratic model fits. In the case of ZTO we clearly see that which growth conditions lead to a maximisation of the carrier concentration or lowest resistivity, which do not coincide due to variations in carrier mobility for the films.

Synthesis and Thermokinetic Analysis of Thermochromic VO_2 Particles for Smart Window Applications

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Vanadium dioxide (VO_2) is often cited as one of the most promising thermochromic materials for energy-efficient smart window applications due to its ability to undergo a reversible, structural phase transition (SPT) from monoclinic VO_2(M) to tetragonal rutile VO_2(R) at 68°C. This transition is accompanied by a distinct change in near-infrared optical transmittance, enabling solar modulation without external power input. However, its practical implementation is hampered by complications such as high switching temperature, optical haze due to large particle size, and reduced functionality by doping and processing. In this work, we report on the scalable synthesis, processing, and thermokinetic characterization of undoped and W-doped VO_2 particles, targeting their application as thermochromic pigments for smart windows. [1,2]

Undoped and W-doped VO_2 powders were synthesized via reduction of V_2O_5 using oxalic acid in aqueous medium, followed by a controlled two-step calcination process. Undoped VO_2 exhibited a switching enthalpy close to the theoretical maximum (55 $J \cdot g^{-1}$) and a narrow hysteresis. The introduction of W dopants in the VO_2 crystal lattice lowered the SPT temperature at an average rate of 23°C per at% of W. The large initial particle size of 24 µm was successfully reduced by subsequent bead milling yielding sub-micron VO_2 particles of approximately 120 nm, though partial amorphization led to a 30-40% crystallinity loss, effectively halving the switching enthalpy. Using the Friedman isoconversional method, the thermodynamic and kinetic profiles of the SPT were investigated as functions of particle size and doping percentage. The milled VO_2 particles were mixed into PVB to make laminates of two glass plates with the nanocomposite thermochromic film as interlayer. The optimal laminates exhibited a luminous transmittance of 54.7% and a solar modulation of 9.4%. Moderate visible light scattering was attributed to the presence of particles exceeding 100 nm in size. A comparison of the switching kinetics between the VO_2 powders and the nanocomposite laminates revealed comparable phase transition rates.

These results illustrate that precise control over VO_2 particle size, crystallinity, and defect structure is critical for optimizing thermochromic performance in smart window applications. The successful integration of VO_2 particles into composite films demonstrates their potential for energy-efficient glazing solutions reducing energy consumption in buildings.

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Influence of Substrate Temperature and Laser Fluence on the properties of $CsPbBr_3$ Thin Films grown by Pulsed Laser Deposition technique

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Inorganic halide perovskites, such as $CsPbBr_3$, have extensively been investigated the recent years, as an emerging new generation class of materials.

Owing to their novel optoelectronic properties [1] such as high carrier mobility, excellent photoluminescence quantum yield and tunable band gap, they have gained enormous interest for their potential use in a wide range of applications, such as in light-emitting diodes [2], photodetectors, photocatalysis [3], solar sells [4] and more recently in sensing technologies [5]. Focusing on their fabrication, the synthesis of halide perovskite nanocrystals based on solution methods [6] is widely reported, the growth of the material in the form of thin film is much less explored. In this work we report on the fabrication and characterization of cesium lead bromide thin films by applying a well-established physical vapor deposition technique, Pulsed Laser Deposition (PLD) [6].

As laser source, a KrF Excimer laser was used (λ=248 nm, τ = 15 ns). The ablated material was collected on silicon and quartz substrates. Particular emphasis was placed on the investigation of the effect of substrate temperature within a broader temperature range extending up to 350 $^{\circ}$C (room temperature, 150 $^{\circ}$C and 250 $^{\circ}$C), alongside two different laser fluences (0.6 and 1.2 J/cm^2), on the films' properties. The as-synthesized cesium lead bromide thin films, were fully characterized in terms of their morphological, structural, optical and compositional properties applying Field Emission Scanning Electron Microscopy (FE-SEM), Energy Dispersive Spectroscopy (EDS), profilometry, X-Ray Diffraction (XRD), UV-Vis and Photoluminescence (PL) Spectroscopy, respectively.

