2023 충남대학교 소재화학연구소 국제학술대회

2023
International Symposium on Materials Chemistry

March 09th (Thursday) 2023

Central Library(N1) Lecture Hall

[주관 Hosts]

충남대학교 소재화학연구소

Research Institute of Materials Chemistry, Chungnam National University

4단계 BK21 4차 산업혁명 대응 융합형 화공소재 교육연구단

Education and research group for convergent chemical materials in the 4th industrial revolution era

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CNU Chemistry Core Facility

충남대학교 화학과

Department of Chemistry, Chungnam National University

충남대학교 응용화학공학과

Department of Chemical Engineering and Applied Chemistry, Chungnam National University

International Chem & ChE Workshop between CNU and QUB

09 March 2023, 9:30~17:30

Central Library, Chungnam National University

International Chem & ChE Workshop between CNU and QUB

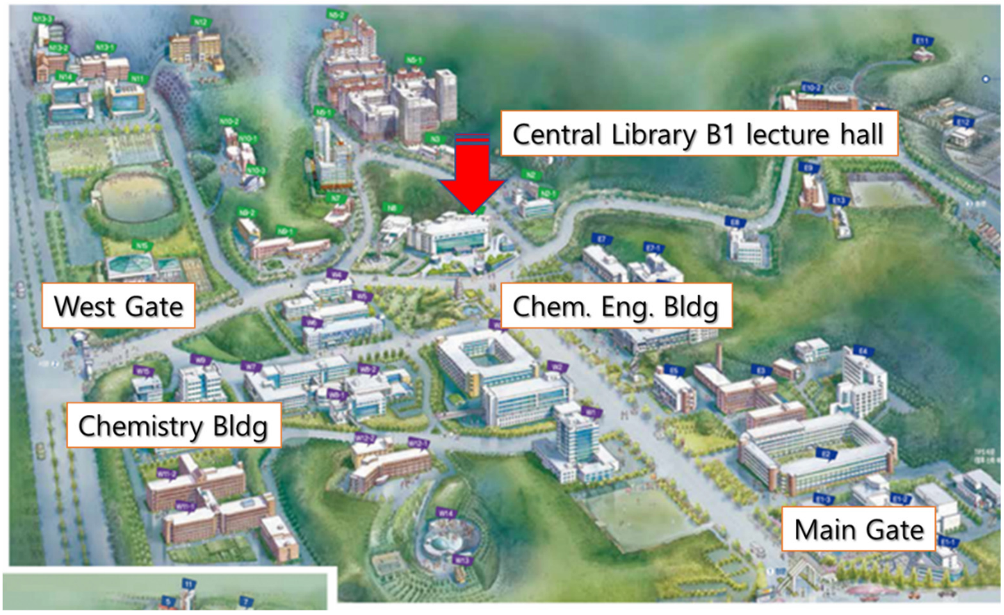
Time: 09 March 2023 09:30
Place: Lecture hall (B1 floor), Central Library, Chungnam National University Daedeok Campus

Tentative schedule

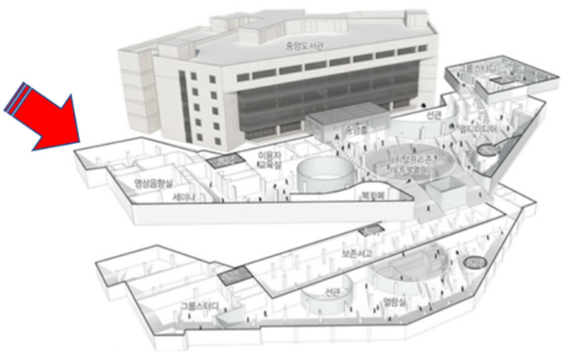
Time	Presenter	Title
09:30		Registration
Welcome Ceremony		Session Chair: Prof. Jaebeom Lee
10:00	Prof. Sung Hi Choi, Prof. Young Jin Kim	Dean of College of Natural Science, Dean of College of Engineering
10:20	Gareth Davies	Head of Science, Innovation and Health, British Embassy Seoul
Session 1	Chair	Prof. Jaebeom Lee
10:30	Prof. Peter K.J. Robertson, QUB	The Photocatalytic Destruction of Cyanotoxins in Water
11:00	Prof. Jaebeom Lee, Chem	Magnetoplasmonic nanoassembly: chiroptical properties and biomedical/energy applications
11:30	Prof. Kosan Roh, CHE	Sustainability analysis and optimization of CCUS technologies using process systems engineering methods
12:00-14:00	Lunch	Young Top Hall
Session 2	Chair	Prof. Lemma Teshome Tufa
14:00	Prof. David Rooney, QUB	Systems approaches to biochar production and valorization of agricultural resources
14:30 (20’)	Dr. Chandra Shakher Pathak, CHE	PTB7 as an ink-additive for spin-coated vs inkjet-printed perovskite solar cells
14:50 (20’)	Dr. Ryan McGhee, QUB	The Development of an in-situ BTEX Water Sensor
15:10 (20’)	Prof. Lemma Teshome Tufa, Chem	Trimetallic-NiCoFeOx Ultrathin Nanostructures for Electrochemical Energy Conversion and Storage
15:30-16:00	Tea & Cookies	
Session 3	Chair	Prof. Jihyun Cha
16:00	Prof. Pilho Kim, KRICT	Discovery of Orally Available BTK Degraders Potent in Murine Xenograft Models, Utilizing Wild-Type and C481S Mutant BTKs
16:30	Prof. Tae Jun Yoon, CHE	Experimental and Theoretical Study on the Technical Feasibility of Supercritical Water Desalination as a Selective Zero-liquid Discharge Process
17:00	Dr. Nathan Skillen, QUB	Photocatalytic Biomass Reforming: *steps towards advancing the technology*
Closing ceremony		
17:30	Director of Research Institute of Materials Chemistry Chair of BK21 Graduate school of Nano Fusion Materials, Chemical Engineering	

Dinner Time address: Chair of Chemistry, ChE of CNU, Chair of Chemistry and ChE of QUB

