



MINISTRY OF  
EDUCATION AND  
SCIENCE



nano<sup>o</sup> | CENTER FOR  
NANOSCIENCE AND  
NANOTECHNOLOGY



# NOMATECH ICMSN-2024

INTERNATIONAL CONFERENCE ON MATERIALS  
SCIENCE AND NANOTECHNOLOGY

ULAANBAATAR, MONGOLIA | JULY 8-9

# BOOK OF ABSTRACTS

7-9 JULY, 2024

## **WELCOME**

### ***Distinguished guests,***

We are grateful that so many international and domestic experts have accepted our invitation to attend in the International Conference on Material Science and Nanotechnology. I warmly welcome each and every one of you.

This International Conference on Material Science and Nanotechnology is especially crucial to achieving our purpose since it provides an exceptional chance to meet colleagues who share our interests and learn from the world's leading experts in the subject. We believe that combining such academic activities with enjoyable times of cultural and social events will create an unforgettable memory for each participant. ICMSN is pleased to provide this unique opportunity to all of you.

The Conference has attracted 84 participants from 7 countries. We will hear 33 oral presentations including 4 plenary lectures, and have an opportunity to see about 50 poster presentations.

Lastly, on behalf of the Scientific Committee of the International Conference on Material Science and Nanotechnology, I wish you all the best in your work and a wonderful stay in Mongolia.



### **GANZORIG Chimed**

Director, Center for Nanoscience and Nanotechnology  
Professor, Department of Chemical and Biological Engineering  
School of Engineering and Technology  
National University of Mongolia



## CONFERENCE COMMITTEES

### Scientific committee

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- Batjargal B. National University of Mongolia
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- Baasansukh B. Mongolian University of Life Sciences
- Battsengel B. German-Mongolian Institute for Resources and Technology
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- Odkhuu D. Incheon National University
- Ganbaatar T. University of Cambridge
- Munkhbayar B. Griffith University
- Battulga M. Technical University of Denmark
- Chinzorig B. Mongolian National Mining Association

### Working group



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## THE CONFERENCE

The core objectives of the NomaTech ICMSN-2024 are to delve deep into the most recent innovations, research, and applications in both material science and nanotechnology, showcasing the forefront of global scientific advancements and also playing a pivotal role in amplifying local collaborations within Mongolia. By providing a platform where Mongolian researchers, institutions, and industry experts could interact directly with international counterparts, the conference has fostered an environment conducive to collaborative partnerships.

## CONFERENCE VENUE

National University of Mongolia – Academic Senate Hall

The Academic Senate Hall at the National University of Mongolia (NUM) is part of the university's main administrative and academic structures. Located in Ulaanbaatar, NUM is the oldest and most prestigious university in Mongolia, founded in 1942. The university offers a wide range of programs and has several schools and research centers under its umbrella.

The Academic Senate plays a crucial role in the governance of NUM, involving faculty, researchers, and administration in decision-making processes. The university's main campus is situated in Sukhbaatar District, which is also home to various other faculties and administrative buildings.



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# Speakers

## Plenary speakers

### Sir Konstantin Sergeevich Novoselov



Sir Konstantin 'Kostya' Novoselov FRS was born in Russia in August 1974. He is best known for isolating graphene at The University of Manchester in 2004, and is an expert in condensed matter physics, mesoscopic physics and nanotechnology. Every year since 2014 Kostya Novoselov is included in the list of the most highly cited researchers in the world. He was awarded the Nobel Prize for Physics in 2010 for his achievements with graphene. Kostya is a director of the Institute for Functional Intelligent Materials and holds a position of a Tan Chin Tuan Centennial

Professor at the National University of Singapore. He is also part time Langworthy Professor of Physics and the Royal Society Research Professor at The University of Manchester.

He graduated from the Moscow Institute of Physics and Technology, and undertook his PhD studies at the University of Nijmegen in the Netherlands before moving to The University of Manchester in 2001. Later Professor Novoselov joined the National University of Singapore in 2019. Professor Novoselov has published more than 400 peer-reviewed research papers. He was awarded with numerous prizes, including Nicholas Kurti Prize (2007), International Union of Pure and Applied Science Prize (2008), MIT Technology Review young innovator (2008), Europhysics Prize (2008), Bragg Lecture Prize from the Union of Crystallography (2011), the Kohn Award Lecture (2012), Leverhulme Medal from the Royal Society (2013), Onsager medal (2014), Carbon medal (2016), Dalton medal (2016), Otto Warburg Prize (2019), John von Neumann Professor from the John von Neumann Computer Society (2022) among many others. He was knighted in 2010 as Knight Commander of the Order of the Netherlands Lion and knighted in 2012 as Knight Bachelor in the United Kingdom New Year Honours for services to science.

### Joe Shapter



Dr. Joe Shapter received his PhD from the University of Toronto in 1990. He subsequently held a NSERC Fellowship at The University of Western Ontario before moving to Australia in 1996 to take up a position at Flinders University. Joe served as Dean of the School of Chemical and Physical Sciences, heading the Flinders involvement in both Microscopy Australia and the Australian National Fabrication Facility (ANFF). He was the Pro- Vice-Chancellor (Research Infrastructure) at the University of Queensland from 2018 to 2022. He is now a member of the Australian National Research Infrastructure Advisory Group.



## Hisao Ishii



Dr. Hisao Ishii received his MS and PhD degrees in chemistry from the University of Tokyo, in 1988 and 1991, respectively. His thesis research focused on the metastable atom electron spectroscopy of clean and adsorbate-covered silicon surfaces. In 1991, he started to investigate the film and interface electronic structure of organic semiconductors at Nagoya University as an assistant professor. In 2002, he was promoted to associate professor in Research Institute of Electrical Communication, Tohoku University, to extend his research to organic device physics. Now, he is working for Chiba University since 2006 as a professor. His current research interests include photoelectron spectroscopy of functional organic materials, electronic structure of organic/ inorganic interfaces, and molecular orientation of thin organic films. His efforts are also focusing on developing new techniques such as high-sensitivity photoelectron spectroscopy and rotary Kelvin probe etc.

## Andreas J. Heinrich



Dr. Heinrich is a world-leading researcher in the field of quantum-coherent nanoscience with a focus on quantum spins on surfaces. He pioneered spin excitation and single-atom spin resonance spectroscopy with scanning tunneling microscopes - methods that have provided high-resolution access to the quantum states of atoms and nanostructures on surfaces. This has culminated in the demonstration of a qubit platform made of atomic spins on a surface (Science 2023) and quantum sensing with atomic-scale spatial resolution (under review 2024). Heinrich is fascinated by the world of atoms and nanostructures, built with atomic-scale precision, and educates the public on nanoscience as demonstrated by the 2013 release of the movie “A Boy and his Atom”.

A native of Germany, Heinrich received his PhD in 1998 from the University of Göttingen and then joined the research group of Dr. Donald Eigler at IBM Almaden as a postdoc. Heinrich spent 18 years in IBM Research, which uniquely positioned him to bridge the needs of industrial research and the academic world. Heinrich became a distinguished professor of Ewha Womans University in Seoul, South Korea in August 2016 and started the Center for Quantum Nanoscience (QNS) of the Institute for Basic Science (IBS) in January 2017. QNS is operating several state-of-the-art STM and AFM systems and combines this atomic-scale approach with ensemble-averaging techniques such as x-ray spectroscopy and ensemble ESR with a surface-science focus. These experimental techniques are rounded off with synthetic chemistry and a well-rounded theory team. QNS’s motto is “engineering the quantum future”. On the goal-oriented side, this implies a focus on developing new qubit platforms for quantum computation with spins on surfaces. On the exploratory side of our research agenda, we continue the decades’ long quest of exploring how the world works on the atomic length scale.



## Masahiro Yamashita



Dr. Masahiro Yamashita received PhD in 1982 from Kyushu University. After his graduation, he was appointed as Assistant Professor at Kyushu University in 1983. In 1989, he was appointed as Associate Professor at Nagoya University, and he was promoted to full Professor at the same university in 1998. He was a full Professor at Tokyo Metropolitan University from 1999 to 2004. Then he moved Tohoku University as a full Professor. He is now Emeritus Professor of Tohoku University. He is also Changjiang Chair Professor of Tongji University (China) and Adjunct Professor of IISER Bhopal (India). He has been honored with the Inoue Scientific Award (2002), the Chemical Society of Japan Award for Creative Work (2005), the Award of Japan Society of Coordination Chemistry (2014), Mukai Award (2018), and the Chemical Society of Japan Award for 2019. He received Award for Honorary Member of Slovakia Chemical Society in 2024. Original Papers: 528. Review Articles: 108. Books: 21. Total 657 publications.

## Session 1 speakers

### Ken Onda



Dr. Ken Onda is a Professor of Chemistry at Kyushu University in Japan. He completed his Ph.D. thesis with Professor Kaoru Yamanouchi at the University of Tokyo in 1994. In 1995 he became a research associate at Tokyo Institute of Technology. In 2002 he joined the research group of Professor Hrvoje Petek at University of Pittsburgh. In 2004 he became a researcher of Non-Equilibrium Dynamics Project of JST. In 2008 he was appointed an associate professor of Environmental Chemistry and Engineering at Tokyo Institute of Technology. His current research interests include ultrafast dynamics in complex and practical chemical systems.

### Odkhuu Dorj



Dr. Odkhuu Dorj received his PhD in Physics from the University of Ulsan, South Korea, in 2012. For the following 2 years, he worked and involved as postdoctoral fellowship and senior scientist in several renowned academic institutions, including InsilicoTech, Samsung Electronics, Ulsan National Institute of Science and Technology, California State University Northridge, and University of California Los Angeles. He joined the Department of Physics in Incheon National University as an assistant professor in 2014 and promoted to associate professor in 2018 and professor in 2023. His research focuses on computational materials design and prediction of 2D materials, permanent magnetic and magnetoelectric materials, and energy storage materials. Currently, he is a member of American Physical Society, Korean Physical Society, and Korean Magnetic Society, and active Reviewer of Physical Review Letters, Physical Review B, Applied Physics Letters, Journal of Applied Physics, Nature Communication, Scientific Reports, etc. He has published more than 100 SCI papers in peer-reviewed journals, and several tens of invited and contributed talks in various scientific meetings.