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Surface Acoustic Waves Gas Sensor for O_3 and CO_2 Applications

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In recent years, humanity has been striving to address various environmental issues caused by excessive energy consumption. The overuse of non-renewable resources, the intensification of the greenhouse effect and the increase in atmospheric pollution, are among these. As a result, the scientific community has directed significant effort toward the development of advanced methods and materials aimed at both reducing the energy footprint of buildings and detecting or neutralizing harmful gases released into the environment.

A critical aspect of this effort is the need to develop low-cost, fast-responding gas sensors capable of monitoring the concentration of toxic and greenhouse gases during production, storage, transportation, usage, and in case of possible leakages. The choice of sensing material plays a key role in the performance of such sensors. Metal oxide semiconductors (e.g., ZnO, CuO) have attracted significant attention due to their high sensitivity, chemical stability, and low fabrication cost. These materials are strong candidates for gas detection, as their interaction with target gases leads to measurable changes in their electrical or acoustic properties, enabling real-time monitoring.

In this work, the method that was used to detected gases is based on Surface Acoustic Wave (SAW). Zinc Oxide (ZnO), as well as Copper Oxide (CuO) films were tested, as sensing layers exposed to different concentrations of ozone (toxic gas) and carbon dioxide (greenhouse gas modified atmosphere packaging gas). The structural and surface properties of the films were investigated using techniques such as X-Ray Diffraction (XRD) and Atomic Force Microscopy (AFM). SAW filters operating at various nominal frequencies showed a response upon ozone and carbon dioxide interaction, which was recorded as a shift a few MHz of the central frequency[1].

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Structure-activity relationships in K-enriched lanthanum ferrite perovskite CO_2 hydrogenation catalysts

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Thermo(electro)catalytic hydrogenation of CO_2 is a promising method for clean and renewable synthesis of value-added chemicals, such as light olefins. It has drawn significant scientific attention as a viable alternative to steam cracking of naphtha. Various metal oxides have been studied as catalysts in composites with alkaline supports, with iron-based catalysts being preferential due to their increased availability and their ability to transform to Fe_3O_4 and FeC_x, which are considered active centers for the modified Fischer-Tropsch route. More specifically, oxides with structures of unique features such as perovskites and spinels can provide abundant oxygen defects, high oxygen mobility, and tunable surface properties for heterogeneous catalysis application. In this work, $LaFeO_3$ perovskite (LFO) and potassium enriched derivatives (K/LFO) have been synthesized by a novel direct salt precursor mechanochemical synthesis[1] and by conventional sol-gel and hydrothermal routes for comparison. The pristine materials have been structurally characterized to derive phase purity, morphology, stoichiometry and metallic active sites oxidation state. The as-prepared samples were then utilized either in powder form for the thermo- catalysis experiments, or as printed electrode films in the case of thermo/electro- catalysis experiments. For the powdered catalysts, an activation under different gasses (CO or H_2) was conducted and materials were studied in-situ to determine their catalytic potential. For the electrode films, thick pastes were developed as colloidal suspensions of the materials and deposited by direct ink writing, a versatile printing method, followed by thermal treatment. The resulting electrodes were characterized structurally and morphologically to observe phase retention and mechanical adhesion to the solid electrolyte substrates. Catalytic experiments for CO_2 hydrogenation showcase the samples to be active towards light olefins and CH_4 under pressurized conditions. Moreover, structural analysis of activated and spent samples (after CO activation and catalysis) indicate an increased carbon activation and structural stability.