Venue: Central Library (N1) Lecture Hall



Space Configuration Plan



1F	• Group Study Room • Conference Room	• Carrel
B1	• Video and Acoustic Room • Multimedia Room • Communication Lounge • Seminar Room	• User Education Room • Laptop Reading room • Book Cafe
B2	• Group Study Room • Carrel	• General Reading Room • Preservation Library

Lunch at **Young Top Hall** (N7),

Brief Introduction of Department and University

Department of Chemistry, CNU

Chemistry is one of the most basic disciplines that satisfies the intellectual curiosity of modern humans and the physical happiness of mankind. It is an important field of basic science that is the basis of high-tech industry as the study of synthesizing materials or predicting new phenomena. Established with the opening of the school, the Department of Chemistry has continued its tradition along with the history of Chungnam National University. There are 42 students in the master's program and 7 students in the doctoral program, and 18 faculty members and students are devoted to research. Currently, 18 faculty members are recognized for their skills not only in Korea but also abroad, and are receiving a lot of research funds from the Korea Science Foundation, Industry-University Foundation, Ministry of Education and Academic Promotion Foundation, etc. and conducting various researches.

Department of Chemical Engineering and Applied Chemistry, CNU

The Department of Applied Chemical Engineering was newly established in 1959 to nurture excellent talents who can acquire core technologies of chemical engineering, a national key industry, and lead the development of related technologies. , Department of Fine Applied Chemistry, which was newly established in 1992 and operated in order to nurture excellent talents who can lead the development of next-generation chemical materials with high added value by acquiring and utilizing advanced technologies in the field of fine chemistry and applying them, was merged in 2015 into the Department of Chemical Engineering We are learning core materials and process technologies in the field and are concentrating on learning and developing new next-generation chemical materials and process technologies by applying them. The Department of Applied Chemical Engineering currently consists of 18 full-time professors, 170 master's and doctoral students, and 400 undergraduate students.

The School of Chemistry and Chemical Engineering, Queen's University, Belfast

QUEEN'S UNIVERSITY BELFAST | SCHOOL OF CHEMISTRY AND CHEMICAL ENGINEERING

we offer degrees in chemistry, medicinal chemistry, and chemical engineering, allowing students to choose a chemical sciences subject which suits them best, whilst at the same time providing an educational and research environment which is cross-disciplinary. Our degrees start from Foundation level and go all the way to Postgraduate Research. Chemists and chemical engineers work in partnership at the School, providing a unique environment which assists our work in making fundamental research discoveries, and our translation of these into real solutions for global challenges.

Our research falls under the broad headings of healthcare and sustainability, with examples of recently-funded keystone projects including those which seek to discover and develop new antibiotics, and reduce the presence of single-use plastics in our environment. The School also leads the Bryden Centre, which focuses on the development of renewable energy systems and infrastructure, as well as the Centre for Advanced Sustainable Energy, and is also home to a world-leading centre for ionic liquids research, QUILL. Our research activities, both theoretical and applied, directly informs our teaching, allowing students to train in a manner which equips them with cutting-edge skills, and prepares them to make a real difference.

CV and Abstract

Brief C.V.
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Experience in reverse chronological order (latest first)
08/2018 - present Professor of Energy and Environmental Engineering, Queen's University Belfast, UK 03/2016 - 08/2018 Head of School, School of Chemistry and Chemical Engineering Queen's University Belfast, UK 01/2015 - 03/2016 Professor of Chemical Engineering, Queen's University Belfast, UK 08/2012 - 12/2014 Vice-Principal and Pro Vice-Chancellor (Research and Academic Support Services), Robert Gordon University, Aberdeen, UK 09/2006 - 07/2012 Vice-Principal and Pro Vice-Chancellor (Research and Commercialisation), Robert Gordon University, Aberdeen, UK 07/2000 - 08/2006 Chair of Energy and Environmental Engineering and Director of the Centre for Research in Energy and the Environment, Robert Gordon University, Aberdeen, UK 09/1995 - 06/2000 Lecturer, School of Applied Sciences, Robert Gordon University, Aberdeen, UK
Education in reverse chronological order (latest first)
D.Sc. "Applications of Engineering for Environmental Sustainability", University of Ulster, 2013 D.Phil, "Photoelectrochemical Reductions using Quinone Radical Anions", University of Ulster, 1989 B.Sc (Hons), Combined Science: Chemistry with Economics, University of Ulster, 1986
Representative publications
1. Carlos J. Pestana, Jianing Hui, Dolores Camacho-Munoz , Christine Edwards, Peter K.J. Robertson, John.T.S. Irvine, Linda A. Lawton, "Solar-driven semi-conductor photocatalytic water treatment (TiO_2, g-C_3N_4, and TiO_2+g-C_3N_4) of cyanotoxins: Proof-of-concept study with microcystin-LR", Chemosphere, 2023, 310, 136828. 2 Christopher W. J. Murnaghan, Nathan Skillen, Bronagh Hackett, Jack Lafferty, Peter Robertson, Gary Sheldrake, "Towards the Photocatalytic Valorization of Lignin: Conversion of a Model Lignin Hexamer with Multiple Functionalities", ACS Sustainable Chemistry & Engineering, 2022, 10, 37, 12107–12116. 3 Nathan Skillen, Helen Daly, Lan Lan, Meshal Aljohani, Christopher W. J. Murnaghan, Xiaolei Fan, Christopher Hardacre, Gary N. Sheldrake and Peter K.J. Robertson, "Photocatalytic Reforming Of Biomass: What Role Will The Technology Play In Future Energy Systems", Topics In Current Chemistry, 2022, 33, 380. 4 Xinzhu Pang, Varaha P. Sarvothaman, Nathan Skillen, Zhe Wang, David W. Rooney, Vivek V. Ranade, Peter K.J. Robertson, "Kinetic Modelling Of The Photocatalytic Degradation Of Diisobutyl Phthalate And Coupling With Acoustic Cavitation," " Chemical Engineering Journal, 2022,444,136494

Abstract (Peter K. J. Robertson)

The Photocatalytic Destruction of Cyanotoxins in Water.

Peter K.J. Robertson[1],

Nathan Skillen, H.Q. Nimal Gunaratne[1], Linda A. Lawton[2] and John T.S. Irvine[3].