### Chao Ming Fu



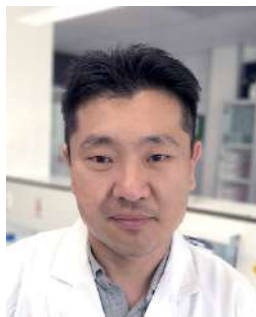
Dr. Chao Ming Fu is an accomplished physicist with a Ph.D. and a Master's in Physics from the Catholic University of Leuven, Belgium. He currently serves as Vice President of Fo Guang University (since August 2021) and has been a Professor in the Physics Department at National Taiwan University since 2006. His previous roles include Director of the Center of Teacher Education at National Taiwan University (2019-2021), Director of the Division at Moscow, Ministry of Science and Technology (2014-2018), Chair of the Applied Physics Department at the National University of Kaohsiung, and Professor at National Kaohsiung Normal University (1995-2006).

Dr. Chao Ming Fu has conducted visiting research at the IBM Almaden Research Center and the Tokyo Institute of Technology. He actively contributes to the academic community as General Secretary of the



Taiwan Association of Quantum Computing and Information Technology, President of SY-A Taiwan, Yuneyama Memorial Foundation, Vice President of the Taiwan Association of Magnetic Society, and a Steering Committee Board Member of the Asia-Pacific Conference of Young Scientists.

### **Tak Kim**



Dr. Tak H. Kim is a lecturer in the School of Environment and Science and serves as an Advance Queensland Industry Research Fellow at Griffith University, Australia. Since the completion of his PhD in nanocarbon materials in 2016, he has dedicated his effort to collaborating with small and medium-sized enterprises, working towards the development of practical solutions, tailored to their specific needs. His research is centered on extracting valuable resources from disposed materials using sustainable processing techniques.

### **Altantuya Ochirkhuyag**



Dr. Altantuya Ochirkhuyag is an Environmental Chemist with a distinguished academic background. She earned her Bachelor's and Master's degrees in Environmental Chemistry from the National University of Mongolia in 2011 and 2013, respectively. Pursuing her passion for environmental science, she completed her PhD in Environmental Science at the University of Szeged, Hungary, in 2021.

Dr. Ochirkhuyag is currently a researcher at the Mongolian Academy of Sciences, working within the Institute of Chemistry and Chemical Technology. Her research is centered on the synthesis of advanced materials derived from natural minerals and waste materials, with a focus on their application in addressing environmental challenges.

## Session 2 speakers

### Nobuhiro Hayashi



Dr. Nobuhiro Hayashi has served as vice president for international affairs since April 2022. He also serves concurrently as professor at the School of Life Science and Technology. Hayashi earned his bachelor's degree in physics from the University of Tokyo in 1989, and then completed his master's and doctoral degrees in life chemistry at Tokyo Tech in 1991 and 1994 respectively. Soon after, Hayashi joined the Institute for Comprehensive Medical Science at Fujita Health University, where he served as lecturer, assistant professor, and associate professor. Hayashi returned to Tokyo Tech in August 2008 as associate professor at the Graduate School of Bioscience and Biotechnology.

### Munkhbayar Batmunkh



Dr. Munkhbayar Batmunkh is an Australian Research Council (DECRA) fellow in Queensland Micro- and Nanotechnology Centre (QMNC) and a Senior Lecturer in the School of Environment and Science at Griffith University, Australia. Dr Batmunkh currently leads an active independent research group working on functional materials, solar cells, catalysis and their integrated systems. He completed his PhD study in School of Chemical Engineering at the University of Adelaide, in 2017. He obtained his “Master of Engineering” degree from Gyeongsang National University, in South Korea in 2012. He completed his “Bachelor of Science” degree in Chemistry at the National University of Mongolia, in Mongolia in 2010.

### Hiroki Ota



Dr. Hiroki Ota received a Ph.D. degree in Mechanical Engineering from Keio University in 2011, and was a postdoctoral fellow in the Tokyo Women's Medical University and University of California, Berkeley from 2011 to 2016. He joined in the Osaka university as an assistant professor from 2016, and was a guest associate professor. He joined the faculty of the Yokohama National University where he is currently an associate professor of Mechanical Engineering. He was a visiting researcher in the National Institute of Advanced Industrial Science and Technology (AIST) in Japan and JST. His research interests include flexible electronics, biosensors, and soft matter.





### **Sina Jamali**



Dr. Sina Jamali is an ARC DECRA Fellow at School of Chemistry. His research centres around electrochemistry of materials and cells. He works closely with Scientia Professor Justin Gooding within the Smart Materials and Surfaces Research Group.

Graduated Ph.D. under Prof Gordon Wallace from ARC Centre of Excellence for Electromaterials Science (ACES) at University of Wollongong (2016), Postdoctoral Research Fellow and Lecturer, University of Wollongong (2016-2020), Project leader at ARC Research Hub for Australian Steel Innovation (2017-2019), Growth and Innovation Technology Leader, Hexion, Melbourne (2020-2021).

### **Yu Lin Zhong**



Dr. Yulin Zhong completed his PhD in Chemistry at the National University of Singapore (NUS) and did his post-doctoral training at Princeton University (2009) and Massachusetts Institute of Technology (2011). After spending three years in the USA, he worked as a Research Scientist at the Institute of Bioengineering and Nanotechnology, A\*STAR Singapore, (2012) and thereafter, as an ARC DECRA Fellow at Monash University (2013). In 2016, he accepted a Senior Lecturer position at Griffith University, was promoted to Associate Professor in 2020 and

awarded the ARC Future Fellowship in the same year. Currently, he serves as the Treasurer in the Electrochemistry Division of the Royal Australian Chemical Institute.

### **Oleg Penyazkov**



Dr. O.G. Penyazkov graduated from the Belarusian State University in 1987. Since 1984, he has been affiliated with the A.V. Lykov Institute of Heat and Mass Transfer, where he became the Head of the Laboratory in 2001, Head of the Department in 2005, Deputy Director for Research in 2006, and Director in 2011. He is also the Chief Editor of the "Journal of Engineering Physics" since 2009 and Editor-in-Chief of the "International Journal of Heat and Mass Transfer" since 2010. His research spans high-temperature thermal physics, gas dynamics, and combustion physics. He has made significant contributions to understanding detonation waves, combustion in heterogeneous systems, and high-temperature oxidation of fuels. Dr. Penyazkov

is a member of several prestigious international scientific institutes and has authored over 270 scientific papers, including 6 monographs and 8 patents. His work has earned him numerous awards, including the V.A. Koptuyug Award (2009), the A.V. Lykov Award (2012), the Russian Federation of Cosmonautics Medal (2014), and the Tsuoshi Asanuma Medal (2016).

## Wei Zhang



Dr. Wei Zhang obtained his Ph.D in University of Leeds, UK in 2008 and then he worked at the Institute of Advanced Technology in University of Surrey, UK. In 2011, he joined Dalian University of Technology. Prof. Zhang's research interests include hyperthermia therapy of cancer, hydrogel for drug delivery and tissue engineering, mechanics of tissue and cell. He has published over 90 SCI journal papers as the first/corresponding author, which have received over 2200 citations with an H-index 24. He has been granted 30 Chinese invention patents, 1 US patent and 10 software copyrights. He is the Associate Editor of Beni-Suef University Journal of Basic and Applied Sciences, Editor of Modern Chemical Research. He is the principal investigator (PI) of one project and one sub-project of National Key Research and Development Project of China. He is also the PI of 13 projects of National Natural Science Foundation of China, Ministry of Science and Technology of China, and Ministry of Education of China, etc.

## Daewon Sohn



Dr. Daewon Sohn, is a professor in the Department of Chemistry at Hanyang University, Seoul, Korea. He received his BS and MS at Hanyang Univ. and PhD (supervisor: prof. Paul Russo) at Louisiana State Univ., Baton Rouge, USA in 1994. After postdoctoral career at Univ. of Wisconsin, Madison (supervisor, prof. Hyuk Yu) and Univ. of Toronto, Canada (supervisor, prof. Eugenia Kumacheva), he joined the department of chemistry at Hanyang Univ. in 1997. He also worked at NIST-Gaithersburg (Dr. Mike Fasolka), Kyushu University (prof. Atsushi Takahara), RIKEN (Dr. Mizuo Maeda), CUHK and USTC (prof. Chi Wu). Sohn's research interests are the characterizations of polymeric materials in solution state, at the air/water interface, and in bulk state. In his laboratory, polymer physical chemistry lab. (PPCL, <https://sites.google.com/view/hyuppcl>), many different techniques are used to characterize the polymer systems, Light scattering, X-ray and Neutron scattering, Langmuir Blodgett, AFM, Surface Force Measurement, BET, DMA, DSC, Viscometry, Cytometry, and etc. He has published 156 peer reviewed journal articles and 17 registered patents. Now, he is a director of the Research Institute for Convergence of Natural Science, and a chair of the Core-Facility Center for Polymers & Composite Materials funded by NRF-Korean. And he has served as an Editor of Polymer Bulletin, Springer, since 2008.

## Session 3 speakers

### Battulga Munkhbat



Dr. Battulga Munkhbat received his PhD in Photonics from Johannes Kepler University Linz, Austria, in 2016. His research focuses on nano- and quantum photonics, quantum light sources, photonic quantum computers, nanofabrication, and strong light-matter interactions. He held Postdoc and Researcher positions at Chalmers University of Technology in Sweden (2016-2021). In 2021, he accepted a tenure-track Assistant Professor position at the Technical University of Denmark (DTU) and moved to Denmark to establish his research group and state-of-the-art quantum optics laboratories. His research has been published in several prestigious journals, including Nature, Nature Physics, Nature Nanotechnology, Nature Communications (3x), and Science Advances, and has resulted in a US Patent (app:17/794,929). He is also a co-founder of SMENA Tech AB. In 2022, he received two prestigious research grants: the ERC Starting Grant (1.5 million Euro) to develop a tunable quantum photonic circuit using a nanoengineered 2D transition metal dichalcogenides platform and the Villum Young Investigator Grant (~0.5 million Euro) to create highly efficient single-photon sources for future optical quantum computers.

### Tomohiro Hayashi



Dr. Tomohiro Hayashi earned his Ph.D. from Ruprecht-Karls Universität Heidelberg in 2003. He later served as an associate professor at the Tokyo Institute of Technology. To date, he has been honored with eleven awards, including the Asahi Kasei Award (2011), JSPS Young Researchers' Award (2018), and JVSS Fellow designation (2023), among others. Recently, his scientific endeavors have centered on advancing surface and interfacial analytical techniques to investigate biointerfaces. This includes the use of atomic force microscopy combined with laser spectroscopy and high-speed signal processing spectroscopy, single-molecule dynamic force measurements, and materials informatics for the design of biomaterials. He is also running a start-up company producing graphene-based supercapacitors (Everon Technologies, Co, Ltd). A comprehensive summary of his scientific contributions and achievements can be found at <http://lab.spm.jp/>.

