## The 7th Southeast Asia Collaborative Symposium

## on Energy Materials (SACSEM 7th)

## 16-17, Nov. 2021

Institut Teknologi Bandung (ITB, Indonesia)							
King Mongkut's University of Technology Thonburi (KMUTT, Thailand)							
Universität Duisburg-Essen (UDE, Germany)							
Universiti Kebangsaan Malaysia (UKM, Malaysia)							
University of the Philippines, Diliman (UPD, Philippines)							
Universiti Teknologi PETRONAS (UTP, Malaysia)							
University of Tsukuba (UT, Japan)							

## 16th November, 2021 (Japan time) Chair: Prof. Dr. Yosahikazu SUZUKI (UT)

Time	No	Affiliation	Presenter	Title
16:00-16:10	OP	UT	Prof. Junji Nakamura	Greeting and opening remark
16:10-16:25	101	ITB	Prof. Brian Yuliarto	Introduction
16:25-16:40	102	KMUTT	Assoc. Prof. Dr.	Introduction to Faculty of Engineering, KMUTT
			Asawin Meechai	
16:40-16:55	103	UDE	Dr. Tobias Teckentrup	Introduction
16:55-17:10	104	UKM	Prof. Dr. Azizan Ahmad	Introduction
17:10-17:25	105	UPD	Prof. Arnel Salvado	Introduction
17:25-17:40	106	UTP	Dr. Hayyiratul Fatimah	Introduction
			Mohd Zaid	
17:40-17:50	107	UT	Prof. Dr. Yohei Yamamoto	Introduction
17:50-18:00	108	UT	Prof. Dr.	Research and Educational Topics in
			Motoyoshi Kobayashi	Bioresources and Environmental Engineering

#### 18:00-18:10 Short break

## Chair: Prof. Dr Hayyiratul Fatimah Mohd Zaid (UTP)

Time	No	Affiliation	Presenter	Title
18:10-18:25	109	UKM	Assoc. Prof. Dr.	Atom-Thick 2H–WS2 Nanosheets' Electron
			Akrajas Ali Umar	Transport Layers for Enhanced Charge
				Transfer in Perovskite Solar Cells
18:25-18:40	S01	ITB	William Budiman	Microwave-assisted preparation of
				photocatalyst based on reduced graphene
				oxide/titanium dioxide nanocomposites
18:40-18:55	S02	UTP	Almila Hassan	Modification of Commercial Defoamers for
				Efficient Foam Mitigation Under Simulated
				Water-Alternating Gas (EWAG) Treatment
18:55-19:10	S03	UTP	Najihah Mazlan	An Insight into Adsorption Mechanism of Fatty
				Hydrazide-Corrosion Inhibitors on Mild Steel
19:10-19:25	S04	KMUTT	Nattida Srisasiwimon	Nanostructured Photocatalysts for Conversion
				of Lignocellulosic Waste to High-Value
				Chemicals

## 17th November, 2021 (Japan time) Chair: Dr. Arie Wibowo (ITB)

Time	No	Affiliation	Presenter	Title
16:00-16:15	S05	UKM	Nabilah Alias	Enhancing the interfacial carrier dynamics by atoms thick 2D TiS <sub>2</sub> passivation of TiO <sub>2</sub> nanograss electron transport layer in perovskite solar cells
16:15-16:30	S06	UPD	Gerald Angelo Catindig	Strain studies on epitaxially-lifted off Gallium Arsenide Films
16:30-16:45	S07	UDE	Dennis Oing	A monolithic, back-gated diamond field-effect transistor for electrically tunable color centers
16:45-17:00	S08	UT	Monika Tsunoda	Peptide beta-sheets/silver ion complex for antibacterial silk fabric without discolouration
17:00-17:15	S09	UPD	Rogie M. Madula	Induced strain influence on monolayer graphene on fluorinated ethylene propylene substrate for flexible gas sensor application
17:15-17:30	I10	UDE	Prof. Corina Andronescu	Electrocatalysis at nanoscale

17:30-17:45 Short break

## Chair: Assoc. Prof. Dr. Loh Kee Shyuan (UKM)

Time	No	Affiliation	Presenter	Title
17:45-18:00	S10	KMUTT	Rattana Muangmora	Photocatalysis Technology for Treatments of
				Emerging Organic Pollutants in Water
18:00-18:15	S11	UDE	<u>Meike Tack</u>	Sub-5 nm iridium oxide nanoparticles from laser
				fragmentation in liquid as catalyst for water
				electrolysis
18:15-18:30	S12	UKM	Dilip K Sarkar	Synthesis of Zn doped $NiO_x$ by simple chemical
				precipitation method using plant extract as a
				complexing agent
18:30-18:45	S13	UT	Sho Aonuki	Notable improvement of the photoresponsivity
				of As-doped n-BaSi2 films by post-annealing
18:45-19:00	S14	ITB	Sarah Zulfa Khairunnisa	Mesoporous gold as a platform for plasmonic
				sensor