[1]School of Chemistry and Chemical Engineering, Queen's University Belfast, David Keir Building, Stranmillis Road, Belfast, BT9 5AG, UK
[2]School of Pharmacy and Life Sciences, Robert Gordon University, Garthdee Road, Aberdeen, Scotland, AB10 7GJ, UK
[3]School of Chemistry, University of St Andrews, North Haugh, St Andrews, Scotland, KY16 9ST, UK

Research in the field of photocatalytic reactor technology has been an area of extensive and diverse research activity over the past thirty years. Photocatalytic reactors have the potential versatility to be applied to the remediation of a range of contaminants in both potable and wastewater. Cyanobacterial toxins produced and released by cyanobacteria around the world have been well-documented. The incidence of cyanobacterial blooms in freshwaters, including drinking water reservoirs, has increased over the past few decades due to rising nutrient levels. Of most significant concern are the hepatotoxic microcystins and nodularins. Microcystins are a family of hepatotoxic peptides produced by freshwater cyanobacteria. Nodularins, produced by the cyanobacterium *Nodularia spumigena*, are structurally and biologically similar to microcystins and both groups of toxins are among the commonly found cyanobacterial toxins detected in water. It has been shown that the mode of action of these toxins at a molecular level is caused by the inhibition of serine/threonine protein phosphatases 1 and 2A. Chronic exposure due to the presence of hepatotoxic cyanotoxins in drinking water is thought to be a contributing factor in primary liver cancer (PLC) through the known tumour-promoting activities of these compounds. Since cyanobacterial toxins pose a considerable threat to human health, various water treatment processes have been evaluated to degrade these toxins. It is believed, however, that conventional water treatment systems may be unreliable for the removal of these toxins. TiO_2 photocatalysis has, nevertheless, proven to be an effective technology for removal of both these class of compounds from water. In this presentation the application of TiO_2 photocatalysis for the removal of these two cyanotoxins is reviewed and the efficacy of the technology as a treatment process for potable waters contaminated with such compounds is considered.

Brief C.V.
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Experience in chronological order
09/2018 - Chemistry Department, Chungnam National University 03/2016 - 03/2018 Professor in the current department, Department Head 09/2013 - Move to Department of Cogno-Mechatronics Engineering 03/2013 - 08/2013 Department Head, Department of Applied Nanoscience 03/2012 - 02/2013 Visiting Scholar, University of Michigan, Ann Arbor, MI. USA 03/2007 - 02/2011 Assistant Professor Director of World Class University (WCU) project (category III) Vice Director of Brain Korea (BK) 21 Nano Fusion Technology
Education in chronological order
2003 - 2007 Post-Doc, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, USA 1999 - 2003 PhD, The Robert Gordon University, Aberdeen, United Kingdom 1991 - 1998 BS, Department of Chemistry, Chungnam National University, Daejeon, South Korea
Representative publications
1. Nanoscale hydroxyapatite particles for bone tissue engineeringH Zhou, J Lee Acta biomaterialia 7 (7), 2769-2781 2. Gold nanoparticle ensembles as heaters and actuators: melting and collective plasmon resonances, AO Govorov, W Zhang, T Skeini, H Richardson, J Lee, NA Kotov, Nanoscale Research Letters 1, 84-90 3. Exciton-plasmon interaction and hybrid excitons in semiconductor-metal nanoparticle assemblies, Nano letters 6 (5), 984-994 4. Bioconjugates of CdTe nanowires and Au nanoparticles: plasmon-exciton interactions, luminescence enhancement, and collective effects, Nano Letters 4 (12), 2323-23 5. Exciton–plasmon interactions in molecular spring assemblies of nanowires and wavelength-based protein detection, Nature materials 6 (4), 291-295, 2007 6. Light-controlled self-assembly of semiconductor nanoparticles into twisted ribbons Science 327 (5971), 1355-1359

Abstract (Jaebeom Lee)

Magnetoplasmonic nanoassembly: chiroptical properties and biomedical/energy applications

Jaebeom Lee

Department of Chemistry, Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, 34134, Korea

One-dimensional hybrid nanostructures composed of a plasmonic gold nanowire core covered by a shell of magnetic oxide nanoparticles (Au@FexOy NWs) were synthesized by a one-pot solvothermal synthesis process. The effects of reaction temperature, time, reducing agent, and precursor as well as postsynthesis treatment were optimized to produce highly uniform NWs with a diameter of 226 ± 25 nm and a plasmonic core aspect ratio of 25 to 82. By exploiting the interaction of NWs with an external magnetic field, precise arrangements into highly periodic photonic structures were achieved, which can generate distinctive structural colors that are vividly iridescent and polarization-sensitive. Furthermore, a Bouligand-type chiral nematic film consisting of multistacked unidirectional layers of achiral NWs was fabricated using a modified layer-by-layer deposition method, which displays circular dichroism (CD) and chiral sensing capability. The addition of bovine serum albumin (BSA) as a model protein analyte induced a concentration-dependent wavelength shift of CD peaks. These intriguing properties of magnetoplasmonic anisotropic NWs and their self-assemblies could be consequently valuable for developing nature-inspired structural color imprints as well as solid-state chiral sensing devices.