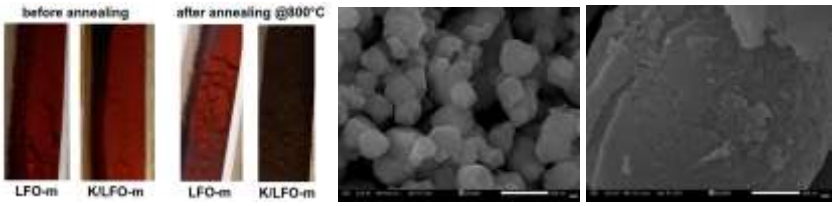

Figure 1. Macroscopic and microscopic observation of $LaFeO_3$ samples and K-enriched derivatives

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Return

$Li_4Ti_5O_{12}$ electrode design: evaluation of synthesis conditions and coating strategies in aqueous lithium-ion batteries

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Lithium-ion batteries (LIBs) have revolutionized the field of energy storage, powering a wide range of applications from portable electronics to electric vehicles and grid-scale storage systems. Their high energy density, long cycle life, and relatively low self-discharge rate make them the preferred technology in both consumer and industrial markets. However, conventional LIBs utilize organic electrolytes, which are flammable, toxic, and pose significant safety risks, particularly under high temperature or mechanical stress [1].

To address these limitations, aqueous lithium-ion batteries (ALIBs) have emerged as a safer and more environmentally friendly alternative. By replacing organic solvents with water-based electrolytes, ALIBs offer enhanced safety, lower cost, and easier recyclability [2]. Despite these advantages, a key challenge remains: the narrow electrochemical stability window of water (~1.23 V), which limits the operating voltage and energy density of aqueous systems [3]. Overcoming this limitation requires the development of suitable electrode materials with stable electrochemical performance within the aqueous window, such as $Li_4Ti_5O_{12}$ (LTO) [4].

LTO is a promising anode material for ALIBs due to its complementary electrochemical properties. LTO, with its spinel structure, is known for its excellent thermal and chemical stability, near-zero volume change during lithiation/delithiation, and a relatively high operating potential of ~1.55 V vs. Li^+/Li (-1.46 V vs.Ag/AgCl), making it particularly suitable for aqueous systems [5].

In this work, LTO powder was synthesized using the sol-gel method, which offers precise control over the morphology and homogeneity of the resulting material. During synthesis, various lithium sources, such as lithium hydroxide, lithium chloride and lithium nitrate were explored, along with different chelating agents, including citric acid and oxalic acid, to optimize the structural and electrochemical performance of LTO. Thermal treatment (annealing) was conducted at 800 °C for durations ranging from 6 to 12 hours in different atmospheres (air, vacuum). These conditions were systematically studied to promote the formation of a pure spinel phase while minimizing undesirable grain growth.

The synthesized LTO was uniformly immobilized onto copper substrates via tape casting process using aqueous slurry.

Electrochemical evaluation was performed using three-electrode systems, investigating the effect of different electrolytes (LiOH, Li_2SO_4, $LiNO_3$) as well as the effect of the final electrode coating (single, double coating, and active material ratio). This investigation is important for selecting the appropriate system to achieve good reversibility, capacity retention, and stability during the cycle.

Keywords: Aqueous lithium-ion batteries (ALIBs), LTO, sustainable materials, cyclic voltammetry, energy storage devices

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Tailoring Noble and Transition Metal Species on Graphitic Carbon Nitride for Enhanced Solar Hydrogen Production

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Photocatalytic hydrogen (H_2) production is a promising approach for addressing the growing global energy demand and transitioning towards sustainable energy systems. Graphitic carbon nitride (g-C_3N_4) and its advanced derivatives, such as exfoliated nanosheets (CNNs) and nucleobase-doped g-C_3N_4 (NB-C_3N_4), have attracted significant attention as photocatalyst supports owing to their metal-free composition, visible-light activity, and excellent thermal and chemical stability [1,2]. Despite these advantages, pristine g-C_3N_4 suffers from rapid charge-carrier recombination and limited active surface sites, which hinder its photocatalytic efficiency.