19:00-19:10 Short break

## Chair: Assis. Prof. Afalla, Jessica Pauline Castillo (UT)

19:10-19:20	CL	To be announced	Award announcement and Closing Remark
19:20-19:40	SE		Student exchange

# **Invited Lectures**

## **102** Introduction to Faculty of Engineering, KMUTT

Assoc. Prof. Dr. Asawin Meechai Associate Dean for International Affairs, Faculty of Engineering, King Mongkut's University of Thonburi (KMUTT), 126 Prachauthit Road, Bangmod, Thungkru, Bangkok 10140, Thailand E-mail: asawin.mee@kmutt.ac.th



The Faculty of Engineering was established concurrently with the Thonburi Technical Institute in 1971, followed by the first master's degrees in 1975 and the doctoral program in 1990. With a proud record of producing engineers with high practical skills, the undergraduate programs in engineering have been designed to archive a solid theoretical basis and professional competence which equips graduates to play an active role in the industry immediately upon graduating. The faculty also believes that research and consulting programs are carried out by faculty staff, separately and sometimes as multi-disciplinary teams. The number of students admitted into the faculty has increased steadily over the last twenty years and has risen dramatically over the last few years, as the university struggles to keep pace with the demand for engineers by a newly industrializing Thailand. At present, the faculty has the following departments: Department of Chemical Engineering, Department of Civil Engineering, Department of Computer Engineering, Department of Electrical Engineering, Department of Electronics and Telecommunication Engineering, Department of Environmental Engineering, Department of Food Engineering, Department of Control System and Instrumentation Engineering, Department of Mechanical Engineering, Department of Production Engineering, Department of Tool and Materials Engineering. The faculty#also has a multidisciplinary program called "Biological Engineering." During the event, achievements, research activities, collaborations, and academic aspects of the Faculty of Engineering will be introduced.

#### 109 Atom-Thick 2H–WS2 Nanosheets' Electron Transport Layers for Enhanced Charge Transfer in Perovskite Solar Cells

#### Akrajas Ali Umar

Institute of Microengineering and Nanoelectronics, Universiti Kebangsaan Malaysia, 43600 UKM bangi, Selangor, Malaysia.



#### Abstract

The structure and the electronic properties of the electron-transport layer (ETL) of perovskite solar cells (PSCs) govern the interfacial charge transfer and charge transportation to the electrode. The ETLs of two dimensions, that are atom thick, and have a planar structure that possesses special electronic properties, such as the surface collective motion of excitons or charge transfer–driven defect state relief, that is 2D transition metal dichalcogenide, allow a highly energetic carrier dynamic process for enhanced photovoltaic effect. Herein, we report that planar, few-atom-thick 2H–WS2 nanosheets' ETLs drive ultrafast charge transfer and transportation along the ETL during the photovoltaic process. The nature of carrier dynamic and the performance of perovskite solar cells utilizing this atoms thik electron transport layer will be discussed.

#### **Biography of Akrajas Ali Umar:**

**Dr. Akrajas Ali Umar** received his PhD in Physics from the National University of Malaysia in 2004 in organic thin film for optical sensing application. He is currently Associate Professor at the Institute of Microengineering and Nanoelectronics (IMEN), the National University of Malaysia since 2011. His research interests are mainly in the field of Nanophysics and Nanomaterial Chemistry with the emphasis for energy conversion application, particularly to investigate the role of atomic composition, surface structure and shape of nanostructures in photoactivity and photoelectrical properties. He served as Kyoto University Venture Business Laboratory Postdoctoral Fellow (2004-2005) and Japan Society for the Promotion of Science (JSPS) Postdoctoral Fellow in Kyoto University, Japan, from 2005-2007. He was appointed as a World Class Professor in Faculty of Mathematics and Natural Sciences, Universitas Halu Oleo-Indonesia in 2018 and 2021 and a visiting scientist in the School of Information Science and Technology, Fudan University, Shanghai, China from 2018 to 2019, working on flexible perovskite solar cells. He was a visiting scientist in Kyoto University from 2008 to 2018. He has published more than 200 papers with H-index 31. Email: <a href="mailto:akrajas@ukm.edu.my">akrajas@ukm.edu.my</a>