Brief C.V.
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Experience in reverse chronological order (latest first)
03/2021 - Present Assistant professor in the Department of Chemical Engineering and Applied Chemistry at Chungnam National University, Daejeon, Republic of Korea 03/2018 - 02/2021 Postdoctoral associate in Chair of Process Systems Engineering (AVT.SVT) at RWTH Aachen University, Aachen, Germany Advisor (Advisor: Prof. Alexander Mitsos) 03/2017 - 02/2018 Postdoctoral associate in the Department of Chemical and Biomolecular Engineering at the Korea Advanced Institute of Science and Technology(KAIST), Daejeon, Republic of Korea (Advisor: Prof.Jay H.Lee) 05/2014 - 11/2014 Visiting researcher in the Department of Chemical and Biochemical Engineering at Technical University of Denmark (DTU), Lyngby, Denmark (Advisor: Prof. Rafiqul Gani)
Education in reverse chronological order (latest first)
09/2011 - 02/2017 Ph. D. in the Department of Chemical and Biomolecular Engineering at the Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Republic of Korea (Advisor: Prof. Jay H. Lee) 02/2007 - 08/2011 B. Sc. in the Department of Chemical and Biomolecular Engineering at the Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Republic of Korea
Representative publications
1. Chung, et int, Roh and Lee, 2022. Computer-aided identification and evaluation of technologies for sustainable carbon capture and utilization using a superstructure approach. J. CO2 Util. 61, 102032 2. Fahr, et int, Parra-Saldivar, Mansouri and Roh, 2022. Mobile On Demand COVID-19 Vaccine Production Units for Developing Countries. Ind. Eng. Chem. Res. 61(35), 13191–13204 3. Roh, et int, Lee and Mitsos, 2020. Early-stage evaluation of emerging CO2 utilization technologies at low technology readiness levels. Green Chem. 22, 3842–3859 4. Roh, et int, Mitsos, 2019. Flexible operation of switchable chlor-alkali electrolysis for demand side management. Appl. Energy 255, 113880 5. Roh, et int, Gani and Lee, 2016. A methodology for the sustainable design and implementation strategy of CO2 utilization processes. Comput. Chem. Eng. 91, 407–421

Abstract (Kosan Roh)

Sustainability analysis and optimization of CCUS technologies using process systems engineering methods

Kosan Roh

Department of Chemical Engineering and Applied Chemistry,
Chungnam National University, Daejeon, Republic of Korea

Excessive anthropogenic greenhouse gas (GHG) emissions have disrupted the global carbon cycle leading to global warming and climate change. Carbon capture, utilization, and storage (CCUS) is expected to play a significant role in reducing the anthropogenic GHG emissions to curb global warming and climate change. CCUS refers to technologies and processes that capture CO2 in a high concentration from flue gases or air and utilize it either directly as carbon compounds in materials or energy carriers or store CO2 in the ground. Due to these advantages, CCUS technologies have been actively studied and also the corresponding R&D has funded by government and industry substantially. More than 100 different chemicals are known to be made from CO2. Also, for a given chemical product, various technologies for CO2 conversion could be applied such as thermochemical, electrochemical, and biological conversion. Therefore, it is critical to rapidly evaluate such a large number of technical candidates for CCUS and identify promising technologies to guide R&D investment. This talk is mainly about systematic and reliable analysis, evaluation, and optimization of CCUS technologies using systems engineering approach. Also, a number of case studies are introduced to demonstrate the ideas presented.

Brief C.V.
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Experience in chronological order
2020 Dean of Internationalisation (EPS) 2012 - Present Professor of Chemical Engineering 2014 - 2017 Vice-dean China Medical University – Queen's College (CQC) 2014 - Present Vice-Chancellors Envoy to China 2012 - 2013, 2016 - 2019 Head of Chemical Engineering Teaching 2009 - 2016 Director of Research (CenTACat) 2016 - Present Director of Sustainable Energy Research Programme 10/2004 - 10/2012 Senior lecturer, School of Chemistry and Chemical Engineering, Queen's University Belfast
Education in chronological order
2002 PGCHET, Queen's University Belfast 1998 PhD Chemical Engineering, Queen's University Belfast 1994 BEng (2.1) Chemical and Food Engineering, Queen's University Belfast
Representative publications
1. Energy Science & Engineering [2022], 10.1002/ese3.1063 2. Renewable & Sustainable Energy Reviews (2021), 10.1016/j.rser.2021.111677 3. Industrial & Engineerign Chemistry Research (2021), 10.1021/acs.iecr.1c01989 4. Energy Economics (2021), 10.1016/j.eneco.2021.105360 5. Chemical Engineering Journal (2021), 10.1016/j.cej.2021.128475 6. Renewable Energy (2021), 10.1016/j.renene.2021.02.027 7. Journal of Energy Chemistry (2021), 10.1016/j.jechem.2020.06.060 8. ACS Applied Materials and Interfaces (2021), 10.1021/acsami.0c19044

Abstract (David Rooney)

Systems approaches to biochar production and valorization of agricultural resources

David Rooney

David Rooney, Ahmed Osman, Samer Fawzy, Stuart James, Queen's University Belfast

In the context of climate change, there is an urgent need for rapid and efficient methods to capture and sequester carbon from the atmosphere. For instance, production, use and storage of biochar are highly carbon negative, resulting in an estimated sequestration of 0.3–2 Gt CO2 $year^{-1}$ by 2050. Yet, efficient biochar production requires enhanced knowledge on feedstocks, thermochemical conversion and end applications. Within, the presentation we will discuss these issues including their impact on the design and development of biochar and complementary systems. Comparisons will be made between the major commercialized technologies offering atmospheric carbon removal including forestation, direct air carbon capture utilization and storage, soil carbon sequestration, wooden building elements and biochar. To achieve success process optimization is imperative to produce an end product that meets application-specific requirements, environmental regulations and achieve ultimate stability for carbon sequestration purposes. The talk will further explore how such systems can be implemented within specific regions to maximise the use of resources and deliver secondary benefits. Here Northern Ireland serves as an interesting case study to evaluate how biochar can complement biomethane from manure and silage material to displace natural gas. Northern Ireland was choses due to the high agricultural intensity, the low penetration of gas relative to the wider UK and the modern pipeline infrastructure. The study includes spatial mapping of biomethane yield and life cycle assessment for processing scenarios. The results demonstrate that current manure management i.e., storage and application of manure to grassland, results in 344 kg CO_2 equivalent/person of greenhouse gases and 9.7 kg/person of ammonia being emitted. In a second scenario where collected manure and underutilised grass silage is routed to anaerobic digestion, the estimated net energy produced is 6124 GWh, with −464 kg CO2 equivalent/person. A third scenario, combining anaerobic digestion and pyrolysis, also produces 6124 GWh and 200 kilo tonnes of biochar (retaining 64% of manure phosphorus), −563 kg CO2 equivalent/person. Finally the talk will demonstrate how new and emerging technologies which can further support this nascent industry. In particular we will show results from work investigating novel CO_2 capture. We will show that current CO_2 separation technologies by liquid solvents suffer from either high regeneration costs or low selectivity/capacity of the solvent. However by dispersing ca. 12.5 wt% CO_2-selective zeolite rho solid into the commercial CO_2 capture solvent Genosorb® converts it into a porous liquid with at least 2.5 times greater CO_2 capacity and CO_2/CH_4 selectivity compared to Genosorb® itself. This is predicted to result in more economical separation processes, particularly for biogas upgrading. Overall the talk aims to demonstrate how systems approaches can maximise the value of the wider supply chain.