### Hsiung Chou



Dr. Chou finished his Ph.D. at the Columbia University in the City of New York 1992 and is a Distinguished Professor of Department of Physics, National Sun Yat-sen University (NSYSU), Taiwan. His main interests are on superconductivity, magnetism, exotic interface and defect physics. He works on the use Synchrotron Radiation and Neutron Scattering. He had served as the Dean of the College of Science and Chair of the Department of Physics of NSYSU. He is the Vice President of the Asia-Oceania Neutron Scattering Association and the Advisor of the Taiwan Neutron Science Society.



## **Battogtokh Jugdersuren**



Dr. Battogtokh Jugdersuren is a research scientist at the US Naval Research Laboratory in Washington, D.C., through Jacobs Engineering Group. He earned his Ph.D. in Physics from The Catholic University of America, Washington D.C., in 2009 and completed postdoctoral research at the Vitreous State Laboratory in D.C. from 2009 to 2010, under a US Department of Energy project. In 2010, Dr. Jugdersuren was awarded the US National Academies Research Fellowship at the US Naval Research Laboratory. Since 2013, he has been a research scientist at Jacobs Engineering Group in Hanover, Maryland. His research focuses on (1) phonon transport and thermoelectricity, including the development of PECVD nanocrystalline silicon thin films with record low thermal conductivity. (2) He also investigates two-level tunneling systems in amorphous, disordered systems, and (3) collaborates on modifying transition metal dichalcogenides to manipulate magnetism, with Mongolian University of Science and Technology. Dr. Jugdersuren has authored over 40 peer-reviewed papers and technical reports and holds 8 US patents, with two additional patent applications pending for approval.



## **Khulan Sergelen**



Dr. Khulan Sergelen is an Assistant Professor (tenure-track) since 2019, with expertise in molecular biosensing and bionanotechnology. She completed a postdoctoral fellowship at the Molecular Biosensing for Medical Diagnostics (MBx) group at Eindhoven University of Technology in 2019. Khulan earned a Ph.D. in Bionanotechnology in 2017 through a joint program between the University of Natural Resources and Life Sciences (BOKU) in Vienna and Nanyang Technological University (NTU) in Singapore. She also holds an MSc in Molecular Medicine from the University of Vienna and a BSc in Biology from the National University of Mongolia.

## Session 4 speakers

### Takeharu Tsuge



Dr. Takeharu Tsuge is a Professor at the Tokyo Institute of Technology. He received his Doctoral Degree in 2000 from Kyushu University. He joined the RIKEN Institute as a Special Postdoctoral Researcher in 2000 and the Tokyo Institute of Technology as an Assistant Professor in 2002. He was promoted to Associate Professor in 2009, then to Professor in 2024. He received the Encouragement Award (Terui Award) from the Society for Biotechnology, Japan (2008) and the SPSJ Asahi Kasei Award from the Society of Polymer Science, Japan (2015). His current research interests include microbial polyester synthesis and bio-based polymeric materials.

### Bolormaa Oyuntsetseg



Dr. Bolormaa received her Ph.D degree in chemistry from Irkutsk State University. Professor at the Department of Chemistry, at the National University of Mongolia since 1995 and from 2023, she started to act as a head of the Department of Chemistry, National University of Mongolia. Dr. Bolormaa worked as a UNESCO visiting researcher and postdoctoral fellow of JSPS at the Tokyo Institute of Technology between 2002 and 2009. Her study focuses on the development of methods for environmental remediation assessment, chemical metrology, surface and groundwater chemistry and soil chemistry. She also collaborates with international research groups from Japan, Korea and Taiwan. She published about 200 research materials and about 150 are research articles published in domestic and international journals.

### Sàpi Andràs



Dr. Sapi Andras is an assistant Professor at University of Szeged, Department of Applied and Environmental Chemistry. His research are focused on heterogeneous catalysis and surface science based on size controlled nanoparticles and 3D transient-metal supports as well as understanding the reactions under reaction conditions. Working together with students is a blessing. His research interests are CO<sub>2</sub> activation and in-situ techniques, Flue Gas Treatment, Size controlled Nanoparticles & 3D mesoporous oxide supports in Surface Chemical Processes, Battery researches, Photocatalytic CO<sub>2</sub> activation and Water treatment, and Other surface chemistry and material science.

## Wei Hu



Dr. Wei Hu, Professor, Fudan University & Inner Mongolia University. Email: huw@fudan.edu.cn. Dr. Hu received her Ph.D degree in Pathogen Biology from Chinese Center for Disease Control and Prevention. She served for National Institute of Parasitic Diseases, Chinese Center for Diseases Control and Prevention from 1996 to 2012; then she became a professor at the department of Microbiology and Immunology in Fudan University from 2012 to now; and from 2020, she started to act as the dean of the School of Life Sciences, Inner Mongolia University. She is interested to understand the invasion, infection and development mechanisms of schistosome, as well as its adaption evolution and genetic variations. Current work in her lab focuses on the developmental biology of schistosome and its interactions with host. In recent years, she has published a number of important papers in journals like Nature Communications, Cell Reports and PLoS Pathogens in these areas. She is an associate editor of Chinese Journal of Parasitology and Parasitic Diseases and the editor of Parasitology.

## Bayar Hexig



Dr. Hexig Bayar, received his Ph. D degree in Biomolecular Engineering Science from Tokyo Institute of Technology. M. Sc. degree in Biological & Chemical Engineering, Gunma University, Japan. B.Sc. in Physics, Inner Mongolia Normal University, China. From 2005 to 2007, He worked as Postdoctoral Researcher, Division of Medical Devices, National Institute of Health Science, Japan (Jointed to Health and Labor Sciences Grants for Research on Advanced Medical Technology and Risk Analysis on Foods and Pharmaceuticals by Ministry of Health, Labor and Welfare, Japan). From 2007 to 2012 Assistant professor, Graduate School of Bioscience and Biotechnology & Frontier Research Center, Tokyo Institute of Technology, Japan; (Evolving Education and Research Center for Spatio-Temporal Biological Network). From 2012-present, Dr HEXIG BAYAR, as a full Professor work in State Key Laboratory of Reproductive Regulation and Breeding of Grassland Livestock, School of Life Science, Inner Mongolia University, P. R. China.

## Nandin-Erdene Mandakhbayar



Dr. Nandin-Erdene Mandakhbayar is a dedicated and ambitious bachelor's student pursuing advanced studies in Biochemistry at the Mongolian National University of Medical Sciences. She has embarked on a journey to expand fundamental and experimental biochemistry. She followed her undergraduate degree in Dentistry with distinction, earning accolades for her education achievements and subsidies to medical and research ambitions. During her undergraduate, she demonstrated excellent analytical skills, communicating with people and problem-solving skills, earning her the respect of her peers and dreams. Nandin-Erdene Mandakhbayar launched her Master and PhD journey focusing on biochemistry engineering and tissue engineering. Under the guidance of her honourable advisors, she has been engaged in cutting-edge research to address some of the most pressing questions about recombinant proteins and tissue engineering. During her graduate and post-graduate, she challenged and questioned her skills in Nano and Bioactive biomaterials, in vivo modelling, and disease modelling



with her great team members. Outside of her academic pursuits, she has collaborated with many teams and knowledge exchange within the scientific community. She is enthusiastic to engage with fellow researchers, exchange ideas, and contribute to the collective advancement of scientific understanding.





## Plenary talk session

### **Enhancing solar cells and catalysts using novel nanomaterials**

**Joe Shapter**

*Australian Institute for Bioengineering and Nanotechnology, University of Queensland*

One of the most important issues facing society is the ability to supply the world's energy requirements via both environmentally responsible and sustainable means. Renewable energy, and in particular solar energy, has the potential to address current issues in energy production but costs, both in terms of the energy required for production and final price to the consumer, as well flexibility in terms of system deployment are problems that will need to be addressed. Reducing the environmental footprint in various chemical processes is also very important. This talk will focus on work using nanomaterials to make new architectures for solar cells or new generation nonmetallic catalysts. Several possible structures including heteroatom doping will be explored and the disadvantages and advantages of each will be examined.

## Spontaneous orientation polarization of amorphous organic films and their applications to devices

Hisao Ishii<sup>1</sup>, Masahiro Ohara<sup>1</sup> and Yuya Tanaka<sup>2</sup>

<sup>1</sup> Center for Frontier Science, Chiba University

<sup>2</sup> Graduate School of Science and Technology, Gunma University

Amorphous films of organic semiconductors have been applied to various types of electronic devices such as organic light emitting diodes (OLEDs). The control of molecular orientation in devices is a key factor to improve device performance. Here we focus on molecular orientation of OLED materials. Most OLED materials have molecular structure with lower symmetry for realizing uniform amorphous film. So their molecular structure often has permanent electric dipole moment (PDM). When these polar molecules are deposited by vacuum vapor deposition, spontaneous orientation polarization (SOP) of their PDM often occurs [1]. SOP is common in the evaporated films of many organic semiconducting molecules with a permanent dipole moment, but the mechanism of SOP formation is still open question. A significant electric field is formed in the film due to SOP. Consequently, the properties of OLEDs incorporating such films are influenced. The polarization charge appearing at hetero-interfaces dominates the charge injection and accumulation properties. Moreover, SOP correlates with device degradation. Recently, these polarized films can be used as electret for vibrational energy generators [2]. In this presentation, we will report on our recent research on SOP. Topics are as follows.

1) *How we can control the orientation order and polarity by changing evaporation conditions and additional perturbation like light illumination?*: The higher deposition rate was found to give higher SOP for Alq<sub>3</sub> and TPBi [3]. Simultaneous UV light illumination during the deposition was found to increase SOP for TPBi [4].

2) *Effect of interval time during evaporation*: Recently we have proposed a novel method, referred to as “**intermittent deposition**”, in which the polarization direction and magnitude are controlled by introducing intervals during physical vapor deposition [5]. The rotary Kelvin probe measurement of the Alq<sub>3</sub> and TPBi films clearly showed a time-dependent decrease in the surface potential owing to the surface relaxation of the molecular orientation immediately after deposition. Through a series of intermittent depositions, in which the deposition shutter is repeatedly opened and closed at certain intervals, a relaxed surface layer was built up, and we could control the polarization magnitude.

3) *Whether wet process deposition induce SOP or not*: By using automatic measurement system of Rotary Kelvin probe method during the film deposition, we have tried to investigate whether



SOP can occur even for wet process deposition in which complete random orientation is expected.[6]

The above results on SOP are useful to control and improve organic electronic devices and vibration generator etc. They are also hints to solve the mysterious mechanism of SOP formation.