To overcome these limitations, we investigate the functionalization of CNNs and NB-C_3N_4 with noble metals (Pt, Pd, Au) and transition metals (Cu, Ni, Mn) via photodeposition and impregnation techniques. This strategy aims to achieve highly dispersed metal species, including single atoms and sub-nanometer clusters, that can promote charge separation and accelerate surface catalytic reactions [3]. Representative catalysts, such as Pt-loaded CNNs (Pt_CNNs), demonstrated significantly enhanced photocatalytic H_2 production. Specifically, optimized 1%Pt_CNNs achieved a remarkable hydrogen evolution rate of 1236.0 μmol/h (61.8 mmol/g·h) under simulated solar irradiation ($\lambda > 360$ nm), while 0.5%Pt_CNNs reached 449.3 μmol/h (22.5 mmol/g·h) under visible light ($\lambda > 420$ nm).

Comprehensive characterization using XRD, TEM, XPS, FESEM-EDS, and UV–Vis DRS revealed strong metal-support interactions, uniform dispersion of metal species, and favorable modifications to the optical properties of g-C_3N_4. These findings underline the synergistic effects of co-catalyst selection and support engineering in optimizing photocatalytic performance. Future work will incorporate advanced structural analysis (XAS, HAADF-STEM) and density functional theory (DFT) calculations to resolve atomic-scale active site configurations and provide mechanistic insights. This combined experimental and theoretical approach is expected to pave the way for designing next-generation photocatalysts capable of efficient solar-driven hydrogen production, contributing to a clean energy future.

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TiO_2-Based Composite Photocatalysts with Metal Sulfides for Improved Hydrogen Evolution Reaction Under Solar Irradiation

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Titanium dioxide (TiO_2) combined with metal sulfide co-catalysts has shown promising performance for the hydrogen evolution reaction (HER) under solar-simulated irradiation [1]. TiO_2, a widely studied photocatalyst due to its stability, abundance, and non-toxicity, suffers from limited visible-light absorption and rapid recombination of photo-generated charge carriers. To address these limitations, metal sulfides such as NiS, CoS, and CuS are integrated as co-catalysts to enhance charge separation and extend light absorption into the visible region. These metal sulfides serve as active sites for proton reduction and improve electron transfer efficiency, thereby significantly boosting hydrogen production [2]. When exposed to a solar simulator light, the TiO_2-metal sulfide system mimics sunlight-driven photocatalytic water splitting, offering a viable pathway toward sustainable hydrogen fuel generation [3].

In this study, TiO_2–metal sulfide composite photocatalysts were synthesized via a hydrothermal method and focused on the effect of varying metal sulfide loadings, as well as the incorporation of bimetallic or trimetallic sulfide systems, where different metal sulfides were combined to enhance the composite's photocatalytic properties. The structural and morphological properties were examined using X-ray diffraction (XRD), in order to confirm phase composition, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) for morphology and particle distribution, and energy-dispersive X-ray spectroscopy (EDS) for elemental mapping. UV–Vis spectroscopy was used to assess optical absorption properties. The hydrogen evolution reaction (HER) performance was tested in a quartz reactor under solar irradiation using a solar simulator, with evolved hydrogen quantified by gas chromatography (GC). The photocatalytic activity was measured over time to assess stability and efficiency.

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Crystalline transitions and point defects in (N, Mg)-doped copper oxide thin films deposited by radio-frequency magnetron sputtering

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Copper oxide is a promising p-type metal oxide compound for a wide range of applications in optoelectronics, as active material for transparent junction transistors and photovoltaic cells. This study aims at analyzing the effects of N and Mg doping on the optical and electrical properties of Cu_2O thin films deposited by radiofrequency magnetron sputtering at room temperature. Additionally, the crystalline phases of copper oxide are examined through complementary X-ray diffraction and energy dispersive X-ray spectroscopy measurements.