## Student / Young Researcher Presentations

## S01 Microwave-assisted preparation of photocatalyst based on reduced graphene oxide/titanium dioxide nanocomposites

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In the past decades, many researchers devoted their efforts to enhance photocatalytic performance of titanium oxide (TiO<sub>2</sub>) to degrade recalcitrant pollutants in water stream. One of attractive strategy is by pairing TiO<sub>2</sub> with reduced graphene oxide (rGO) to become rGO/TiO<sub>2</sub> nanocomposites, because rGO has high surface area that prevent agglomeration of TiO<sub>2</sub> particles and allowing electron transfer from TiO<sub>2</sub> to rGO to prevent fast recombination. However, most of the mentioned studies used graphene oxide (GO) synthesized through Hummers method which might be harmful to environment because it may produce toxic NO and NO<sub>2</sub> gas from decomposition of HNO<sub>3</sub>. In this study, rGO/TiO<sub>2</sub> nanocomposites was prepared by green and simple method, where GO precursor was synthesized by Tour method and GO reduction was performed by microwave irradiation. We hope that the simple and green synthesis of rGO/TiO<sub>2</sub> nanocomposites and their utilization as a promising photocatalyst for photocatalytic degradation of dyes and other recalcitrant pollutants in water stream.

#### **Publication**

1. Andri Hardiansyah, William J. Budiman, Nurfina Yudasari, Isnaeni, Tetsuya Kida, and Arie Wibowo, "Facile and green fabrication of microwave-assisted reduced graphene oxide/titanium dioxide nanocomposites as photo-catalyst for rhodamine 6G degradation", under revision to be resubmitted to ACS Omega

## S02 Modification of Commercial Defoamers for Efficient Foam Mitigation Under Simulated Water-Alternating Gas (EWAG) Treatment



<u>Almila Hassan<sup>1</sup></u>, Khairulazhar Jumbri<sup>1</sup>, Noorazlenawati Borhan<sup>2</sup>, Mohd Sofi Numin<sup>1</sup> <sup>1</sup> Fundamental and Applied Sciences Department, Universiti Teknologi PETRONAS, 31750 Tronoh, Malaysia <sup>2</sup> PETRONAS Research Sdn. Bhd, 43000 Bangi, Malaysia

The excessive formation of foam caused by the injection of surfactant foams in FAWAG application has led to significant problems in the oil well production and separation facilities. Over the years, the development of defoamers has reached its fourth generation, referring to modified silicone defoamers. Several studies have shown that modified defoamer gives better performances under harsh conditions and have greater solubility and efficiency. Besides, studies also reveal that a Gemini-based modified defoamer can give good antifoaming ability and remain active even when dissolved in a solvent. Unfortunately, not all defoamer composition is suitable for every application since different oilfields may have different treatment methods and conditions. Consequently, several different compounds should be examined to determine the most appropriate defoamer for specific treatment. For this reason, various commercially available defoamers with different family types were screened under simulated EWAG treatment to select the best chemicals and then characterized to determine the best parent chain for modification into Gemini based chemicals. Four modified siliconebased defoamers were successfully synthesized, characterized and the performance was evaluated using TECLIS Foamscan under simulated EWAG treatment. Results show that all four modified silicone-based defoamers, especially amide modified defoamer (S2), showed excellent performance as a defoaming agent to mitigate foam under simulated conditions. The study on the factor affecting the performance of defoamers has proved that the best-case condition for the modified defoamer was at high temperature (60°C), gas flow rate of 1.0 L/min, and low ratio concentration of surfactant polymer-to-brine (30:70). The study on bubble counts and distributions using KRÜSS Dynamic Foam Analyzer revealed that S2 excellently contributes to the formation of unstable foams that can fasten foam destruction in the foaming system. The observation also showed that the bubble count and distribution of S2 were found to decrease as the average bubble size increases, therefore leading to a rapid coalescence and collapsing of foams. Overall, the synthesis of new Gemini based modified defoamers derived from commercial defoamers with high performance under simulated conditions can contribute to a new perspective in the synthesis approach for defoamers specific to separation application and highly concentrated foam surfactants.