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## Towards quantum computing with spins on surfaces

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There is a strong international research effort in the area of quantum information science. Here, the concepts of quantum coherence, superposition and entanglement of quantum states are exploited. These concepts were originally shown with photons as well as atoms and ions in vacuum traps. Over the past two decades, many advances at studying such quantum coherence in solid-state and molecular architectures have evolved [1].

In this talk we will focus on quantum-coherent experiments in Scanning Tunneling Microscopy (STM). STM enables the study of surfaces with atomic-scale spatial resolution and offers the ability to study individual atoms and molecules on surfaces. To study qubits with STM, we recently learned how to combine STM with electron spin resonance [2,3]. Spin resonance gives us the means to quantum-coherently control an individual atomic or molecular spin on a surface. Using short pulses of microwave radiation further enables us to perform qubit rotations and learn about the quantum coherence times of our spins [4]. Finally, we will demonstrate multi-qubit operations with spins on surfaces and discuss their performance measures [5]. Future directions for improvements will wrap up the talk.

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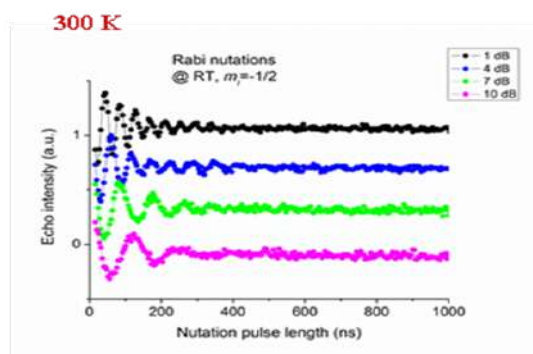
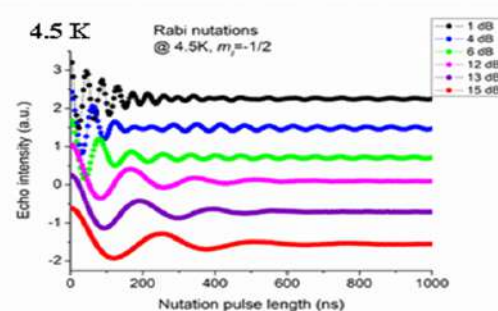
## Molecular spin qubits toward quantum computer and high-density memory devices based on molecular magnets

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Spintronics, based on the freedoms of charge and spin of the electron, is a key technology in the 21<sup>st</sup> century. Magnetic random access memory (MRAM), which uses giant magnetoresistance (GMR), has several advantages compared with electronics. Although conventional magnets composed of transition metals are normally used, in our study, we use single-molecule magnets (SMMs) to overcome “Moore’s Limitation”. SMMs are also available for quantum computer. I will talk about the molecular spin qubits for quantum computer as well as high-density memory devices such as single-molecule memory device, SMMs encapsulated into SWCNT, and metallic conducting SMMs with negative magnetoresistances.

As for molecular spin qubits for quantum computer, we must increase  $T_1$  (spin-lattice relaxation time) and  $T_2$  (spin-spin relaxation time). Therefore, we will focus on the following three strategies: **(1) Crystal Engineering Method;** To compare 0D [VO(TPP)] and 3D [VO(TCPP-Zn<sub>2</sub>-bpy)] (3D-MOF) to investigate the influence of the spin-lattice relaxation ( $T_1$ ) in 0D and 3D lattices. Due to the rigid lattice of 3D-MOF, the Rabi nutation was observed even at room temperature (Fig.1). **(2) g-Tensor Engineering Method;** To compare [VO(TPP) and [CrN(TPP)] to investigate the contribution of the anisotropy of their g-values for the spin relaxation. Due to the large anisotropy of g-values, [CrN(TPP)] shows the short life time. **(3) Orbital Engineering Method;** To compare [Ni(cyclam)X<sub>2</sub>]ClO<sub>4</sub> and TBA[Ni(mnt)<sub>2</sub>] to investigate the relationship between the different occupied orbitals and spin relaxation. [Ni(cyclam)X<sub>2</sub>]ClO<sub>4</sub> has the longer life time due to the rigid molecular structure.





As for the single molecule memory, we have used STM and STS for TbPc<sub>2</sub> SMM. By using tunnelling magnetoresistance, we have realized the single memory effect of up-spin and down-spin on TbPc<sub>2</sub>. As for the negative magnetoresistances for high-density memory devices, we have synthesized (BEDO-TTF)<sub>3</sub>[Co(pmdt)<sub>2</sub>] (**BO3**) and (BEDO-TTF)<sub>4</sub>[Co(pmdt)<sub>2</sub>] (**BO4**). **BO3** show the metallic behavior around room temperature and M-I transition around 12K. Moreover, **BO3** shows the negative magnetoresistance for the first time by the interaction between conducting electron and SMMs. We have succeeded the encapsulation of DySc<sub>2</sub>N@C<sub>80</sub> SMMs into Single-Walled Carbon Nanotubes (SWCNTs). After encapsulation, the coercivity increase by one order by suppression of the quantum tunnelling.



# Session 1: Next-Generation advanced materials: Fundamentals & Applications

## Fundamental processes in photofunctional materials studied by ultrafast spectroscopy

**Ken Onda**

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Photofunctional materials are the materials that exhibit useful functions via a change in optical, electrical, or chemical properties by photoirradiation. To develop new photofunctional materials, it is necessary to know the fundamental processes in the materials induced by photoirradiation. It is, however, difficult to attain this because the processes span in a wide temporal range from femtoseconds to milliseconds and in a wide energy range from meV to eV. Thus, we have developed time-resolved analytical methods applicable to such photofunctional materials using ultrashort pulse lasers, and revealed many important processes in photo-functional materials (Fig. 1). In this talk, we focus on our two recent topics: CO<sub>2</sub> photoreduction processes in artificial photo-synthesis [1,2] and luminescent processes in organic light emitting diode (OLED) [4-6].

Artificial photosynthesis mimics natural photo-synthesis and produces high energy materials from CO<sub>2</sub> and H<sub>2</sub>O using sunlight energy. It is really challenging to analyze the fundamental processes due to their multi-electron and multi-step processes. We have developed time-resolved infrared vibrational spectroscopy (TR-IR), which has high selectivity for chemical species and high temporal resolution, and elucidated many essential processes such as the electron transfer mechanism between a photosensitizer and a catalyst [1] and photocarrier dynamics in the hybrid systems of semiconductor and metal complex [2].

OLEDs are still under development for improving their cost, durability, and environmental load. To achieve these, the processes in the electronically excited states in the devices must be known. We have explored the fundamental emission processes related to OLED using transient absorption and time-resolved luminescent spectroscopies in a wide temporal and energy ranges. To date we revealed the role of structural change in spin-flip processes in a solution and a thin film [3] and the detailed intermolecular energy transfer mechanism in host-guest films [4].

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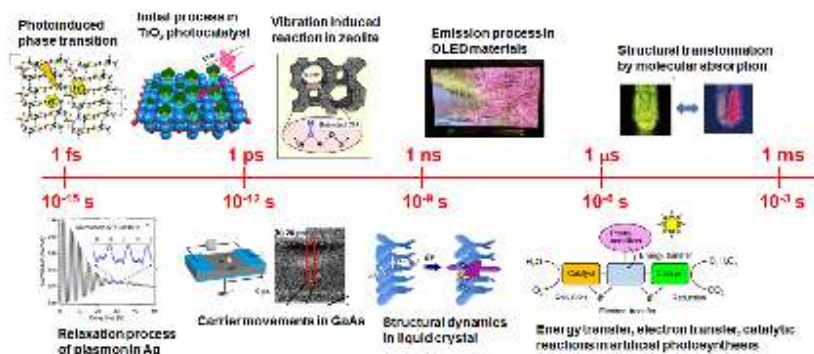


Fig. 1. Fundamental processes we revealed in various photofunctional materials.



## **Towards nanomagnetic materials design and characterization\***

**Odkhuu Dorj**

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Magnetic materials are important components in many applications today. In particular, permanent magnets are vital for energy conversion and storage sectors, while 2D magnetism is expected desirable in spintronics.

Since  $\text{Nd}_2\text{Fe}_{14}\text{B}$  permanent magnet was developed in 1982, a permanent magnet with higher performance has not been reported yet. Ever since, search for permanent magnet materials that do not contain rare-earth elements, but compatible to ferrites in price, is underway.

In the first half of this talk, we will briefly review the properties that make a material good permanent magnet, including saturation magnetization, magnetocrystalline anisotropy, maximum energy density product, Curie temperature, and thermodynamic stability, and then discuss on our recent approaches to designing and characterizing permanent magnets free or reduced content of rare-earth elements, namely  $\text{SmFe}_{12}$ ,  $\text{Fe}_2\text{P}$ ,  $\text{FeNi}$  based alloys, while retaining a comparable performance with  $\text{Nd}_2\text{Fe}_{14}\text{B}$ .

In the second half, with our comprehensive theoretical and experimental results we will emphasize towards the possibility of achieving room-temperature ferromagnetism in 2D  $\text{MoSe}_2$  versus  $\text{WSe}_2$  by simply manipulating vacancy defects. In order to consider 2D magnet more practical and more robust ferromagnetism, other promising efforts explored thus far, that are, various doping impurities (i.e., Fe, Co, Sm, and Nd), strain effect, or applying an electric field, will also be discussed.

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## Synthesis and optimization of Fe<sub>3</sub>O<sub>4</sub> nanoparticles for hyperthermia application

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Magnetic nanoparticles of Fe<sub>3</sub>O<sub>4</sub>, exhibiting superparamagnetic characteristics, are pivotal in the realm of biomedical applications. This research delineates the synthesis of Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles via the co-precipitation technique, followed by their exposure to an alternating current (AC) magnetic field to assess their potential in hyperthermia treatments. The efficiency of heat absorption, quantified by the Specific Absorption Rate (SAR), is a critical factor influenced by the synthesis process parameters. The study utilizes an orthogonal experimental design to systematically explore and optimize these parameters, aiming to enhance the SAR for effective hyperthermia. The findings, which provide insights into the influence of process parameters on the heating efficacy of Fe<sub>3</sub>O<sub>4</sub> nanoparticles under an AC magnetic field, will be expounded upon in the ensuing report.