Brief C.V.
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Experience in chronological order
01/2023 - Present Postdoctoral fellow, Department of Chemical Engineering and Applied Chemistry, Chungnam National University Daejeon, South Korea 01/2021 - 09/2022 Postdoctoral fellow, Department of Chemical engineering, Ben – Gurion University of the Negev, Beer Sheva, Israel 05/2018 - 12/2020 Kreitman postdoctoral fellow, Ben-Gurion National Solar Energy Center, Department of Solar Energy and Environmental Physics, Ben-Gurion University of the Negev, Midershet Campus, Midershet, Israel
Education in chronological order
Doctor of Philosophy (Ph.D., 2018) Department of Physics, Indian Institute of Technology (IIT) Delhi, New Delhi, India, Thesis Title "Investigation of PEDOT:PSS/Si Heterojunctions and Graphene/Si Schottky Diodes for Potential Application in Photovoltaics" Master of Technology (M. Tech., 2011), (Advanced Materials Science and Technology) Gold Medalist for securing highest CGPA, CGPA 9.49, National Institute of Technology (NIT) Durgapur, India. Thesis Title "Synthesis and Characterization of ZnS Nano particles by Mechano-chemical Route
Representative publications
1. Yuval Harari, C.S. Pathak, Eran Edri, Molecular Relays in Nanometer Scale Alumina: Effective Encapsulation for Water-Submersed Halide Perovskite Photocathodes, *Nanoscale,* (2023) 2. C.S. Pathak*, "Probing the photo degradation of MAPI perovskite with concentrated sunlight" *Optical Materials*, 133, (2022) 113012 3. C.S. Pathak*, G. Paramasivam, F. Mathies, K. Hirselandt, O. Maus, J. Dagar, C. Klimm, Eva L. Unger, Iris Visoly-Fisher, "PTB7 as an ink-additive for spin-coated versus inkjet-printed perovskite solar cells" *ACS Applied Energy Materials,* 5, 4 (2022) 4085-4095 4. Stav Alon, Mayaan Siohmer, C.S. Pathak, Iris Visoly-Fisher, Lioz Etgar, "Photovoltaic recovery of all printable mesoporous carbon-based perovskite solar cells" *Solar RRL* 5,4 (2021) 2100028 5. C.S. Pathak*, J.P. Singh and R. Singh, "Optimizing the electrical properties of PEDOT:PSS films by co-solvents and their application in polymer photovoltaic cells" *Applied Physics Letters,* 111,10, (2017) 102107- 5

Abstract (Chandra Shakher Pathak)

PTB7 as an ink-additive for spin-coated vs inkjet-printed perovskite solar cells

Chandra Shakher Pathak

Department of Chemical Engineering and Applied Chemistry,
Chungnam National University Daejeon, South Korea

We report on the fabrication and optimization of triple cation perovskite solar cells from inks containing the polymer PTB7 as an additive, comparing spin-coating and inkjet printing as deposition methods. Spin-coated devices exhibited maximum power conversion efficiency of 17.75% but showed little difference between samples with and without the polymer ink additive. For inkjet-printed devices, the combined optimization of printing parameters and the amount of the polymer additive in the precursor ink enabled a perovskite layer with increased quality. In comparison, devices with added PTB7 improved the power conversion efficiency to 10.35% as compared to 8.0% for cells prepared without the polymer additive. The effect is attributed to the modified crystallization dynamics of perovskite layer by the PTB7 addition after inkjet printing, and improved quality of the resulting perovskite layers. We found that the effect of the polymer additive on film formation in spin-coated samples was obscured when using an anti-solvent drip, but the incorporation of PTB7 has a positive effect on the opto-electronic quality of thin films indicated by increased grain size and photoluminescence quantum yield. Our results emphasize the technological potential of polymer additives in perovskite precursor inks, when using scalable manufacturing processes, such as inkjet printing, where the control and induction of controlled crystallization is more difficult to implement by additional quenching steps.

Brief C.V.	
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Experience in reverse chronological order (latest first)	
10/2021 - present	PhD student, Chemistry, Queen's University Belfast, Northern Ireland, UK.
01/2020 - 09/2021	Chemist, McQuillan Environmental, Northern Ireland, UK.
07/2017 - 12/2019	Synthetic Organic Chemist, Almac Sciences Ltd, Northern Ireland, UK.
06/2015 - 06/2016	Bioconjugation Chemist (University placement), Randox Laboratories Ltd, Northern Ireland, UK.
Education in reverse chronological order (latest first)	
09/2021 - present	PhD student, Chemistry, Queen's University Belfast, Northern Ireland, UK. Thesis: The Development of an in-situ multi-analyte Water Sensor.
09/2012 - 07/2017	MSci Medicinal Chemistry with Industry (1st Class Honours), Queen's University Belfast, Northern Ireland, UK. Thesis: The Catalytic Asymmetric Alkylation of α-Branched Aldehydes.
Representative publications	
N/A	

Abstract (Ryan McGhee)

The Development of an in-situ BTEX Water Sensor

Ryan McGhee[b]

Prof. Peter Robertson,[b] Prof. Steven Bell,[b] and Prof. Daniel McStay,[a]
Inov8 Systems Ltd, 6 Edgewater Road, Belfast, BT3 9JQ, Northern Ireland, UK.[a]
School of Chemistry and Chemical Engineering, Queen's University, Belfast, BT9 5AG, Northern Ireland, UK.[b]

BTEX and PAH are major components of crude and refined oils, which become contaminants in many water systems due to ongoing produced water discharge and oil spillages. These compounds have been shown to cause deleterious health effects at trace levels in humans. Therefore, it is imperative that a reliable and portable means of detection can be developed so that these compounds can be discovered at their source of contamination, which will usher in strict regulative systems to define strategies for BTEX/PAH contamination.