#### Publication

 Physio-Chemical Analysis of Amide and Amine Poly(dimethylsiloxane)-Modified Defoamer for Efficient Oil-Water Separation. Almila Hassan, Khairulazhar Jumbri, Anita Ramli, and Noorazlenawati Borhan ACS Omega 2021 6 (23), 14806-14818. DOI: 10.1021/acsomega.1c00350

# **S03** An Insight into Adsorption Mechanism of Fatty Hydrazide-Corrosion Inhibitors on Mild Steel

<u>Najihah Mazlan<sup>1</sup></u> and Khairulazhar Jumbri<sup>1</sup> <sup>1</sup>Department of Fundamental and Applied Sciences, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia. \*Corresponding author: khairulazhar.jumbri@utp.edu.my



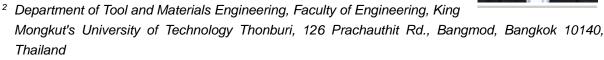
Corrosion of metals in pipelines is a gigantic concern in industrial performance, resulting in environmental pollution and economic loss. The implementation of a cost-effective technology in using waste palm oil as biobased corrosion inhibitors (CIs) has risen. However, the inhibition mechanism of CIs remains unclear due to lack of comprehensive review and small number of existing experimental data. Molecular dynamics (MD) simulation was employed to provide significant insights into adsorption mechanism and the influence of fatty acid hydrazide derivatives as effective CIs on ferrous (110) metal surface in 1.0 M HCl medium at temperature ranging from 298K to 383K. Simulation data showed that the inhibition efficiency increases at low concentration of CIs, 0.04M and together with increasing of temperature, which is suggestive of chemical adsorption mechanism from -200 kJ/mol up to -400kJ/mol. The result further suggested that thermal stability of CIs at high temperature was increased due to activation energy of CI-metal interaction from heat supplied. All the molecular simulation results were consistent with the experimental findings. The understanding of the adsorption mechanism of fatty acid hydrazide derivatives on metal surface could be used as a basis for future development of specific biobased CIs for cost-effective corrosion control technology.

*Keywords:* corrosion inhibitors (CIs), molecular dynamic (MD) simulation, adsorption, inhibition efficiency

## S04 Nanostructured Photocatalysts for Conversion of Lignocellulosic Waste to High-Value Chemicals

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Green chemical production from lignocellulosic waste is widely considered attempted to produce the desired products economically and substituting fossil fuels. Especially, lignin, low-value waste of lignocellulosic biomass which is abundant aromatic structure components and can be also useful for high-value chemical production. In this work, the conversion of lignin to high-value chemicals was investigated by photocatalysis. TiO<sub>2</sub> has been successfully exposed as a famous photocatalyst under UV light stimulation. Nevertheless, the limitation of the TiO<sub>2</sub> photocatalytic system is the suitable light energy to activate electrons. Therefore, the utilization of lignin as carbonaceous materials to modify TiO<sub>2</sub> composited photocatalysts (TiO<sub>2</sub>/lignin) to enhance the photocatalytic activity is our attempt. The carbon composite photocatalysts were synthesized by the sol-gel microwave technique. The effect of lignin loadings showed good characteristic properties for improvement of the performance of TiO<sub>2</sub>, including small crystallite size (7 nm of TiO<sub>2</sub>/lignin 1:0.5, compared with pristine TiO<sub>2</sub>-air 24 nm and TiO<sub>2</sub>-N<sub>2</sub> 9 nm) which are corresponding of grain size in TEM results, raise the photoabsorption in the visible and UV region, and decrease PL intensity which is significant of the lower rate of recombination. TiO<sub>2</sub>/lignin 1:0.5 shows the highest surface area (92.89  $m^2/g$ , compared with pristine TiO<sub>2</sub>-air 6.15  $m^2/g$  and TiO<sub>2</sub>-N<sub>2</sub> 46.74  $m^2/g$ ) and shows the best photocatalyst with enhanced photocatalytic activity by increasing lignin conversion up to 40.28% under UVA irradiation and 15.73% under visible light. Finally, High-value chemicals, such as vanillin, were found after photocatalysis.



## S05 Enhancing the interfacial carrier dynamics by atoms thick 2D TiS<sub>2</sub> passivation of TiO<sub>2</sub> nanograss electron transport layer in perovskite solar cells

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Photoelectrical dynamics i.e. an efficient interfacial charge transfer and facile charge transportation of the electron transport layer (ETL) of Perovskite solar cells (PSCs), are desperately administered by the ETL properties. Despite the excellent energy alignment with most perovskite materials, TiO<sub>2</sub> nanograss (NG) having a large density of surface defects as a result of sub-lattice vacancies has made them hurdle in the facilitation of enhanced photogenerated carrier transport to the electrode. Herein, it is discovered that an atom -thick 2D TiS<sub>2</sub> synthesized directly onto TiO<sub>2</sub> nanograss ETL have effectively passivated the defects allowing a facile interfacial charge transfer and transports as the PSCs produced a PCE as high as 18.73% with short-circuit current density (*Jsc*), open-circuit voltage (*Voc*), and fill-factor (FF) values as high as 22.04 mA/cm2, 1.13 V, and 0.752, respectively, a 3.3% improvement from the pristine TiO<sub>2</sub>-NG-based PSCs. This efficacious approach hence can be the basis for the photoelectrical dynamics development of high-performance PSC devices.