## **Processing of carbonaceous residue from waste tyre pyrolysis plants for the production of high-quality carbon and its potential uses**

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Pyrolysis of tyres produces fuel oil and recyclable steel, representing a renewable energy technology that directly reduces the associated risks of stockpiled waste tyres. Thus, pyrolysis is one of the economically feasible solutions for addressing the stockpiling of waste tyres. Despite the unmet and urgent demand from the industry, most of the research has focused exclusively on processes for fuel oil extraction[1] and dedicated carbon production.[2] Subsequently, commercial activities have focused on the recovery of fuel and steel. Unfortunately, the pyrolysis process inevitably produces a secondary carbonaceous waste, known as low-quality tyre char, containing not only carbonaceous residues but also toxic by-products. Consequently, tyre char is not suitable for other uses or landfilling.[3] The tyre char is therefore stockpiled, adding further environmental concerns to an already overburdened environment.

To address the issues arising from tyre char, we demonstrated that tyre char can be further processed to improve the quality of the carbon. At each stage of processing, changes in the tyre char were evident, including a reduction in mass and changes in morphology. Subsequent investigation using inductively coupled plasma optical emission analysis revealed alterations in the overall composition of heavy metals, while X-ray photoelectron spectroscopy indicated shifts in surface elemental composition and bonding characteristics. The heavy metal analysis indicated that concentrations of lead, cadmium, mercury, arsenic, and zinc in the processed tyre char fell below the guidelines set by the International Biochar Initiative.[4] Surface analysis further confirmed morphological changes during the processes, with noticeable shifts in elemental composition and an increase in  $\pi$ - $\pi$  interactions as the process stage progressed. These results indicated that the processed tyre char may have the potential to be applied to environmental remediation and energy applications, replacing conventional activated carbon and graphite.

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## From waste to nanomaterials: synthesizing mesoporous silica from briquette coal ash for advanced applications

**Ochirkhuyag Altantuya<sup>1,2</sup>, Tserenpil Otgonjargal<sup>1</sup>, Tuuguu Enkhdul<sup>1</sup>, Lhuvsandagva Mandakhsaikhan<sup>2</sup>, Rentsennorov Ulambayar<sup>2</sup>, Gendenjamts Oyun-Erdene<sup>2</sup>**

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Ulaanbaatar, the capital city of Mongolia, heavily depends on briquette coal as a source of heating, leading to the production of 2-3 million tons of coal ash every year from around 220,000 households. The study aims to repurpose a substantial amount of waste ash for the synthesis of mesoporous silica nanoparticles (MSNPs).

The briquette coal ash primarily consists of SiO<sub>2</sub> (69%) and demonstrates its potential as a raw material for silica nanoparticles (SNPs). SNPs were synthesized and characterized after undergoing thermal treatment at a temperature of 900 °C, followed by chemical processing. The surfactant-free synthesized silica nanoparticles (SNPs) possess a surface area of 115 m<sup>2</sup>/g and a microporous structure with a diameter of 1 nm. Consequently, they exhibit a mere 2% adsorption capacity for methylene blue dye (MB) at a concentration of 50 mg/l over a duration of 80 minutes. On the other hand, SNPs produced using cetyltrimethylammonium bromide (CTAB) have a surface area of 317 m<sup>2</sup>/g and a pore diameter of 7.8 nm, resulting in an 83% capacity to adsorb MB. The SNPs, which are synthesized using polyethylene glycol (PEG), have a surface area of 121 m<sup>2</sup>/g and a pore diameter of 8.1 nm. As a result, they exhibit a lower adsorption capacity for MB, with only 12% of MB being adsorbed. This emphasizes the significance of choosing the appropriate surfactant to create mesoporous structures and improve the properties of SNP.

In addition, incorporating SNPs into briquette coal ash significantly enhances the density of construction foam blocks, increasing it from 876 kg/m<sup>3</sup> to 943 kg/m<sup>3</sup>. This demonstrates the promising potential of utilizing ash in construction materials. This study highlights the significance of utilizing briquette coal ash for sustainable MSNP production, providing prospects for environmental remediation and enhanced construction material quality.

**Keyword:** mesoporous silica nanoparticle, briquette coal ash, methylene blue, foam block





## Session 2: Emerging functional materials & devices

### **Sustainable futuristic healthy society realized through AI-assisted personalized healthcare**

To consider BIOMATERIALS & BIOMEDICAL MATERIALS required by society in the future

**Nobuhiro Hayashi**

*School of Life Science and Technology, Tokyo Institute of Technology*

The life sciences have experienced several paradigm shifts in the past, including the discovery of the cell and the rise of molecular biology with the discovery of DNA as a gene. With the recent breakthrough in AI capabilities, the life sciences are now at another turning point. The speaker and colleagues have been working on the generalization of proteomics, a method for comprehensive analysis of the health status of living organisms. Its potential is expanding from cutting-edge researches and clinical studies to daily health care [1,2]. We have recently succeeded in using AI to decipher images (proteomic data) containing comprehensive information about living organisms [3]. After this technology in society will be implemented in society, by using machine learning with records of daily life, such as what people eat, what they do, and what happens to them, as teacher data, it is now possible to prepare an AI that will work with each individual to figure out what they should eat and how they should live that day in order to become the person they each want to be. To achieve this, it is essential to develop the data acquisition devices as well as open innovation through data sharing based on the understanding of stakeholders (citizens, companies, and government).

This presentation will explain how we can create an AI that will partner with us in our daily lives, including food, and present several activities for achieving this goal. In the future society presented here, people will be able to ask their AI partner about their own health status and performance anytime they want. To realize such a future, it is necessary to develop materials for devices that enable comprehensive health checkups to be performed at hand at any time. On the other hand, such a future requires new materials for the development of devices that allow people to control their own health and performance in their daily lives. Furthermore, it will be desirable to switch the materials of existing products to materials that can contribute to the individual's daily health management and performance control.

I hope that this presentation will provide an opportunity for consideration of the invention of new functional materials.

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## Engineering two-dimensional (2D) materials for energy applications

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Organic/inorganic metal halide perovskites attract substantial attention as key materials for next-generation photovoltaic technologies due to their potential for low cost, high performance, and solution processability. Despite their great promises, perovskite solar cells do have some disadvantages such as use of expensive electrode materials, the high temperature required during production and poor operational stabilities. Two-dimensional (2D) layered nanomaterials such as black phosphorus and metal carbide MXene have shown great promise for use in a wide range of energy related applications including perovskite solar cells. The high degree of tunability in the properties of these unique nanomaterials offers an abundance of opportunities for next generation solar cells. In this talk, Dr Batmunkh will present the recent contributions he and his colleagues made to this cutting-edge research area and also highlight the future promises in this area.



## Highly deformable smart device for healthcare and medical application

**Hiroki Ota**

*Yokohama National University*

With the development of IoT (internet of things), various smart devices have been proposed. In particular, the development of smart devices for healthcare and medicine, mainly wearable devices, has been focused. In our laboratory, we develop highly deformable electrodes based on flexible and stretchable materials. Flexible and stretchable electrodes are highly deformable and lightweight, which can significantly reduce the physical load and enable acquisition of biological signals with high signal-to-noise ratio. It is possible to measure body temperature, electrocardiogram, electroencephalogram, SpO<sub>2</sub>, etc. with high stability. However, research is still limited to the electrodes themselves and electronic components. Research on smart devices with a view to social implementation and the realization of killer applications are required in the current flexible and stretchable electronics.

Smart devices using flexible electrodes and flexible substrates are gradually used in society, including smartphones. On the other hands, it is difficult to say that social implementation of healthcare and medical devices, which are expected to demonstrate the significant advantages of deformability, has progressed. In the future, stretchable devices using stretchable electrodes, which are made of even more flexible materials, are expected to be introduced to society as next-generation electronic devices. In this presentation, we report on the flexible smart devices that are being developed in our laboratory for social implementation in healthcare and medical applications, and also report on stretchable devices, which are expected to be the next generation of smart devices, from development of electronic elements to systemization.



## Stochastic electrochemistry: a powerful emerging analytical tool for real time characterization

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Stochastic electrochemical measurement has come of age as a powerful analytical tool in corrosion science, and recently gaining momentum in electrophysiology and single-entity electrochemistry. The technique relies on the fundamental trait that most electrochemical processes are stochastic and discrete in nature. Stochastic measurement of a single entity probes the charge transfer from a few or even one electroactive species and employs strategies for signal amplification and analysis<sup>1,2</sup>. In corrosion science, the stochastic measurements capture either the average amplitude/frequency of many redox events that take place spontaneously and independently or they probe discrete transients signifying localized dissolution<sup>3,4</sup>.

The methodology of stochastic measurements varies in corrosion, single-entity sensing, batteries and electrophysiology, yet they share the aspect that the main quantifiable values in the data are frequency and amplitude of events<sup>5</sup>. Herein, we introduce a new application where the formation of a biofouling layer is quantified using stochastic electrochemistry<sup>6</sup>. This is showcased on gold as the electrode of the choice, and albumin as the biofouling agent. The technique uniquely affords thermodynamic and kinetic information without applying an external bias (potential and/or current) hence allowing the system to be appraised in its innate state. The technique relies on the analysis of non-Faradaic current and potential fluctuations that are intrinsically generated by the interaction of charged species at the electrode surface. We will lay theoretical foundations for the parameters extracted from the stochastic data and how they relate to physical aspects of the system being studied. We will then use experimental data and complementary techniques to validate our findings. Adsorption of a fouling layer on the surface of sensors decreases the electrochemical activity and hence shortens the service life of sensors. Real time quantification of the loss of activity is important for in situ assessment of performance while presenting an opportunity to compensate for the loss of activity and recalibrate the sensor to extend the service life.

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## **Electrochemical engineering and direct ink writing 3D printing: cost-effective production of 2D nanomaterials and their bespoke assemblies**

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Electrochemical engineering is a powerful technique that has been applied on industrial scale to cost-effectively produce valuable chemicals and materials that are otherwise difficult to produce via traditional chemical synthesis (i.e. utilising heat or catalysts). As such, it is a highly viable method to overcome the bottleneck in the commercialisation of novel 2D nanomaterials (production cost) and enabling them, through in situ modifications, for their niche application in flexible and energy-related devices.[1] We have employed a combination of highly robust boron-doped diamond (BDD) with a wide electrochemical potential window and commercially available fused deposition modelling (FDM) 3D printing to fabricate a scalable packed-bed electrochemical reactor (PBER) for GO production.[2] In our recent work, the niche feature of two - dimensional carbides and nitrides of transition metals (MXenes) was capitalised in our packed - bed electrochemical reactor to produce MXenes at an unprecedented reaction rate and yield with minimal chemical waste.[3] A simple NH<sub>4</sub>F solution was employed as the green electrolyte, which could be used repeatedly without any loss in its efficacy.