It is shown that nitrogen incorporation enhances both the electrical conductivity and the optical transparency, with resistivity reaching values as low as 1.15 Ωcm and an average transmittance in the visible range of 31.7%. Raman spectroscopy measurements indicate an increase in the number of $(N_2)_{Cu}$ shallow acceptor point defects, which can be associated to the enhancement of the hole concentration. Furthermore, we report a marginal improvement of the optoelectrical properties of Mg-doped samples. Conversely, we demonstrate that (N, Mg) co-doping leads to a degradation of the material crystallinity, along with a reduction of film conductivity, which could be attributed to high levels of nitrogen incorporation. The influence of dopants on the electrical and optical properties is discussed via a detailed analysis of the correlation between defects and Raman activities.

This work contributes to the assessment of Mg and N as doping species, unveiling the dominant behavior of specific point defects[1]. The results obtained in the study can therefore benefit future developments in copper-based p-type semiconducting oxides with enhanced optical and electrical properties.

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Self-Powered Transparent Photodetector for Broadband Vision and Wide-Field Subretinal Function

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Human color vision is facilitated by natural photoreceptors that detect colors and their corresponding intensities through cone and rod cells, respectively. In this study, we have developed an artificial broadband photoreceptor that mimics the light-color intensity detection functions of natural photoreceptors. This self-powered photoreceptor operates across a broad spectral range (365–940 nm) and is designed to perceive a variety of colors. It features a metal-oxide heterojunction (n-ZnO/p-NiO) with a thin tin sulfide interlayer, offering excellent transparency in the visible spectrum and seamless integration with flexible substrates, making it ideal for use in flexible electronics. The fabricated device demonstrates an exceptional response time of approximately 1 ms and a wide field of view (150°), surpassing the human eye's sensing range (50–100 ms response time and 108° field of view). Functioning similarly to cones and rods, the transparent photoreceptor can detect wavelength-dependent signals and accurately differentiate signal intensities. This capability is further validated through real-time color detection, where the photoreceptor generates distinct signals for each color. These results provide a proof of concept for self-biased, flexible bioelectronics that replicate the advanced visual functions of artificial eyes.

Deposition of Dense, Smooth, and Amorphous Ta_2O_5, Al_2O_3, and TiO_2 Thin Films via Gas Flow Sputtering

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Facilitating adatom mobility through high substrate temperatures is frequently unsuitable for materials exhibiting low melting or crystallization points. Gas Flow Sputtering (GFS)[1] technique emerged to address this limitation and achieve the desired deposition outcomes at reduced substrate temperature. This method involves a modification of the target geometry in the sputtering process, specifically transforming it into a hollow cylindrical configuration. This alteration enables the benefits associated with the hollow cathode effect to be realized. By enhancing ion bombardment energy, the GFS technique facilitates the engineered transition between structure zone model (SZM)[2] regions at lower temperatures.

Despite its innovative nature, the application of GFS for oxide deposition in dielectric media presents several challenges. Notably, the deposited oxide films must be both dense and smooth while remaining amorphous. Achieving such film characteristics necessitates the careful optimization of multiple process parameters. To date, the precise values for these parameters remain undetermined.

In this project, seven parameters were systematically optimized for the deposition of Tantalum, Aluminium, and Titanium oxides. These parameters include chamber pressure, target size, reverse voltage, frequency, argon flow rate, the distance between the substrate and cathode, and oxygen flow rate. Each oxide was deposited independently. The density of the films was evaluated using X-ray reflectivity (XRR), while surface roughness was measured using atomic force microscopy (AFM). X-ray diffraction (XRD) was employed to determine the crystallinity of the deposited films.

The results of the study are noteworthy. A dense Tantalum oxide film with a density of 8 g/cm³ and a surface roughness of 478.9 pm (RMS) was achieved. An Aluminium oxide film with a density of 3.36 g/cm³ and a surface roughness of 820 pm (RMS) was also obtained. For Titanium oxide, a density of 3.98 g/cm³ and a surface roughness of 485.5 pm (RMS) was achieved. All films remained amorphous despite their high density and smoothness.