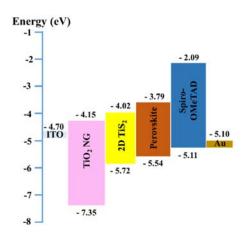
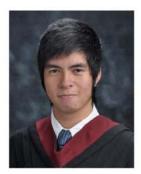


Figure 1- Energy diagram of PSC with the addition of 2D TiS<sub>2</sub> passivation layer.

**Key Words:** photoelectrical dynamics, perovskite solar cell, defect passivation, TiO<sub>2</sub> nanograss, TiS<sub>2</sub> atom thick

## S06 Strain studies on epitaxially-lifted off Gallium Arsenide Films



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Strain is a property that quantifies the deformation of a material under a variety of conditions. Strain applied onto semiconductors greatly affect not only physics properties such as the semiconductor lattice constant but also electronic properties such as the semiconductor band structure. The effects of strain on semiconductors are not always detrimental to the semiconductor's performance. Strain is sometimes used as a method of enhancing carrier mobility in high electron mobility transistors as well as modulating the emission wavelength of diode lasers. In this work, strain is introduced onto gallium arsenide (GaAs) films through a technique called epitaxial lift-off. The GaAs thin films are removed from their host GaAs substrates via a technique called epitaxial lift-off (ELO). The GaAs thin films are then bonded onto acetate, silicon (Si), and magnesium oxide (MgO) substrates. The strain on the GaAs film is induced through cooling the bonded films, thereby inducing a thermal mismatch due to the difference between the thermal expansion coefficients of the GaAs thin film and its new host substrate. At low temperatures, MgO is known to induce compressive strain onto GaAs while Si is known to induce tensile strain onto GaAs. The effect of tensile and compressive strain on the photoluminescence spectra of the bonded films is investigated. We demonstrate a band gap blueshift (relative to unstrained GaAs) of 3.1 meV for the GaAs film bonded on MgO and 19.6 meV for the GaAs film bonded on acetate at a temperature of 11 K. Similarly, we demonstrate a redshift of 8.7 meV relative to unstrained GaAs for the GaAs film bonded onto Si. The findings presented in this work show the possibility of using the ELO technique to conduct strain-related studies using spectroscopic techniques such as Raman and reflectance spectroscopy.

#### A monolithic, back-gated diamond field-effect transistor for electrically tunable color centers

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Diamond is a promising wide bandgap semiconductor [1], where a two-dimensional hole gas (2DHG can be formed on the hydrogen terminated diamond surface [2]. The 2DHG can be used for transistor structures and for tuning color centers in diamond [3]. Here, we present an innovative device structure for a back-gated, diamond-based field-effect transistor. It is monolithic in the sense that all essentia

a)

components consist of diamond. The back gate-electrode is realized by a buried, degenerately boron-doped diamond layer with a resistance of  $10^{-2}$   $\Omega$ cm, while the dielectric material consists of lightly nitrogen-doped diamond. The 2DHG on the hydrogen terminated surface serves as a conductive channel. The structure, its components and the calculated band structure are shown in Figures la and b.

In this contribution, we will discuss the band structure of this device, the function of each individual component, and the device preparation routine. Furthermore, we investigate the electrical and optical tunability of a sample that is prepared using that routine. The corresponding IV-characteristics are shown in Figure 1c. Additionally, we use the field effect to manipulate the charge state of color centers in the nitrogen-doped film.

This device structure opens a range of applications. not only in the diamond semiconductor and quantum information technology, but also for sensing applications where the back-gating is advantageous or where an all-diamond layer sequence is beneficial (e.g. for biocompatible devices or high temperature gradients).

Boron Nitrogen-doped diamond doped diamond [eV] 0.5 Band 0 b) -0.5 /alence -1.0 -250 -200 -150 -100 -50 -300 0 Growth direction [nm] -80 c) -13 V T=303 K -60 [hA] · lso L Steps -40 0.5 V Current / 05-4 V 0  $V_{a}$ 0 -3 -5 -1 -2 -4 Voltage V<sub>sp</sub> [V] Figure 1: a) Stacking sequence and b) band

structure of the presented device. c)

IV-characteristic of the transistor.

