





INFRACHIP SCHOOL

October 2024 – February 2025 Organised by the Hellenic Mediterranean University (HMU) **2D Materials for Flexible Energy Harvesting and Storage Devices**

October 14-18th, 2024/series of webinars

Abstracts

"An introductory 2D Materials Seminar"

Prof. Adam Babiński (University of Warsaw)

Two dimensional materials have been at focus of researchers for almost 20 years. The success of studies of graphene, a monolayer-thick carbon structure sparked research on other materials (called 2D materials) which consist of layers of atoms connected with strong ion-covalent bonds which are kept together with much weaker van der Waals forces. The main feature of those materials is the strong dependence of their properties on the structure thickness in a few layers limit. Out of hundreds of stable 2D materials the layers of transition metal dichalcogenides (TMDs) MX_2 , where M = transition metal, X = S, Se, Te, seem to best investigated. In this presentation the properties of semiconductor **TMDs** will be reviewed. insight their will provided. An in lattice dynamics be The excitonic resonances will be introduced and their rich families explained. The effect of dielectric environment on their properties will be discussed. It will be shown how vertical heterostructures of TMDs can be produced with additional degree of freedom - the twist angle. Finally, information on current topics from the cutting edge of 2D materials research will be provided.

"Enabling the Transition of Perovskite Single Junction and Perovskite/Silicon tandem Technologies from lab to fab: the role of bi-dimensional (2D) materials"

Prof. Antonio Agresti (Università di Roma Tor Vergata)

Recently, the increasing energy demand pushes the scientific community in developing new technologies for the exploitation of the renewable energy sources, such as new generation photovoltaics. Indeed, organic and hybrid photovoltaic technologies such as Perovskite Solar Cells (PSCs) dominated the PV scientific research, by developing efficient and stable devices, produced by employing scalable and low-cost printing techniques, easily embedded in roll2roll or sheet2sheet production lines.

Despite the astonishing advancements in power conversion efficiency -PCE-(overcoming 26% over small area devices) and long-term stability, PSC technology still requires to demonstrate the transfer from lab to fab, pushing the scientific community in finding brilliant solution for drawing a feasible and reliable route toward its commercialization. Moreover, the impressive potentiality of perovskite technology has been already demonstrated to compete on equal footing with traditional inorganic PV or to work in synergy with established silicon technology in tandem cell configuration.[1] As a matter of the fact, the astonishing PCE recently achieved by small area perovskite/silicon tandem solar cells (PCE>34%) demonstrated the technology potentialities to be appealing for the PV market.[2] However, such technology should keep the promise to be easily manufactured by employing the exiting silicon cell production line and by minimizing the Levelized Cost of Electricity (LCOE). Thus, the synergetic development of large area perovskite devices fitting the standard silicon wafer dimensions and the optimization of perovskite/silicon tandem architectures can definitively open up new horizons for winning the commercialization challenges.

In general, when moving to large area substrates, the use of crystallization processes from the liquid phase tends to the formation of imperfections and defects in the bulk and surfaces that could give rise to non-radiative charge recombination.[3] Moreover, energy levels in halide perovskite semiconductors and materials for the transporting layers cannot be simply controlled by chemical doping as for Si and III-V semiconductors. Here, the use of interface engineering based on bi-dimensional (2D) materials is proposed as an efficient tool for trap passivation and energy level alignment, by mitigating the performance losses induced by the scaling-up process for both single junction perovskite and perovskite/silicon tandem devices.[4] On one side, the successful application of 2D materials, i.e., graphene,[5] functionalized MoS₂,[6] and MXenes [7,8] in opaque perovskite solar modules (PSMs) allowed to achieve PCE overcoming 17% and 14.5% over 121 and 210 cm² substrate area respectively.[9] An ad-hoc lamination procedure employing low temperature cross linking EVA (at 80°C-85°C) allowed to fabricate several 0.5 m² panels, finally assembled in Crete Island, in the first worldwide fully operating 2D material-perovskite solar farm.[10] On the other side, the 2D material engineered structure employed for the opaque perovskite modules composing the solar farm, has been further modified and optimized for realizing small (0.1 cm^2) [11] and large area semi-transparent modules (PCE>16% on active area = 60) cm²) suitable for perovskite/silicon tandem application, in four-terminal (4T) architecture. The as-optimized 2D material-engineered PSK modules (16 parallelconnected modules) have been coupled with four wafer sized (15.7x15.7 cm²) silicon heterojunction (Si-HJT) bifacial cells produced by 3 Sun company (Catania, Italy) and connected in series, in a 4T architecture by realizing a 0.2 m² PSK/silicon tandem panel. Notably, PCE approaching 20% has been achieved over the as-designed tandem panel, while the same PCE has been estimated to be > 23% employing the albedo radiation (ranging from 15% to 30%) thanks to the bifacial leading-edge Si-HJT technology employed as bottom cells. The modular architecture proposed for the tandem mini-panel, can represent a building block to develop larger 4T tandem panels, with minimized PCE losses. Following this approach, on one side the PSK solar modules can be independently optimized, realized and stacked atop the commercial Si-HJT cells employing an ad-hoc developed lamination process. On the other side, the as-proposed panel architecture does not require any modification in the Si production lines, making the tandem technology appealing for the already exiting Si cell producers.