This project not only successfully demonstrated the potential of the GFS technique for depositing high-quality dielectric oxides but also provided valuable insights into the relationships between process parameters and the resulting film properties. These findings contribute to the broader understanding of GFS as a viable deposition method for dielectric applications.

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Metallic nanowire based transparent electrodes: Fruits of collaboration between chemists, physicists and engineers in two French laboratories

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Metallic nanowire (MNW) networks have received special attention as a transparent conductive material for solar cells, displays, touch screens, smart windows, transparent heaters and low-emissivity applications due to their outstanding optical, electrical and mechanical properties.[1] Among various MNW, the most studied one has been silver nanowire (AgNW), but recently, copper based MNW (such as core-shell structures[2]) have become an appealing alternative to silver ones[3] due to their comparable electrical properties, material abundance, and low-cost production.

Nevertheless, in all cases, morphological instabilities induced by thermal or electrical stress and high surface roughness constitute the main bottlenecks for further long-term operating performance of MNW based TCMs[4]. Metal oxide layers have been proven to be efficient protective coatings around nanowires with excellent results in terms of stability enhancement as well as flatness improving capability as compared to bare nanowires[5]. The nature of the metal oxides (such as SnO_2, Al_2O_3, TiO_2 and ZnO…) and how they affect concrete device performance is an aspect to be investigated for each application in order to tune and design more efficient device structures[5,6]. There are other aspects that deserve attention such as coating thickness and conformability, which should be considered for instance when optimizing the collection of photo-generated charge carriers for high photovoltaic efficiency or the absence of localized hot spots for transparent heaters. Thanks to this metal oxide surface passivation, AgNW networks have been efficiently integrated in electrochromic devices[7].

This contribution presents the main features related to a collaboration between chemists, physicists and engineers in two French laboratories (ICMCB at Bordeaux and LMGP at Grenoble) in order to present the main benefits, drawbacks and challenges of using different MNW[8] as well as protective metal-oxides, in relation to the chosen application.

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p-$Cu(OH)_2$/n-$SrTiO_3$ Heterojunction for Efficient Photocatalytic Hydrogen Production

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Improving the efficiency of well-known photocatalysts in the hydrogen evolution reaction is contingent upon the development of cost-effective and highly efficient co-catalysts [1]-[4]. The rapid recombination of photogenerated charges within semiconductor materials, such as $SrTiO_3$ (STO), results in reduced photocatalytic efficiency. To address this, copper-based co-catalysts have garnered considerable attention due to their relative low-cost, natural abundance of constituents and promising reactivity [5],[6]. In this work, p-$Cu(OH)_2$/n-$SrTiO_3$ heterojunctions were prepared for efficient photocatalytic hydrogen production. The $SrTiO_3$ photocatalysts with a flower-like morphology decorated with $Cu(OH)_2$ at different weight percentages of Cu (0.1, 0.5, 1, 2 and 5 wt%) were successfully prepared using a simple solvothermal and photodeposition process. The p-$Cu(OH)_2$/n-$SrTiO_3$ composite with 1 wt.% Cu content exhibits significant enhancement toward photocatalytic hydrogen production compared to the pristine STO, achieving a rate of ~139 μmol h^{-1} (~6950 μmol g^{-1} h^{-1} mass activity) under $\lambda > 360$ nm light irradiation which is about 3.5 times higher than that of single-component STO. X-ray photoelectron spectroscopic studies indicate formation of $Cu(OH)_2$ phase. Moreover, UV-vis/NIR, EIS spectroscopy and photocatalytic evaluation studies indicate that the improved photocatalytic performance arises from the formation of p-n junction at the $Cu(OH)_2$/STO interface which promotes enhanced charge carrier transfer and separation within the heterojunctions.