#### References

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- [2] F. Maier, M. Riedel, B. Mantel, J. Ristein, L. Ley, Phys. Rev. Lett. 85, 3472-3475 (2000)
- [3] C. Schreyvogel, V. Polyakov, R. Wunderlich, J. Meijer, C. E. Nebel, Scientific Reports 5,12160 (2015)

**S08** 

## "Peptide beta-sheets/silver ion complex for antibacterial silk fabric without discolouration"

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#### Introduction

Silver ions and silver nanoparticles show excellent antibacterial properties and are easy to handle, so they are often used not only in academic fields but also in broad applications [1]. However, the silver particles produced by the reduction of silver ions and the relatively large particles obtained by the aggregation of silver nanoparticles have a wide absorption in the visible light region, and are avoided because they present a black color, thus damaging the appearance. In fact, silver is loaded onto inorganic materials in commercial products to reduce the blackness. In this study, we found that complexing silver ions with peptides suppressed the black coloration while maintaining the same antibacterial properties as silver ions.

#### Experiment

The oligopeptide Fmoc-VKVVC (Fig. 1) was synthesized by the Fmoc method, one of the peptide solidphase synthesis methods. When Fmoc-VKVVC was dispersed in methanol and left to stand at 25 °C for 7 days, the peptide chains aggregated to form a β-sheet structure and precipitated as a fibrous solid [2]. The Fmoc-VKVVC β-sheet dispersion was then mixed with aqueous AgNO<sub>3</sub> solution (0.01 mM) with a molar ratio of 1:1. A portion of this mixture (0.2 mL) was drop casted onto a 2 cm square silk cloth (cloth A), which was then irradiated with white light (500 W) emitted from a solar simulator. As a control experiment, the same experiment was conducted on a silk cloth (cloth B) with only AgNO3 solution (0.01 mM) drop casted on it. Resultant fabric specimens were characterized by means of SEM, EDX, TEM, diffuse reflection, antibacterial test (bacterial solution absorption method), and XPS.

Fig. 1 Molecular structure of Fmoc-VKVVC

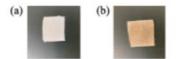


Fig. 2 (a) Silk/Peptide/Ag complex (Cloth A), (b) Silk/Ag complex (Cloth B)

#### **Results and Discussion**

After white light irradiation, the coloration of cloth A was less than that of cloth B (Fig.2). The diffuse reflectance spectrum showed a slight broad absorption band at 450 nm, and SEM and EDX images showed that silver atoms were evenly deposited to the entire silk fabric in both cloth A and cloth B. TEM images showed that silver particles were the cause of the color change. The XPS spectrum of fabric B showed the presence of Ag (0), while cloth A showed the presence of ionic silver atoms. Cloth A showed excellent antibacterial properties with a bactericidal activity value of 3.56.

#### Conclusion

We found that silver ions complexed with Fmoc-VKVVC can exist as silver ions without photoreduction when exposed to light. This is in clear contrast with the peptide-free system in which silver nanoparticles are produced upon photoirradiation. On the other hand, antimicrobial properties are maintained. As a method for applying high concentrations of silver without compromising the appearance, we plan to explore its application in future.

#### References

- [1]. Y. Wu et al., Advanced Powder Technology 2018, 29, 407-415.
- [2]. T. Mizutaru et al., ACS Appl. Mater. Interfaces 2017, 9, 9996-10002.

# S09 Induced strain influence on monolayer graphene on fluorinated ethylene propylene substrate for flexible gas sensor application



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We examine the influence of induced strain on monolayer graphene transferred on flexible fluorinated ethylene propylene (FEP) substrate and fabricated into a chemiresistive gas sensor. A strain of 0.77 % and 1.05 % were applied using a mechanical bender and characterized by Raman spectroscopy before, during, and after. Significant red shifts during bending were observed up to 13 cm<sup>-1</sup> and 33 cm<sup>-1</sup> for the G and 2D peak of graphene, respectively. The calculated rate of change of Raman shift per strain was -10.3 cm<sup>-1</sup>/% for the G peak and -30.4 cm<sup>-1</sup>/% for the 2D peak. The sensing capability of the fabricated graphene gas sensor was tested in an open system with individual exposure to 20 ppm concentration of ammonia (NH<sub>3</sub>) and 20 ppm concentration of nitrogen dioxide (NO<sub>2</sub>) with a gas flow rate of 400 sccm. A notable change in resistance was observed during exposure with values of -34  $\Omega$  for NH<sub>3</sub> and -295  $\Omega$  for NO<sub>2</sub> with calculated percent sensitivity of 1.2 % and 1.1 %, respectively. The influence of strain on the sensing capacity of graphene gas sensor was also studied. Upon application of strain to the device during gas exposure, a remarkable change in resistance were observed with values of up to -93.7  $\Omega$  for NH<sub>3</sub> and -791  $\Omega$  for NO<sub>2</sub>.