References

- [1] Z. Zhang, Z. Li et al., Adv. Function Mater., 30, Art. no. 2001904, (2020)
- [2] https://www.nrel.gov/pv/cell-efficiency.html (accessed on October 2024)
- [3] Agresti A. et al., Nano Energy, 122, 109317 (2024)
- [4] Bellani S., Bartolotta A., Agresti A., et. al., 50, 11870 (2021)
- [5] Agresti A. et al., ACS Energy Lett., 2 (1), 279–287 (2017)
- [6] Agresti A. et al., ACS Energy Lett., 4 (8), 1862-1871 (2019)
- [7] Agresti A. et al. Nature Materials, 18, 1228–1234 (2019)
- [8] Saranin D. et al. Nano Energy, 82, 105771 (2021)
- [9] Pescetelli S., Agresti A. et al., Nano Energy 95, 107019 (2022)
- [10] Pescetelli S., Agresti A., et al., Nature Energy, 7, 597 (2022).
- [11] Agresti A. et al., IEEE Journal of Photovoltaics ,12, 1273 (2022)

"Wearable smart edge devices for personal assistance and health monitoring"

Prof. Luigi G. Occhipinti (University of Cambridge)

Printable sensors, electronics and AI technologies are unique enablers of wearable smart edge devices for personalised diagnostics and assistive care.

Solely powering these autonomous IoT devices with batteries may not sustain the growing complexity and computational requirements of these devices. For that leveraging energy storage with ambient energy harvesting technologies helps mitigate the sustainability challenge. Also, when it comes to sensors and electronics for data acquisition and processing, the design and development of ultra-low power printed electronic circuits and sensors, made of eco-friendly materials and manufacturing processes, plays a critical role in managing the power budget at the system level, and reducing the burden of batteries and conventional electronics to the environment.

In this talk I will introduce emerging technologies for wearable electronics and energy harvesting [1]-[4], providing examples of application use cases founded on multimodal analysis of chemical, mechanical and optical sensors data, with edge AI-assisted [5] and neuromorphic-based signal processing [6] and human body digital twin modelling [7]. I will also discuss routes towards ultra-low power electronics [8],[9] and integration of smart components in e-fibres and e-textiles [10]-[11].

References

[1] Tang, C. *et al.* Ultrasensitive Textile Strain Sensors Redefine Wearable Silent Speech Interfaces with High Machine Learning Efficiency. *npj Flex. Electron* **8**, 27 (2024)

[1] Jabri, M. *et al.* Flexible Thin-Film Thermoelectric Generators for Human Skin-Heat Harvesting: A Numerical Study. *Nano Energy* **129** Part A, 110001 (2024)

[2] Zhang, K. *et al.* Nanosheet-Doped Polymer Composites with High Intrinsic Piezoelectric Properties for Energy Harvesting. *Energy & Environ. Mater.*, e12789 (2024)

[3] Pecunia, V. *et al.* Emerging Indoor Photovoltaic Technologies for Sustainable Internet of Things, *Adv. Energy Mater.* **11**(29), 2100698 (2021)

[5] Tang, C. *et al.* WMNN: Wearables-based Multi-column Neural Network for Human Activity Recognition. *IEEE Journal of Biomedical and Health Informatics* **27**(1), 339-350 (2023)

[6] Wang, S. *et al.* Memristor-based adaptive neuromorphic perception in unstructured environments. *Nat Commun* 15, 4671 (2024)

[7] Tang, C. *et al.* A Roadmap for the development of human body digital twins. *Nat Rev Electr Eng* 1, 199 (2024)
[8] Portilla, L. *et al.* Ambipolar Carbon Nanotube Transistors with Hybrid Nanodielectric for Low-Voltage CMOS-like Electronics, *Nano Futures* 5, 025001 (2021)

[9] Portilla, L. *et al.* Ambipolar Deep-Subthreshold Printed-Carbon-Nanotube Transistors for Ultralow-Voltage and Ultralow-Power Electronics, *ACS Nano* 14(10): 14036–14046 (2020)

[10] Lee, S. *et al.* Truly form-factor-free industrially scalable system integration for electronic textile architectures with multifunctional fiber devices. *Science Advances* **9**, eadf4049 (2023). DOI: 10.1126/sciadv.adf4049 (2023)

[11] Choi, H. W. *et al.* Smart Textile Lighting/Display System with Multifunctional Fibre Devices for Large Scale Smart Home and IoT Applications. *Nat Commun* **13** (1), 814 (2022)

"Solution-Processed Carbon-Based Electrodes for Fully-Printed Solar Cells"

Ass. Prof. George Kakavelakis (Hellenic Mediterranean University)

This presentation will explore advancements in solution-processed carbon electrodes as alternatives to traditional metal electrodes in solar cells and modules. The focus will be on the development of carbon pastes and inks that facilitate the creation of efficient, paintable, and flexible solar cells. Key performance metrics, including power conversion efficiency (PCE) and operational lifetimes, will be discussed, alongside challenges and future prospects for integrating carbon electrodes into commercial photovoltaic technologies.