This presentation outlines the current research surrounding the development of a portable sensor for BTEX, which is one of the most critical water analytes that requires an in-situ solution. This is a collaborative project based between Inov8 Systems Ltd and the School of Chemistry and Chemical Engineering at Queen's University Belfast.

Inov8 Systems Ltd specialises in the development of online oil-in-water analysers that can be used in a variety of water bodies, and are fitted with robust protective housing to withstand demanding temperatures and pressures. Their core products utilise a 405 nm laser as an excitation light source on crude oil/water samples which then emit in the 500 nm range and beyond. The components of crude oil can be detected and equated to a concentration value based on a calibration curve. A deep-UV option is also offered within the EXP analyser that excites finer oils such as petroleum, diesel and hydraulic oils at 280 nm. These oils emit into and above 350 nm wavelength range, and detection limits range from 1 ppb to 10,000 ppm. The application of Inov8's unique RapidWave ultrasonics ensures that the optical window remains clean to provide accurate and reliable results at all times.

At the early stages of the project, much of the work focused on the characterisation of BTEX fluorescence spectra using a high resolution spectrofluorometer. These results were then used to design and assemble a compact fluorescence sensor, using deep-UV LED excitation and a miniature spectrometer for detection. Ongoing progress is reported here and many steps have been made towards understanding the benefits and limitations of the current hardware. We also report results from studies on the impact of varying sample handling parameters on the status of samples and the fluorescence measurements from said samples. The results from this work have enabled improved sample acquisition and handling protocols to be developed, thus enhancing the quality of the sensor data generated.

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Experience in chronological order

2019 - Present	Assistant Professor, Adama Science and Technology University, Ethiopia
2022 - Present	Researcher Professor, Institute of Materials Chemistry, Chungnam National University, Korea
2019 - 2020	Postdoctoral Researcher, Institute of Materials Chemistry, Chungnam National University, Korea
2011 - 2013	Lecturer, Adama Science and Technology University, Ethiopia

Education in chronological order

2014 - 2019	Ph.D. in Nano Fusion Technology, Colledge of Nanoscience and Vanotechnology, Pusan National University, Korea
2004 – 2010	B.Sc. in Chemistry and M.Sc. in Physical, Jimma University, Ethiopia.

Representative publications

1. Molla,C.F., Gonfa, B.A.,Sabir,F.K., Gicha,B.B., Nwaji, N., <u>Tufa, L.T.*</u>, Lee, J.*.Ni-Based Ultrathin Nanostructures for Overall Electrochemical Water Splitting. *Materials Chemistry Frontiers*,2023
2. Tufa, L.T., Tran, V.T., Jeong, K.J., Gicha, B.B., Gonfa, B.A. and Lee, J.* Electrochemical Investigation of Porosity in Core–Shell Magnetoplasmonic Nanoparticles. *The Journal of Physical Chemistry Letters*, 2022, *13*(26), pp.6085-6092.
3. Gicha, B.B., Tufa, L.T., Goddati, M., Adhikari, S., Gwak, J. and Lee, J.* Non□Thermal Plasma Assisted Fabrication of Ultrathin NiCoOx Nanosheets for High□performance Supercapacitor. *Batteries & Supercaps*. 2022
4. Gicha, B.B., Tufa, L.T., Choi Y., Lee, J.* Synergistic Effect of Bulk and Surface Fe in $Ni_{1x}Fe_{x}$ Oxyhydroxide Nanosheets for Highly Efficient and Stable Oxygen Evolution Reaction. *ACS Applied Energy Materials*, June 22, 2021
5. Tufa, L.T., Gicha, B.B., Wu, H., Lee, J.* Fe-Based Mesoporous Nanostructures for Electrochemical Conversion and Storage of Energy. *Batteries & Supercaps,* 2020, *3*, pp.1 –17. Including Cover Feature: 2021*,* 4(3), pp.429-444.
6. Gurmessa,S.K.,¶ Tufa,L.T.,¶ Kim,J., Lee,K-I., Kim,Y-M., Tran,V.T., Nguyen,H-N., Shim,T.S., Kim,J., Park,T.J., Lee,J.*, and Kim, H-J.* Colorimetric Detection of Mycobacterium tuberculosis ESX-1 Substrate Protein in Clinical Samples Using Au@Pd NanoparticleBased Magnetic Enzyme-Linked Immunosorbent Assay. *ACS Applied Nano Materials,* 2021, 4 (1) pp 539–549.

Abstract (Lemma Teshome Tufa)

Trimetallic-NiCoFeOx Ultrathin Nanostructures for Electrochemical Energy Conversion and Storage

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The process of large scale hydrogen production and supercapacitors entails highly active and stable electrocatalysts for electrochemical energy conversion and storage. The engineering of electrocatalysts' electronic structures and surface properties can improve their catalytic and energy storage performances. Thus, the construction of a highly active and cost-effective catalyst with abundant oxygen vacancies is critical to enhancing reaction efficiency and decreasing required overpotential. Due to earth-abundance and electrocatalytic activities, Ni-based ultrathin Nanostructures (Ni-utNSs) have attracted immense attention for overall water splitting and energy storage. Herein we present electrochemical, Ar-plasma, and hydrothermal synthesis approaches and green exfoliation strategy to obtain a boundary defect-rich ultrathin bi/trimetallic oxy/hydroxide nanosheets network of NiCoOx/NiCoFeOx. Detailed information on Ni-utNSs is presented, including their properties and crystal structure, manufacturing techniques, as well as in-situ and ex-situ characterization, and computer modeling. This work can help researchers understand the Ni-utNS catalyst's recent progress and get insight into the rational design of Ni-utNS catalysts with high electrocatalytic and energy storage activities.