## S10 Photocatalysis Technology for Treatments of Emerging Organic Pollutants in Water

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With the progress of environmental analysis technology, a variety of unexpected organic compounds have been detected in natural water worldwide. Emerging organic pollutants (EOPs) are unregulated water pollutants that may contribute to negative effects on living organisms even though their concentrations are low. Caffeine is one of the EOPs. It is commonly found as a constituent in various consumer products (e.g., coffee, tea, soft drink, and energy drink). The occurrence of caffeine in water bodies is mainly due to routine excretion from humans and incomplete removal from conventional wastewater treatment processes. Photocatalysis technology is gaining interest as an alternative approach for water purification. Organic pollutants can be degraded by the attack of free radicals in which produced from light irradiation on photocatalytic materials. This study aimed to evaluate the efficacy of the photocatalytic process for the degradation of caffeine in water. Titanium dioxide (TiO<sub>2</sub>) was chosen as a photocatalyst because of its high chemical stability, availability, and safety to the environment. Concentrations of caffeine in water were determined by high-performance liquid chromatography (HPLC). The results showed that TiO<sub>2</sub>-based photocatalysis is potentially able to remove caffeine from the water. 20 mg/L of caffeine was found to be degraded with efficiencies up to 100% under ultraviolet-C irradiation for 3 h. The degradation rate decreased with increasing caffeine concentration thus more reaction time was required to achieve its complete removal. TiO<sub>2</sub> coated circular glass sheet can greatly overcome the separation problem of nanosized-TiO<sub>2</sub> from the treated water, and it can be reused for fifteen cycles without a significant loss of its activity.

## Sub-5 nm iridium oxide nanoparticles from laser fragmentation in liquid as catalyst for water electrolysis

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Laser fragmentation in liquids enables the production of surfactant-free, ultrasmall nanoparticles which then can be used for catalytic applications [1]. While the fragmentation of nanoparticles for the production of sub-5 nm particles is already established [2] there are only few general studies available about the fragmentation of microparticles. Microparticle fragmentation enables a one-step synthesis of nanoparticles because the step of producing the educt colloid via laser ablation is omitted. This makes the fragmentation less time consuming, cheaper, and therefore the better choice for upscaling.

In the present talk recent breakthroughs in the synthesis of surfactant-free sub-5 nm iridium oxide nanoparticles by pulsed laser fragmentation in liquid flow starting with laser-generated iridium nanoparticles (IrNP,  $\sim 60$  nm) as well as commercially available iridium microparticles and iridium oxide microparticles will be presented. By using a liquid-flow setup it can be shown that the iridium microparticles are predominantly reduced to the catalytically important size fraction which is smaller than 10 nm after just one passage [3]. Below this size and especially below 5 nm the surface to volume ratio increases distinctly which enhances the catalytic activity [4]. Because the expensive and rare iridium oxide is known as the best catalyst for the electrocatalytic oxygen evolution reaction (OER) in acidic media [5,6], such an intervention is one way for making large scale applicability possible.

It will be shown that the produced particle size clearly depends on the pH-value of the fragmentated colloids. The best results can be achieved when operating at a pH-value of 11,5 because there the surface groups of the nanoparticles are deprotonated, and the ionic strength of the liquid is optimized. The resulting particle sizes are, independent of the educt size, between 3 and 4,5 nm and have a narrow size distribution (an example is shown in Figure 1). Finally, OER measurements of the generated particles show differences in the overpotential depending on the educt and the laser treatment.

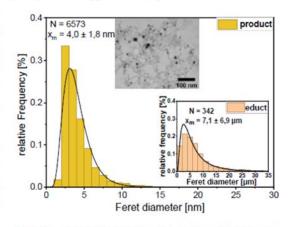


Figure 1: Size distribution of partly oxidized IrNP (product) synthesized via fragmentation of iridium powder (educt).

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# S12 Synthesis of Zn doped NiOx by simple chemical precipitation method using plant extract as a complexing agent

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#### Abstract

NiOx is a promising candidate as the hole transporting material (HTM) for perovskite solar cells (PSCs) due to its suitable bandgap, deep valence band and high stability. At normal temperature, solution-processed NiOx as HTM for PSCs is required to be improved since it has been reported as very low conductivity. In this work using plant extract as a complexing agent, Zn doped NiOx has been synthesized by a simple chemical precipitation method. The prepared materials were calcined at 500°C and characterized by XRD, UV-Vis and FESEM to confirm material composition and properties. The crystallite size, lattice parameter, dislocation density and strain were calculated from XRD results. The preferred orientation 100 and 101 planes were found at two theta angles 31.56 and 36.06 degrees, respectively, shown in figure-1. The FESEM result shows the synthesised material's morphological structure, which is composed of almost uniform spherical particles with an average size 52.1 nm. The optical band gap has been calculated from UV-Vis spectroscopy as a function of wavelength. The calculated band gap is found to be 3.24 eV.