"2D Nanomaterials Synthesis and Applications in Flexible Supercapacitor Manufacturing"

Dr. João Coelho (Universidad de Sevilla)

2D nanomaterials, including graphene and MXenes, are revolutionizing flexible supercapacitors by providing high-performance, lightweight, and robust energy storage solutions. Prominent synthesis methods include liquid phase exfoliation (LPE) and laser-induced graphene (LIG), both scalable for industrial production. LPE is cost-effective and simple, while LIG transforms carbon-rich precursors into porous graphene on flexible substrates using lasers. This work discusses these synthesis techniques and their application in supercapacitor fabrication, emphasizing efforts to enhance sustainability and environmental responsibility.

"Development of novel Two Dimensional (2D) Layered Materials via Wet Chemistry"

Dr. Ali Shaygan Nia (Technische Universität Dresden & Max Planck Institute of Microstructure Physics)

The emergence of two-dimensional (2D) layered materials has transformed various fields in materials science and nanotechnology due to their unique physical and chemical properties. This talk will focus on innovative approaches to synthesizing novel 2D materials through wet chemistry techniques. We will explore methods such as liquid-phase exfoliation, chemical vapor deposition, and solution-based synthesis, highlighting their advantages in producing high-quality materials with tailored properties. Emphasis will be placed on the characterization of these materials and their potential applications in flexible electronics, energy storage, and sensing technologies. This presentation aims to provide insights into the future of 2D materials and their role in advancing modern technology.

"Two-dimensional materials: From powder to device"

Dr. Adam Kelly (CENIMAT|i3N)

The field of two-dimensional nanomaterials has exploded over the past two decades, driven by the isolation of graphene from graphite and the demonstration of its superlative properties, such as high carrier mobility, tensile strength, and thermal transport. Beyond graphene, there are over 5000 materials in the 2D family, which contain almost all the properties relevant to electronics, from conductors to dielectrics, thermoelectrics to piezoelectrics, and so on. The ability to synthesise and process these materials in solution allows us to apply similar techniques to the entire 2D family, produce 2D nanosheets at scale, and create networks of nanosheets that can be used as electronic devices using high throughput printing techniques. For such devices, the two-dimensional geometry of the nanosheets provides distinct advantages for printed devices compared to other materials with 1D and 0D geometries. In this presentation, I will discuss state-of-the-art solution-processing techniques, covering various exfoliation techniques, techniques for sorting nanosheets by length and thickness, the requirements for creating high performance networks of nanosheets, the benefits of the 2D geometry, and a range of electronic applications.

"Flexible Electrochemical Capacitors and Sensing"

Dr. Libu Manjakkal (Edinburgh Napier University)

Wearable energy autonomous sensing systems are gaining significant attention in applications ranging in health monitoring. In the case of wearables, multiple sensors for monitoring the physical, chemical, and biological parameters are highly necessary. The continuous operation of wearable sensors and related electronics demands sustainable sources of energy. When designing wearable sensors, and energy systems, the consideration of sustainable and eco-friendly materials will be a real advantage for disposable devices. This talk presents an overview of the importance of advanced functional materials based on flexible and wearable electrochemical capacitors and sensing. Our major aim is to fine-tune the ionic and electronic conductivity of the electrodes to develop the next generation of flexible and wearable devices.

"Publishing applied sciences and engineering research at Nature Electronics"

<u>**Dr. Stuart Thomas</u>** (Senior Editor of Nature Electronics) [talk integrated with ATHENA European University's colloquial talks]</u>

My talk will introduce the Nature Research portfolio of journals with a focus on applied sciences and engineering research publishing. I will talk about Nature Electronics and some of our recently launched engineering focused journals, what we hope to achieve and their editorial scope. I will then give an overview of the editorial processes and the journey an article undergoes between submission and publication, discussing what the editors are looking for in a Nature paper.

"Printable and biocompatible 2D material inks based on supramolecular chemistry"

Prof. Cinzia Casiraghi (University of Manchester)

Solution processing of 2D materials allows simple and low-cost techniques, such as ink-jet printing, to be used for fabrication of heterostructure-based devices of arbitrary complexity.

In this talk I will show that supramolecular chemistry is able to achieve in one-pot approach both liquid-phase exfoliation in water and non-covalent functionalization of 2D materials, hence enabling to produce a wide range of printable and biocompatible 2D material-based inks with specific surface chemistry. I will discuss fabrication of several printed devices, based on these 2D material inks, such photodetectors, capacitors, transistors and memristors as well as wearable sensors for breath monitoring made on rigid and flexible substrates.

"Inkjet printing of nanofunctional inks and graphene"

Dr. Giulio Rosati (Institut Català de Nanociència i Nanotecnologia (ICN2))

The lesson will discuss the potential of 2D materials and in particular of graphene. An important focus will be given to inkjet printing showcasing this method's characteristics and the process needed to adapt metal nanoparticles and graphene dispersions to it, in order to grant printability and good electrical properties. Finally, applications in biosensing and energy harvesting will be briefly demonstrated.