Keywords: Ni-based Nanostructures, Ultrathin, Water splitting, supercapacitor, Oxygen vacancy

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09/1997 - 01/2002 Ph. D. in the Department of Chemistry at the University of California, Davis, California, USA (Advisor: Dr. Mark J. Kurth) 03/1991 - 02/1993 M. Sc. in the Department of Chemistry at Korea University, Seoul, Korea (Advisor: Dr. Bong Young Chung) 03/1987 - 02/1991 B. Sc. in the Department of Chemistry at Korea University, Seoul, Korea (Advisor: Dr. Bong Young Chung)
Representative publications
1. Lim, Y. S.; Yoo, S.-M.; Patil, V.; Kim, H. W.; Kim, H.-H.; Suh, B.; Park, J. Y.; Jeong, N.-R.; Park, C. H.; Ryu, J. H.; Lee, B.-H.; Kim, P.*; Lee, S. H.*, “Orally bioavailable BTK PROTAC active against wild-type and C481 mutant BTKs in human lymphoma CDX mouse models” Blood Adv. 2023, Jan. 10, 7, 92-105. 2. Hyesu Yeom, Raghavendra Achary, Yunha Choi, Chi Hoon Park, Joo-Youn Lee, Heung Kyoung Lee, Pilho Kim*, Sung Yun Cho*; Pyrazolo[3,4-d]pyrimidine derivatives as irreversible Bruton’s tyrosine kinase inhibitors. Bull. Korean Chem. Soc. April 6, 2022, 43 (4), 577-584. 3. Yunha Choi, Sang Hee Ji, Vineet Patil, Eun Hye Kim, Hoyeong Park, Seong Hwan Kim, Pilho Kim*; Discovery of harmalanium halides as anti-ovarian cancer agents. Bull. Korean Chem. Soc. April 6, 2022, 43 (4), 559-563

Abstract (Pilho Kim)

Discovery of Orally Available BTK Degraders Potent in Murine Xenograft Models Utilizing Wild-Type and C481S Mutant BTKs

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Inhibition of B-cell receptor (BCR) signaling pathways could be considered well-validated strategies for the treatment of chronic lymphocytic lymphoma (CLL), mantle cell lymphoma (MCL), and other B-cell related cancers. In this context, Bruton's Tyrosine Kinase (BTK) plays an important role in BCR pathway and its activation leads to growth, survival, and proliferation of leukemic B-cells. Hence, targeting BTK has proven to be a practical way for the treatment of hematological tumors. Ibrutinib, the first approved irreversible BTK inhibitor in 1993, deactivates BTK by covalently binding with the C481 present in the ATP binding site of BTK, providing a breakthrough therapy in the treatment of leukemia and lymphomas. Along with ibrutinib, FDA has approved acalabrutinib and zanubrutinib in 2017 and 2019, respectively, as irreversible BTK inhibitors for the treatment of MCL and CLL. However, due to the C481 mutations in the binding site of BTK, the patients treated with irreversible BTK inhibitors acquire resistance leading to tumor progression. Therefore, a novel approach, such as reversible inhibitors or PROteolysis-TArgeting Chimeras (PROTACs), could be solutions to overcome this issue.

Contrary to the small molecule inhibitors, PROTACs are heterobifunctional molecules, which degrade the target protein by hijacking natural ubiquitin proteasome system (UPS). A typical PROTAC compound is composed of a target protein binder, E3 ligase binder, and a linker that connects both of the binders. In 2019, two clinical trials were launched using protein degraders, ARV-110 and ARV 471 by Arvinas. While ARV-110 is targeting androgen receptor for the treatment of prostate cancer, ARV-471 is targeting estrogen receptor for breast cancer. Currently, clinical trials are underway with 2 BTK degraders, NX-2127 and BGB-16673 by Nurix and Beigene, respectively.

Through collaboration with Ubix Therapeutics, our team has designed and synthesized novel BTK degraders which have shown activity in both wild type and diverse mutant BTKs. Among them, TD-1082 showed in vitro activities far better than those of a reported BTK degrader, MT-802. We also found that TD-1082 had superior pharmacokinetics and *in vivo* efficacy in murine xenograft models, compared with ibrutinib and other reported BTK degraders. In this lecture, our journey to discover TD-1092 will be discussed.

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03/2023 - Present Assistant Professor, Chungnam National University 09/2019 - 01/2023 Directors Postdoctoral Fellow, Los Alamos National Laboratory 01/2019 - 09/2019 Postdoctoral Research Associate, Los Alamos National Laboratory 03/2018 - 12/2018 Postdoctoral Research Associate, Seoul National University
Education in reverse chronological order (latest first)
03/2014 - 02/2018 Ph.D., School of Chemical & Biological Engineering, Seoul National University Advisor Professor Youn-Woo Lee / Professor Won Bo Lee Thesis Statistical methods for the description of the structural transition in supercritical fluids 03/2007 – 09/2013 B.Sc., School of Chemical & Biological Engineering, Seoul National University
Representative publications
1. Yoon, T. J., Maerzke, K. A., Currier, R. P., & Findikoglu, A. T. (2023). PyOECP: A flexible open-source software library for estimating and modeling the complex permittivity based on the open-ended coaxial probe (OECP) technique. Computer Physics Communications, 282, 108517. 2. Yoon, T. J., Sharan, P., Craddock, E. P., Lewis, J. C., Matteson, J. A., Seong, J. G., ... & Findikoglu, A. T. (2022). Selective recovery of critical materials in zero-liquid discharge supercritical water desalination. Desalination, 537, 115849. 3. Yoon, T. J., Vigil, M. J., Raby, E. Y., Singh, R. P., Maerzke, K. A., Currier, R. P., & Findikoglu, A. T. (2020). Dielectric relaxation of neodymium chloride in water and in methanol. Journal of Molecular Liquids, 308, 112981. 4. Yoon, T. J., Craddock, E. P., Maerzke, K. A., Currier, R. P., & Findikoglu, A. T. (2022). Electrical Conductivities and Association Constants in Dilute Aqueous NdCl3 Solutions from 298 to 523 K along an Isobar of 25 MPa. Journal of Chemical & Engineering Data, 67(3), 568-579. 5. Yoon, T. J., Ha, M. Y., Lazar, E. A., Lee, W. B., & Lee, Y. W. (2018). Topological characterization of rigid–nonrigid transition across the Frenkel line. The Journal of Physical Chemistry Letters, 9(22), 6524-6528.