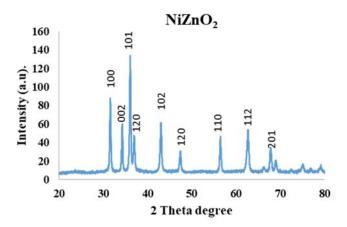


Figure-1 XRD pattern of NiZnO<sub>2</sub> material prepared by chemical precipitation method **Key words:** doping, plant-extract, bandgap, absorbance, precipitation

## S13 "Notable improvement of the photoresponsivity of As-doped n-BaSi<sub>2</sub> films by post-annealing"



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We have been paid special attention to barium disilicide (BaSi<sub>2</sub>) which has been expected as a new candidate for thin-film solar cell materials. Its band gap of 1.3 eV is suitable for solar cell applications.<sup>1</sup><sup>1</sup> The most striking characteristics of this material are achieving both large absorption coefficient ( $3 \times 10^4$  cm<sup>-1</sup> @1.5 eV) and prominent minority carrier diffusion length (~10 µm).<sup>1</sup>) The operation of a BaSi<sub>2</sub> homo-junction solar cell was demonstrated; however, its conversion efficiency was quite low.<sup>2</sup><sup>1</sup> This is because the quality of n-BaSi<sub>2</sub> layers degrades the solar cell performances. Recently, it was revealed that post-annealing is a very effective means to improve the optical properties of BaSi<sub>2</sub> films.<sup>3</sup> In this study, we thereby aim to improve the optical properties of n-BaSi<sub>2</sub> films by post-annealing.

We fabricated 500-nm-thick As-doped n-BaSi<sub>2</sub> films on Si(111) substrate by molecular beam epitaxy.<sup>4</sup> After the growth of As-doped n-BaSi<sub>2</sub> films, post-annealing was conducted in Ar gas flow by rapid thermal annealing system. The samples were cut into pieces and put together face-to-face to prevent oxidation. Pre-annealing was performed at 200 °C for 30 min to remove water in the furnace, followed by post-annealing at temperatures (*T*) of 850 – 1000 °C for 2 min.

Figure 1 shows the photoresponse spectra of As-doped BaSi<sub>2</sub> films after post-annealing. The photoresponsivity increased after post-annealing and reached a maximum of 4.0 A/W at T = 1000 °C.

This value is one order higher than that of As-grown sample.

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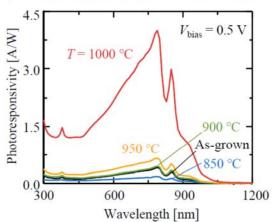


Fig. 1 Photoresponse spectra of As-doped  $BaSi_2$ films after post-annealing with different *T* of 850 – 1000 °C. The photoresponsivity measured under bias voltage of 0.5 V.

# S14 Mesoporous gold as a platform for plasmonic sensor

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Until today, sensor technology is still developing to optimize detection of any substances that is needed in many applications, such as health care, environmental applications, and biotechnology-based industries. As one of the methods, optical sensors offer many advantages in detecting biological substances or chemical molecules. Optical sensors give a real-time and label-free detection, has a high specificity and sensitivity, also its size can be made compactly with affordable cost.

Gold materials are widely known of its application in working as a platform for optical sensor since it has a good plasmonic property and biocompatible. The plasmonic property of gold arises since gold material is a metal and containing lots of free electrons that could collectively oscillate when given incident light. The propagation of plasmon of a gold thin film will occur along its surface and the phenomena is known for surface plasmon resonance (SPR) while for gold nanoparticles, the plasmon resonance will be localized (called LSPR) and gives higher sensitivity detection.

In both SPR and LSPR, the effect of refractive index changes in the environment will introduce transduction mechanism in sensing since there will be a shift of the plasmonic peaks. Moreover, to continue optimize of the sensor system, plasmonic response could be tuned based on the changes of the size, shape, or composition of gold nanoparticles. With this, there are a wide variety of options to be explored based on the gold dimension. The selection gold mesoporous structure potentially supports the plasmonic sensor since it offers many active sites on the surface stably and results in larger surface to volume ratio. The fabrication of the gold mesoporous will be presented by exploiting electrochemical deposition method which gives uniform porous structure with the help of the block-copolymer as the porogens.