Regarding bespoke assembly, we have demonstrated a new effective formulation for 3D printing of conductive PDMS/graphene ink by using an emulsion method to form a uniform dispersion of PDMS nanobeads, EGO and PDMS precursor binder.[4] Due to the unique hybrid structure of PDMS and EGO sheet, the 3D printed EGO/PDMS nanocomposite possesses high, linear and reproducible sensitivity that is suitable for application as skin-attachable wearable health monitoring device. To power the wearable devices, we have introduced a highly printable MXene ink that was prepared by incorporating a surfactant (C12E9) into the MXene hydrogel.[5] The incorporation of C12E9 offers amphiphilicity to the MXene flakes and produces a 3D interlinked network of the MXene flakes. The formulated nanocomposite ink facilitates the alignment of the MXene flakes during extrusion as well as the formation of the aligned micro- and sub-microsized porous structures, leading to the improved electrochemical performance of the printed microsupercapacitor.



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## Flame deposition technology for high purity fused silica generation

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Fused silica glass is manufacturing from pure liquid precursor compounds, thereby minimizing impurities and maximizing refractive index homogeneity, transparency range, low thermal expansion, and resistance to optical damage. That is why this synthetic glass are using as an optical material for deep UV lens elements, which are using for photolithography. This report describes our studies in developing flame deposition technology for high purity fused silica formation during OMCTS/CH<sub>4</sub>/O<sub>2</sub> combustion process. Different aspects of the technology and fused silica glass characterization is considered.





## **Application of magnetic nanoparticles in cancer therapy**

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Magnetic nanoparticles has great promise in cancer therapy and drug delivery. Herein, we developed magnetic nanoparticles with low Curie temperature. When used in magnetic induction of hyperthermia, those nanoparticles can self-regulate the hyperthermia temperature in 42-46°C without any temperature controlling system. To improve the therapeutic effects, we investigated the factors e.g. mechanical properties of cell and particle size on the endocytosis of nanoparticles by cancerous cells. We also developed magnetic nanoparticle based microspheres for photothermal therapy of cancer and drug delivery.



## Structure and properties of hydrogels prepared by coordination bonds

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We developed hyaluronic acid (HA) hydrogels by regulating the gelation kinetics of Fe(III) and a catechol cross-linker, including Fe(III)-induced covalent bonding and coordination bonding. Dual roles of Fe(III) in catechol-modified HA (HA-CA), Fe(III)- catechol coordination, and catechol oxidation followed by a coupling reaction, were selectively applied for different gelations. Tetra-poly(ethylene glycol) with catechol end groups (4-PCA) was also crosslinked through coordination bonds between catechol moieties and Fe(III) ions, which produce bis-complex and tris-complex depending on pH levels. The structure and property of 4-PCA gels were examined upon the bonding types controlled by pH levels and molar ratios between catechol groups and Fe(III) ions. The coordination bond types were probed by UV absorption peaks and Raman spectra. The correlation lengths ( $\xi$ ) were determined in the semi-dilute solution regime and the PCA gel networks using light scattering, small-angle X-ray scattering, and neutron scattering measurements. For the gels with bis- complex units,  $\xi$  values correspond to the size of a single polymer chain. Otherwise, they increased in the gels consisting of tris-complex units, indicating that the matrices have partial crosslinks. The results show structure and property of gels can be controlled by geometries of crosslinking units as a strategy to develop novel polymer gels.

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## Session 3: Novel trends in nanostructures & nanomaterials: design, characteristics, & applications

**To be announced**

**Sir Konstantin Sergeevich Novoselov**

## Nanoengineered transition metal dichalcogenides platform for quantum photonics: generation and interference of single photons

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Transition metal dichalcogenides (TMDs) have attracted significant attention as a unique excitonic and photonic platform for nano- and quantum photonics. One remarkable feature of TMDs is their easy exfoliation via the scotch tape, thanks to their van der Waals stacking nature. This feature opens the door to assembling and stacking various TMD materials to possess new properties and integrating them into other photonic platforms. Additionally, TMD mono- and bilayers can yield single photons through strain- and defect-engineering, ranging in visible [1] and telecom [2]. Integrating these TMD quantum emitters with photonic nanostructures and cavities promises efficient single-photon generation [3-5]. In addition, multilayer TMDs possess exceptional optical properties, e.g., high index ( $n \geq 4$ ) and low loss ( $k \leq 10^{-4}$ ) [6], despite their indirect bandgap. These exceptional optical properties combined with optimized nanostructuring offer new possibilities to exploit multilayer TMDs in developing novel photonic components [7-8] for fully integrated quantum photonic circuits.

In the first part of my talk, I will present our recent advancements in fabricating highly polarized mono- and bilayer TMD single photon emitters through strain engineering [9]. This technique allows precise control over the polarization of these quantum emitters, a crucial step in their integration into desired photonic cavities for developing efficient single-photon sources. Our fabricated quantum emitters not only feature a high degree of single photon purity but also exhibit narrow zero-phonon lines with visible phonon sidebands [10]. This provides crucial details on the exciton-phonon coupling of the system and allows us to predict exciton preparation under different excitation schemes [11]. Moreover, we have explored experimentally various optical excitation schemes [10], including quasi- and resonant excitations, to understand their impact on single photon characteristics and the stability of emission lines, especially when compared to above-band excitation.

In the last part of my talk, I will discuss our ongoing research activities in developing on-chip TMD photonic components such as nanobeam cavities, on-chip beam splitters, and



waveguides, harnessing the unique properties of nanoengineered multilayer TMDs. These novel photonic components combined with our TMD quantum emitters could be a promising platform for realizing fully integrated quantum photonic circuits.

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## Water at Biointerfaces

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In biological systems, water plays an important role in governing intra and inter molecular processes, which maintain the homeostasis of our lives. In the cases of biointerfaces of artificial materials and devices with proteins, cells, tissues, etc, the interactions should be precisely controlled depending on their applications. Here, we discuss the anti-biofouling (bioinert) surfaces used for surface coatings to prevent blood coagulation and non-specific adsorption and adhesion of proteins and cells. Our surface force measurements revealed that non-fouling surfaces possess a barrier of water preventing the approaches of proteins and cells. Our interface-sensitive vibrational spectroscopy also unveiled a unique hydrogen bonding state of the interfacial water. In this presentation, we discuss how interfacial water molecules affect the interactions at biointerfaces.[1] Furthermore, we also introduce the design of biomaterials using informatics.

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## Spin-triplet superconductivity at LSMO/YBCO interfaces

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Spin-triplet superconductivity can be generated at superconductor/ferromagnetic interfaces where both the superconducting proximity effect and the magnetic exchange coupling are mixed, and exhibits several potential advantageous properties such as enabling a spin-polarized superconducting current in the ferromagnetic layer, establishing a long-range quantum entanglement of carriers, and possibly forming Majorana particles. Reorienting induced Cu moments at the  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  (YBCO)/  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) interface via a field-cooling process enhances the transformation of superconducting pairs into triplet states around the interface region. These spin-triplet pairs at the parallel state then can exist inside the ferromagnetic LSMO layers, enhancing their magnetization and modifying their electronic structures. In this paper, we used Polarized Neutron Reflectivity (PNR) and X-ray Absorption Near Edge Structure (XANES) measurements to investigate these changes in the LSMO layers. We found an average of 9% enhancement of the magnetization and a 38 meV increase in the O K-edge in the LSMO layers when spin-triplet pairs emerge in LSMO layers. These findings suggest a very efficient rate of spin-triplet pair generation and the spin-triplet pairs may not be converted from the spin-single pairs in YBCO layers but are generated in other source of holes for forming spin-triplet pairs due to the complex magnetic and superconducting proximity effects around the interfaces. These results provide important insights into the development of triplet pairs in a ferromagnetic/superconducting heterostructure and how they engage with the ferromagnetic electronic structure.



## **PHONON TRANSPORT IN NANOSTRUCTURED MATERIALS.**

**Battogtokh Jugdersuren**

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To address the global energy crisis, it is imperative to tailor the thermal conductivity of materials. Advanced technologies such as thermoelectrics and thermal barrier coatings rely on low thermal conductivity. This study explores phonon transport in nanostructured materials, emphasizing fundamental principles and recent advancements. Nanostructured materials—such as nanowires, nanoparticles, and thin films—exhibit unique characteristics due to interfaces, grain boundaries, and reduced dimensions, altering thermal energy transport mechanisms. Multiple scattering mechanisms, particularly at grain boundaries, significantly reduce the mean free path of phonons in these materials compared to bulk materials, thereby leading to lower thermal conductivity. Recent advances in material fabrication, like plasma-enhanced chemical vapor deposition, offer considerable control over nanostructure parameters, including size, shape, composition, and interface characteristics. This capability enables tailored engineering of thermal properties, promising enhanced energy efficiency and effective thermal management solutions across various industries.





## Continuous molecular monitoring: Development of optical biosensors

**Khulan Sergelen**<sup>1</sup>

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The continuous detection of molecular levels are vital in various applications ranging from basic research, healthcare to environmental monitoring. Particularly in healthcare, conditions require patient monitoring for early decision making for efficient and life-saving treatments and procedures, such as therapeutic drug monitoring for narrow therapeutic range drugs [1]. Although various technologies are developed to face the challenge of drug or biomolecular monitoring, many fail at stable and sensitive detection in practice, aside from the singular successful technology called continuous glucose monitoring. The limit of this technology is the utilization of glucose oxidase to generate detectable electrochemical signal. This cannot be applied to other analytes due to lack of available enzymes specific to a wide range of molecules [2]. Several electrochemical biosensors are demonstrated for continuous monitoring applications in healthcare, but lack long-term stability over a few hours [3].

I will present the approach of developing optical technologies to tackle continuous molecular monitoring challenges from developing reversible detection assay, sensitive optical readout mechanisms to tackling stability and biocompatibility for in vivo applications using biomaterials. These include designing aptamer bioreceptors to tune kinetic ranges suitable for reversible biosensing, as well as application of aptamers to enhance optical signals [4]. Several transduction mechanisms based on optical technologies, such as surface plasmon resonance (SPR) and fluorescence signal enhancement, particle motion and soft polymer materials will be presented [5]. I will present my current research focusing on developing implantable biosensor device for in vivo pharmacokinetic measurements for preclinical studies in neuropsychiatric disease treatment.