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Heterostructures for advancing properties of p-type TCOs: growth and characterisation of V2O3/Cu2O bilayer

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The optimization of n-type TCOs is a well explored field, with materials such as Sn:In_2O_3 (ITO) and InGaZnO (IGZO) displaying impressive conductivities and mobilities and as such they see regular use in applications such as thin film transistors, photovoltaics and gas sensors. In comparison, the performance of p-type TCOs lags behind their n-type counterparts. This is typically due unsatisfactory charge carrier concentrations or hole mobilities intrinsic to the O 2p nature of the VBM in many oxide materials[1,2,3]. If p-type materials with sufficiently high performance could be achieved, it would result in a number of important applications, such as the transparent p-n junction and an increase in the efficiency of OLEDs. Recently groups have tried novel approaches to circumvent this issue such as Chemical Modulation of the Valence Band (CMVB) leading to new families of p-type materials such as delafossites, spinels and layered oxychalcogenides[1]. Despite small advances in conductivity, overall, their performances remain unsatisfactory for large scale industrial applications, requiring different approaches to the modulation of the valence band, such as the use of correlated metal oxides[4] as in this study. In order to achieve the required performance, a novel approach to p-type TCOs is proposed. In this work we synthesize a multi-layer film that alternates two p-type TCOs, V_2O_3 and Cu_2O, each possessing high carrier concentration and high carrier mobility, respectively[4,5]. In theory, the structure, as a whole, exhibits the desired properties of the constituent materials.

We demonstrate that the ideal growth temperature of Cu_2O is 600ºC or higher resulting in a mobility of 21 cm^2/Vs. However, growing Cu_2O at this temperature on V2O3 results in oxidation of the V_2O_3 layer and reduction of the Cu_2O layer, along with intermixing at the boundary between the two materials. The substrate temperature must be reduced to avoid this interdiffusion, however the mobility of Cu_2O at this growth temperature is only 1 cm^2/Vs. To circumvent this issue we examine the effectiveness of 1) low temperature grown Cu_2O buffer layers prior to the high-temperature, high-mobility Cu_2O layer and 2) post annealing of the low-temperature, low-mobility multilayers. We also report results on the electrical and optical properties of the multilayers measured by ellipsometry, UV-vis spectroscopy, and Hall effect measurements, and compare these results to individual layers as well as the bilayers grown at lower, non-ideal temperatures.

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Membrane Electrode Assembly Inks Utilizing Antimony-Doped Tin Oxide Support Particles for Water Electrolysis

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Replacing noble metal catalysts in water electrolyzers and photoelectrocatalytic systems is critical for scaling these technologies. Non-noble metal alternatives for the oxygen evolution reaction (OER) typically operate at higher overpotentials and suffer from degradation and rapid equilibria between the solution and solid phases. These shortcomings can be attenuated by various supporting effects.[1] Therefore, stable, conductive, and chemically resistant support electrode materials are crucial. TCOs are attractive catalyst support candidates. While doped TCOs offer sufficient conductivity, minimizing ohmic drop in real applications, dopant corrosion can lead to gradual performance loss. Metal oxidation and anodic dissolution further complicate stability, particularly during the OER.

We have successfully employed TCO-coated anode supports, specifically ITO and FTO, in evaluating non-noble molecular pre-catalysts.[3-5] In previous research, TCO supports provided the experimental flexibility and high reproducibility needed for *operando* and post-catalysis tests, aiding the detailed analysis of molecular pre-catalysts and their side reactions during the OER.

We are currently investigating TCOs, primarily antimony-doped tin oxide (ATO) powder, as an ink constituent for membrane electrode assembly (MEA) fabrication to advance the anodic OER in proton-exchange membrane (PEM) single water electrolysis cells. Developing such ink compositions is a complex process. This work introduces methods for combining ATO particles or other support materials with the catalyst, Nafion, and optional additives in varying ratios and undergoing different treatments to produce catalyst inks for spray-coating onto the PEM. This contribution presents a comprehensive evaluation of the pros and cons of different supports, focusing on their utilization in MEAs. Most importantly, it examines their adsorption stability, homogeneity, charge transfer properties, and degradation onset potentials in combination with various Fe- and Ni-containing molecular pre-catalysts.