Abstract (Tae Jun Yoon)

Experimental and Theoretical Study on the Technical Feasibility of Supercritical Water Desalination as a Selective Zero-liquid Discharge Process

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Supercritical water desalination is one of the promising technologies that can remove salts from saline water without discharging any concentrated brines. In this process, the brine's temperature and pressure are elevated above the critical point of pure water (374 and 221 bar) so that the salts are precipitated or concentrated in the brine. The concentrated liquid collected at the bottom of the cell is depressurized, resulting in the formation of steam and dry salts.

Compared to conventional zero-liquid discharge techniques, this technology has several advantages, including lower energy consumption with high-concentration inputs, high efficiency, and the ability to treat a variety of resources. Moreover, considering that the salt solubility in water is sensitive to the local aqueous environment (e.g., dielectric constant), this technique has a great potential to be utilized for recovering strategic elements (e.g., lithium, cobalt, manganese, rare earth elements, gold, etc.) while removing common salts.

Despite these promising aspects, some areas of research still require further investigation before this technology can be implemented on an industrial scale. Specifically, our understanding of the aqueous electrolyte system over a wide range of thermodynamic conditions still needs to be completed.

In this talk, we would like to address a recent series of our theoretical and experimental works to examine the potential of the supercritical water desalination technique as a selective zero-liquid discharge technology. We measured the complex conductivities of aqueous neodymium chloride solutions by installing and operating an in-situ conductometric cell and supercritical water desalination process. Based on a state-of-art Monte Carlo technique and molecular dynamics simulations, the obtained conductivity spectra were analyzed to calculate the thermodynamic and dynamic properties of neodymium salts in mixed electrolytes. These theoretical and experimental efforts were combined to interpret the precipitation behavior of neodymium salts in electrolyte solutions during the supercritical water desalination process.

All results suggest that supercritical water desalination can be a promising technique for recovering neodymium as a hydroxide salt while removing common salts without any liquid discharge.

Brief C.V.

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Experience in reverse chronological order (latest first)

2022 - Present	Lecturer & Programme Director (MSc Net Zero Engineering), QUB
2021 - 2022	UKRI Supergen Bioenergy Hub Research Fellow, QUB
2020 - 2021	Post-Doctoral Research Associate, University of Manchester
2017 - 2020	Post-Doctoral Research Associate, QUB
2013 - 2017	Post-Doctoral Research Associate, Robert Gordon University

Education in reverse chronological order (latest first)

2009 - 2013	PhD at the Centre for Research into Energy and the Environment (CRE+E), Robert Gordon University. Title: Directly enhancing the photocatalytic transformation of CO_2 and water to renewable fuels. EPSRC funded incollaboration with University of St. Andrews and California Institute of Technology
2005 - 2009	BSc (first class, first division) in Biology with Molecular Biosciences, Robert Gordon University

Representative publications

1. Skillen, N., Daly, H., Lan, L., Aljohani, M., Murnaghan, C. W. J., Fan, X., Hardacre, C., Sheldrake, G. N., & Robertson, P. K. J., 2022. 'Photocatalytic Reforming of Biomass: What Role Will the Technology Play in Future Energy Systems'. Topics in Current Chemistry (I.F 9.06, 4 citation)
2. Murnaghan C., Skillen, N., Hackett B., Lafferty J.H., Robertson, P.K.J. & Sheldrake G., 2022 'Towards the Photocatalytic Valorization of Lignin: Conversion of a Model Lignin Hexamer with Multiple Functionalities' ACS Sustainable Chemistry & Engineering (I.F. 9.224))
3. Murnaghan, C. W. J., Skillen, N., Hardacre, C., Bruce, J., Sheldrake, G. N., & Robertson, P. K. J. 2021. 'Exploring lignin valorisation: the application of photocatalysis for the degradation of the β-5 linkage'. Journal of Physics: Energy (I.F 7.56, 7 citations)
4. Pang X., Skillen N., Gunaratne H.Q.N., Rooney D., Robertson P.K.J., 2021 'Removal of Phthalates from Aqueous Solution by Semiconductor Photocatalysis; A review' Journal of Haz Mat (I.F 10.588, 67 citations)
5. Osman I.A., Skillen N., Robertson P.K.J., Rooney D., Morgan K., 2020 'Exploring the photocatalytic hydrogen production potential of titania doped with alumina derived from foil waste', Intl. J. Hydrogen Energy (I.F 7.139, 28 citations)
6. Kelly, J., Morrison, G., Skillen, N., Manesiotis, P. & Robertson, P.K.J., 2019, 'An investigation of the role of pH in the rapid photocatalytic degradation of MCPA and its primary intermediate by low-power UV LED irradiation', Chemical Engineering Journal (I.F 16.744, 21 citations)
7. McCullagh, C., Skillen, N., Adams, M., Robertson, P.K.J., 2011. 'Photocatalytic Reactors for Remediation: A Review' Journal of Chemical Technology and Biotechnology (I.F 3.709, 291 citations)

Abstract (Nathan Skillen)

Photocatalytic Biomass Reforming: *steps towards advancing the technology*

Nathan Skillen*[a], Peter Robertson[a], Gary Sheldrake[a], Chris Murnaghan[a], Helen Daly[b], Christopher Hardacre[b], Padraig McDonagh[c] & Denis McCrudden[c]

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Photocatalytic reforming of biomass has emerged as an area of significant interest within the last decade. The number of papers published in the literature has been steadily increasing with keywords such as ‘hydrogen’ and ‘visible’ becoming prominent research topics. There are likely two primary drivers behind this, the first of which is that biomass represents a more sustainable photocatalytic feedstock for reforming to value-added products and energy. The second is the transition towards achieving net zero emission targets, which has increased focus on the development of technologies that could play a role in future energy systems. Therefore, this presentation provides an overview of the work conducted within the Photocatalytic Technology Research Group at QUB in relation to the reforming of biomass. Producing energy via photocatalytic biomass reforming is very desirable due to the ambient operating conditions and potential to utilize renewable energy (e.g., solar) with a wide variety of biomass resources. As both interest and development within this field continues to grow, however, there are challenges being identified that are paramount to further advancement. Our work is primarily focused on two key research streams: improving our fundamental understanding of the reforming process and developing technology platforms for energy production. These research priorities underpin the enhancement of photocatalytic technology with a view towards improving the technology readiness level and promoting engagement between academia and industry.