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## Session 4: Current and future prospects of bio & nanotechnology

**The present situation in materials research activity in Mongolia and possible future directions emphasise utilising natural resources and various wastes.**

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In the modern world, a country's development is determined by its science and technological achievements and innovation activity. High-developed countries' science and technological policies focused on high-end products in modern technological development such as AI, biomedical, chip design, environmental technology, etc. In developing countries, the main research topics are the supply of raw materials for high-end products, high-purity materials production, sustainability, etc. In Mongolia, where the main income is generated via mineral resource exploration, an increase in the income from mineral resources by value addition and reduction of environmental stress through environmentally benign technology is becoming a very important task. In this paper, we report the latest research results on the value addition of mineral sources such as molybdenite by using mechanochemical technology, using industrial wastes such as floatation waste of the copper minerals for substitution of the natural sand for mortar production and ashes of the thermal power stations for preparation of geopolymer type binder preparation. These results are crucial in our efforts to address the environmental challenges associated with mineral resource exploration in Mongolia, and they reiterate the importance of our work in the context of global environmental issues, making it clear that our research is not just about local solutions, but about contributing to the global efforts in environmental sustainability.

The used raw materials were characterised by various analytical techniques, such as XRD, DTA-TG, SEM, TEM, PSD, BET, and mechanical testing methods.

The alkali activation technique was used for the production of geopolymer materials. For the binder preparation, fly ash and pond ashes from the various thermal power stations in the central region of Mongolia and fluidised bed combustion ash from the Amgalan thermal station were used. Research revealed that it is better to use fly ash instead of pond ashes for the binder



preparation because of the low moisture content and the virgin surface of the original ashes. The use of floatation waste for mortar preparation should also be limited at a certain value because the chemical reagents used for floatation negatively influence the waste surface's and polymeric binder's binding properties. Mechanochemical reduction of the molybdenite can occur during the milling of the wolframite with the Mg metal. However, the outcomes of the process were sluggish to consider it an alternative technology to traditional molybdenite processing.



## Biosynthesis, physical properties, and biodegradability of $\alpha$ -methylated polyhydroxyalkanoates

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Petroleum-based plastics have become indispensable in human life, serving a multitude of purposes. However, their widespread utilization poses significant environmental and health hazards. Indeed, petroleum-based plastics contribute significantly to greenhouse gas emissions, including CO<sub>2</sub>, throughout their manufacturing and processing stages, intensifying the challenges of global warming and climate instability. Furthermore, their resistance to degradation and challenges in recycling further exacerbate resource depletion and pollution concerns. Consequently, there is an urgent need to develop biodegradable renewable alternatives.

Polyhydroxyalkanoate (PHA) is a microbial polyester recognized for its exceptional biodegradability, which makes it a promising environmentally friendly plastic [1]. The structure and characteristics of PHA vary according to their monomers, with poly[(*R*)-3-hydroxybutyrate] [P(3HB)] being the most common and basic form. However, P(3HB) faces challenges, such as high crystallinity and low elasticity, which limit its practical applications. To address these limitations, various PHA copolymers have been developed by copolymerizing 3HB with other monomers such as 3-hydroxyvalerate (3HV), 3-hydroxy-4-methylvalerate (3H4MV), and 3-hydroxyhexanoate (3HHx). 3HB-based copolymers enhance the overall material properties of PHA, surpassing the limitations associated with P(3HB) alone. PHAs incorporating  $\alpha$ -methylated monomers, 3-hydroxy-2-methylbutyrate (3H2MB) [2], 3-hydroxy-2-methylpropionate (3H2MP) [3,4], 3-hydroxypivalate (3HPi) [5], and 3-hydroxy-2-methylvalerate (3H2MV) [6,7], epitomize pioneering bio-based materials. These monomers confer superior crystallization behavior to polymers and exhibit high thermal stability, rendering them tough.

In the presentation, I will talk about the biosynthesis method of  $\alpha$ -methylated PHA, its physical properties, and biodegradability.

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## *Cenococcum geophilum* sclerotia: a key biomaterial in diverse environment

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*Cenococcum geophilum* is the most common and globally abundant ectomycorrhizal fungus, which dominates in forests of arctic, temperate, subtropical zones and particularly in extreme environments with abiotically stressful habitats such as high drought stress, phytotoxic stress, and fire stress. *Cg* has a unique life cycle forming spherical melanic resistant propagules called “sclerotia”, with its long-life (>1000 years) to maintain genetic diversity of the fungus and provide habitat of endophytic bacteria required for natural ecosystem. *Cg* sclerotia is materially characterized as dominance of sugar chains (Watanabe et al. 2007), key sources of forest soil polysaccharides (Sugiura and Murayama 2017), pigment with dihydroxyperylenequinone structure (Kumada and Hurst 1965), and precursors of perylene trapped in lacustrine sediments and sedimentary rocks (Ito et al. 2012). The biochemical properties of *Cg* sclerotia that allow them to remain in soil and retain their structure are unclear. *Cg* sclerotia is a key material to deepen our knowledge on environmental regeneration and conservation.

In this paper, we focus on metal accumulation in *Cg* sclerotia in various soil environment and discuss the function of *Cg* sclerotia in soil ecosystem. Biotransformation pathways in terms of sclerotia development stage were pointed out to explain the mechanism of metal accumulation for *Cg* sclerotia.



## **Towards a green future with structured catalysts; fluegas treatment and CO<sub>2</sub> activation at near-industrial level**

**Sàpi Andràs**

Billions of dollars are investigated into the information industry. It is less known that a similar budget is used for planning catalysis and industrial catalytic processes. The increasing demand for high activity and selectivity products needs new technologies and understanding of heterogeneous catalysis. The former trial-and-error method can be exchanged with new techniques using in-situ methods for molecular level understanding under reaction conditions as well as controlled nanotechnology. These techniques could be exploited in CO<sub>2</sub> activation towards e-fuels to solve energy and climate crises.

In our research, we are focusing on direct hydrogenation of carbon-dioxide with high activity and controlled selectivity of C<sub>1</sub> as well as C<sub>5+</sub> products using designed nanoparticles and supports as well as interfaces followed by molecular level understanding of the reactions. I will show plenty of results on CO<sub>2</sub> activation towards CO and CH<sub>4</sub> with high activity and >99% selectivity beside showing novel catalysts of production of C<sub>5+</sub> liquid fuels with tunable selectivity of catalyst moderation, e.g demonstrated FeZnCeO<sub>x</sub> catalyst with >99% of C<sub>5+</sub> iso-paraffins or tunable jet-fuel catalyst from designed Fe-based systems. Beside regular characterization techniques (HRTEM-ED-EDX, SEM-EDX, DRIFTS, XRD, BET, H<sub>2</sub>-TPR, NH<sub>3</sub>-TPD etc.) NAP-XPS, in-situ RAMAN, XRF as well as DRIFTS techniques helped for molecular level understanding of the processes for future catalysts design.

Under the umbrella of RRF-2.3.1-21-2022-00009, titled National Laboratory for Renewable Energy by the Recovery and Resilience Facility of the European Union within the framework of Programme Széchenyi Plan Plus, we are scaling up Fe-catalyst based C<sub>5+</sub> production to 5-10 kg liquid product/day based on solar power-motored H<sub>2</sub> generation. Also, I will speak about our TRL-7 level retrofit ceramic supports for flue gas treatment of fireplaces.



## Identification and functional analysis of key proteases involved in *Schistosoma japonicum* cercariae penetration

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*Schistosoma japonicum*, a zoonotic parasite with a wide range of mammalian hosts, is one of the major pathogens of schistosomiasis. Cercaria is the only stage that can infect the mammalian hosts. Proteases secreted by cercariae are specifically adapted to effectively degrade host tissues to aid penetration and migration of the larvae. In this study, based on RNA-Seq, we first mapped the detailed transcriptome profiles of four *S. japonicum* larval stages (eggs, miracidia, sporocysts and cercariae). By analyzing the stage-specific/enriched genes, we identified functional genes associated with the biological characteristics at each stage, and found elastase (*SjCE2b*) and leishmanolysin might contribute to the cercariae invasion. Through the comparative analysis of miracidium and cercaria, we found that different groups of proteases were highly expressed in these two stages. Leishmanolysin, neplilysin and trypsin may be involved in the miracidia invasion, while cathepsin B, elastase and leishmanolysin may be involved in the cercariae invasion. We used linoleic acid and mouse skin as stimulants to induce cercariae to release their acetabular glands contents, and identified the protein components by mass spectrometry. Both stimulants can induce the secretion of *SjCE2b* by cercariae, but leishmanolysins were only presented in skin-induced group. Through the venn diagram analysis of the proteome and secretome, we identified 9 proteins that were highly expressed in cercaria and would be secreted in large quantities during the invasion process, including elastase (*SjCE2b*), leishmanolysins (*SjLeish-1/2/3*), calcium-binding protein (*CaBP*) and venom allergen-like proteins (*VAL4/5*). We focused on three key protease - one elastase (*SjCE2b*), one cathepsin (*SjCB2*) and one leishmanolysin (*SjLeish-1*), and studied their functions during the cercariae invasion process. Our results revealed that *SjCE2b* plays a





pivotal role in the *S. japonicum* penetrating process, and *SjCB2* not only can help digesting the skin, but also can cleave immunoglobins and complement proteins, suggesting that it may play other roles in the host-parasite interactions, *SjLeish-1* may play important roles in inhibiting the host's immune response. This study not only improves the transcript and protein information of the *S. japonicum* larval stages, but also deeply explores the molecular mechanisms of *S. japonicum* cercariae invasion, and provides many new targets for the development of anti-schistosomiasis vaccines and drugs.

**Key words:** *Schistosoma japonicum*, invading, proteases



## **Directed-differentiation of neural stem cells into normal and abnormal astrocytes based on bio-nano interface**

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The discovery of neural stem/progenitor cells (NSPCs) in the central nervous system (CNS) of adult mammals, along with significant achievements in *in vitro* culture systems utilizing cell-cell aggregated neurosphere assay under defined conditions, have revealed that NSPCs can repair brain injuries and diseases by generating neurons, astrocytes, and oligodendrocytes. Astrocytes, the most abundant glial cells in the mammalian CNS, play a crucial role in maintaining the homeostasis of the entire CNS. Reactive astrocytes are abnormally induced by various neurological diseases *in vivo*, in which the specific protein glial fibrillary acidic protein (GFAP) has been found to be upregulated. However, its role and functions are poorly understood. Here, we have developed a serum-free monolayer culture system for NSPs that can avoid heterogeneity issues caused by traditional neurosphere assay. Based on this culture system, we successfully differentiated the neural stem cells into two types of astrocytes, typical GFAP-expressing and high GFAP-expressing. Our findings provide a platform for characterizing the function of abnormal astrocytes and regulating their morphogenesis, which leads to intrinsic and extrinsic signaling of synaptic dysfunction. More importantly, the novel highly efficient directed-differentiation of neural stem cells into normal and abnormal astrocytes is achieved in the absence of any soluble factor in culture.