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Investigation of various designs of prototype silicon dioxide – based memristors for applications in advanced communications.

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With communication technology rapidly evolving, driven by increased incentive for higher data speeds and less energy consumption, oxide-based memristors have emerged as promising candidates to aide in pushing communication technology forward. Memristors are solid-state devices, theorized by Prof. Leon Ong Chua in 1971 [1]. Among the main reasons for this is that they exhibit both volatile and non-volatile memory, rapid switching capabilities and low power consumption, allowing for communication systems that are faster and more energy efficient [1]. Our work has primarily focused on silicon dioxide based memristors, with a goal being to develop a memristor-based switch applicable to communication systems. Silicon oxide / dioxide based memristors are of high interest given that such memristors would already be fully compatible with modern complementary metal oxide-based semiconductor (CMOS) technology [2]. In this work we have focused on characterizing the I-V properties of a variety of different types of these memristors, specifically experimenting with different types of electrodes such as gold and silver. We have made memristors in which both the top and bottom memristors were made of gold, where the top electrode was made of silver and the bottom made of gold, and vice versa. What all these memristors have had in common is that the oxide layer has consistently been silicon dioxide. We have also utilized atomic force microscopy (AFM) to analyze the surface topography of our devices, allowing for the observation of physical degradation on each device after prolonged use. Our work over the next few months will include an expansion of what we have done up until this point, testing new silicon dioxide – based memristors with additional combinations of electrodes, with the goal being to find a combination of materials that results in a memristor optimum for applications in communication systems.

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Tuning Wettability and Electrochemical Properties of Graphene Thin Films via PECVD Process Parameter Control

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Enhancing the performance of energy storage devices, particularly in terms of capacity, remains a significant challenge in the development of modern energy systems. Sodium-ion systems have emerged as a promising alternative to lithium-based technologies due to sodium's natural abundance, low cost, and environmental advantages. However, achieving conformal material deposition through scalable, low-temperature fabrication techniques continues to be a major obstacle. This study explores the relationship between Plasma Enhanced Chemical Vapor Deposition (PECVD) parameters and the structural and functional properties of graphene thin films synthesized on copper substrates (50 mm × 50 mm × 0.025 mm). By systematically varying key deposition conditions including substrate temperature (400 °C to 1000 °C), gas flow ratios of hydrogen (H_2) and methane (CH_4), and RF plasma power, we were able to tune the crystallinity, defects, and uniformity of the resulting graphene layers.

Characterization using Scanning Electron Microscopy (SEM), Raman Spectroscopy, and X-ray Photoelectron Spectroscopy (XPS) confirmed that these PECVD parameters significantly impact the material's structural and chemical features. In particular, it was found to strongly influence defect formation and overall film quality, highlighting a clear correlation between processing conditions and graphene characteristics. To evaluate the electrochemical performance, 1 cm × 1 cm electrodes were cut from the coated copper sheets and tested in an aqueous sodium-based enhancing or impairing electrochemical reversibility based on their impact on the electronic and structural properties of the graphene electrolyte using a standard three-electrode configuration (graphite as the counter electrode and Ag/AgCl as the reference). Cyclic voltammetry (CV) measurements, performed with an Autolab potentiostat, showed that electrochemical behavior is directly influenced by the PECVD parameters, with redox reversibility strongly affected by the structural defects. These defects were found to control ion transport pathways and influence charge transfer efficiency.

Additionally, contact angle measurements were performed to assess the surface wettability of the films, providing further insight into their interaction with the electrolyte. Overall, this study underscores the importance of precise PECVD process control in tailoring graphene films and demonstrates a pathway toward the rational design of materials with enhanced characteristics for energy storage applications.

Keywords: PECVD, graphene, sodium-ion supercapacitor, copper substrate, electrochemical performance, layers.

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