**Key words: biomaterials, neural stem cells, astrocytes, bio-nano interface.**



## **Double hits with bioactive nanozyme based on cobalt-doped nanoglass for acute and diabetic wound therapies through anti-inflammatory and pro-angiogenic functions**

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Regeneration of pathological wounds, such as diabetic ulcers, poses a significant challenge in clinical settings, despite the widespread use of drugs. To overcome clinical side effects and complications, drug-free therapeutics need to be developed to promote angiogenesis while overcoming inflammation to restore regenerative events. This study presents a novel bioactive nanozyme based on cobalt-doped nanoglass [1] (namely, CoNZ), which exhibits high enzymatic/catalytic activity while releasing therapeutic ions. Cobalt oxide “Co<sub>3</sub>O<sub>4</sub>” tiny crystallites produced *in situ* through a chemical reaction with H<sub>2</sub>O<sub>2</sub> within CoNZ nanoparticles play a crucial role in scavenging ROS. Results showed that CoNZ-treatment to full-thickness skin wounds in mice significantly accelerated the healing process, promoting neovascularization, matrix deposition, and epithelial lining while reducing pro-inflammatory signs. Notably, CoNZ was highly effective in treating pathological wounds (streptozotocin-induced diabetic wounds). Rapid scavenging of ROS by CoNZ and down-regulation of pro-inflammatory markers while up-regulating tissue healing signs with proliferative cells and activated angiogenic factors contributed to the observed healing events. *In vitro* experiments involving CoNZ-cultures with macrophages and endothelial cells exposed to high glucose and ROS-generating conditions further confirmed the effectiveness of CoNZ. CoNZ promoted angiogenesis was attributed to the release of cobalt ions, as evidenced by the comparable effects of CoNZ-extracted ionic medium in enhancing endothelial migration and tubule formation via activated HIF-1  $\alpha$  [2]. Finally, we compared the *in*



*vivo* efficacy of CoNZ with the clinically-available drug deferoxamine. Results demonstrated that CoNZ was as effective as the drug in closing the diabetic wound, indicating the potential of CoNZ as a novel drug-free therapeutic approach [3].

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## **From local to global R&I: practices in next generation material development for bio-medical applications**

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In this talk, I will present our currently ongoing experience in the development of next generation bio-nano materials, focused on the characterization, toxicity & efficacy assessments and design of next generation bio-nano materials, along with our strategy to transform smoothly our research and innovation (R&I) from local to global. In our “Institute for Next Generation Material Design (INGMD)”, we aim to develop safe, sustainable and high-performance nanomaterials for biomedical applications. To achieve this goal, we are conducting research R&I on the following topics. 1) Perform proteomics and transcriptomics analyzes to characterize molecular mechanisms of the interactions between the biological cells and nanoparticles, using in vitro cells, organoids, and 3D models to predict the toxicity of nanoparticles. 2) In vitro and in silico analysis to replace animal testing, so alternative animal testing methods are performed to reduce animal testing. 3) Prediction of interaction between nanoparticles and cells using new approach methodologies (NAMs) and long-term toxicity of nanoparticles, development of an effective experimental data analysis pipeline to evaluate the stability of nanoparticles. Under the umbrella of the INGMD, domestic industry-academia-research collaboration clusters, such as the Center for Next Generation Cytometry (CNGC), the Safe and Sustainable Nanotechnology community (S2NANO), and the artificial intelligence-based exosome (exosome.AI) consortium were created. For the smooth transition of our R&I capabilities from local to global, we are participating various multilateral collaborative research consortia, as a part of the European H2020 and Horizon Europe programs (e.g., ACEnano, NanoSolveIT, SABYDOMA, CompSafeNano, CHIASMA, INSIGHT), which include 20+ research institutes and universities from various EU countries.



## Poster session

### **Studies on fabrication of nanostructured few-layer MoS<sub>2</sub> and their physicochemical characterization**

**Narangerel Adiyasuren**

In this research work, mono-mineral fraction and 2D MoS<sub>2</sub> nanomaterials were extracted from molybdenite-bearing minerals, and their physicochemical properties were studied. A single crystal was extracted from the molybdenite-containing minerals of the "Erdenet Plant" copper-molybdenum deposit by petrographic method, and it was determined to be highly pure with 2H phase by X-ray diffractometer analysis. Furthermore, by using a ball mill to produce powder with an average size of 2.89  $\mu\text{m}$ , 2D MoS<sub>2</sub> nanomaterials with 5-layer-to-bulk and 4-layer dimensions, with bandgap energy of 1.86 eV and 1.92 eV, were obtained by ultrasonication with probe and salt-assisted in liquid medium. In the future, it is possible to carry out research on obtaining potential mono-layer-MoS<sub>2</sub>, establishing optimal conditions for mass production, and applying it to various biomedical applications by modifying and stabilizing the surface.

## Some results of formulation of nano calcium supplements with cholecalciferol and rhodiola extract for treatment of osteoporosis

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**Introduction:** Osteoporosis is a skeletal condition characterized by decreased density (mass/volume) of normally mineralized bone [1]. The reduced bone density leads to decreased mechanical strength, thus making the skeleton more likely to fracture [2]. Calcium nanocomposites, cholecalciferol, and the *Rhodiola* extract are known to have antiosteoporotic effect [3]. The current study aimed to investigate the development of chewable tablets with nano calcium, cholecalciferol and rhodiola extract for treatment of osteoporosis.

**Methods:** Chewable tablets by using nano-calcium carbonate, cholecalciferol, *Rhodiola* dry extract leveraging on findings from Mongolian traditional medicine. The chewable tablet had an average weight of around 680 mg with an active content percentage of calcium ion 68.17% and salidroside - 0.94 mg/tab. The physicochemical properties of chewable tablets satisfied the pharmacopoeial requirements for tablets.

**Results:** We assessed the manufacturability of powders based on their flow and compaction properties by using the compressibility index and Hausner ratio, respectively. We selected the wet granulation process based on the poor flow properties of API and its blends with common compaction excipients. The different formulations (F1–F6) of chewable tablets were evaluated according to their palatable properties and facilitation of dissolution.

Formulation 1 (Nano calcium carbonate, Rhodiola extract, Vitamin D, citric acid, sorbitol, orange powder, polyvinylpyrrolidone (Kollidon® 30), sodium croscarmellose, magnesium stearate, cacao powder, aspartame) satisfied the requirements of a chewable tablet. The average weight of the chewable tablets was 676.5± 1.13 mg. The weight variations of all measured tablets were <1.92 % and far below the pharmacopoeial limit. Salidroside, the active compound of *Rhodiola rosea* was about 0.94 mg per each tablet. These results were near the theoretical values as calculated according to the input amounts of the components. The hardness of the tablet was 0.8 MPa. The friability of chewable tablets was 99%, which was notably below the pharmacopoeia limit of 97%. The disintegration time of chewable tablets was 2 minutes.



**Conclusion:** We developed chewable tablets containing calcium nanocomposites, cholecalciferol and, *Rhodiola* extract. The physicochemical properties of chewable tablets satisfied the pharmacopoeial requirements for tablets.

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## **Antioxidant and antibacterial properties of *artemisia sieversiana* Willd. extracts: a focus on ethyl acetate extract**

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This study investigates the antioxidant and antibacterial properties of *Artemisia sieversiana* Willd. extracts, focusing on the ethyl acetate extract. Five groups of extracts (hexane, chloroform, ethyl acetate, n-butanol, and water) were obtained from the thick methanol extract of *Artemisia sieversiana* Willd. Each extract was evaluated for antioxidant and antibacterial activity. The ethyl acetate extract, which showed the highest biological activity, was further analyzed for its total phenolic content (TPC) using the Folin-Ciocalteu reagent method and total flavonoid content (TFC) using the aluminum chloride colorimetric method.

Antioxidant activity was assessed using DPPH, ABTS, and FRAP assays. The ethyl acetate extract exhibited significant antioxidant properties, with an IC<sub>50</sub> value of 54.8±0.47 µg/mL in the DPPH assay and high inhibitory percentages in both ABTS and FRAP assays, indicating superior efficacy compared to extracts obtained with butanol, chloroform, and hexane.

Antibacterial activity was tested against Gram-positive (*Bacillus subtilis*, *Staphylococcus aureus*) and Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*) using the disc diffusion method. The ethyl acetate extract demonstrated significant antibacterial effects, with inhibition zones measuring 12.32±0.21 mm for *Bacillus subtilis* and 13.21±0.16 mm for *Staphylococcus aureus*, highlighting its potential as an effective antibacterial agent. Phytochemical analysis identified substantial amounts of secondary metabolites in the ethyl acetate extract, including 23.4±0.07 mg GAE/g of phenolic compounds and 0.084±0.25 mg RE/g of flavonoids. The analysis also revealed a low alkaloid content, suggesting a moderate toxicity profile for the extract.

These findings highlight *Artemisia sieversiana* Willd. as a promising source of natural antioxidant and antibacterial agents. The study underscores the need for further research to isolate and characterize the specific bioactive compounds responsible for these beneficial activities, which could pave the way for their potential therapeutic applications.



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## **Aspen plus simulation of copper cathode production by L-SX-EW processing**

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With the decline in both the number and quality of high-grade copper ore mines and the increasing demand for copper, it has become imperative to process oxidized, low-grade ores and previously unextracted minerals. This study utilizes the L-SX-EW (Leaching-Solvent Extraction-Electrowinning) process, simulated through Aspen Plus® modeling software. A theoretical model was developed reflecting actual plant operations, incorporating reagent and output data. The results indicate a deviation of 1.22% in the leaching process and 4.45% in the SX-EW process when compared to real-world data. Additionally, a sensitivity analysis of copper extraction was performed, examining the impact of variations in acid and organic solvent concentrations. The results of this analysis were thoroughly evaluated and discussed.



## **Superhydrophobic modification and morphological characterization of camel wool fiber surfaces with silica nanoparticles by AFM method**

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Camel wool possesses numerous advantages, including heat and cold insulation, minimal environmental impact, suitability for use as insulation material, and high textile versatility. By applying a superhydrophobic layer to the surface of camel wool, the durability and lifespan of the textile can be extended, while also imparting resistance to water and other pollutants. This attribute is crucial for reducing the frequency of textile washing and for the preservation of archaeological artifacts of textiles.

Superhydrophobic fibers were formed using the dip-method in a solution containing silicon dioxide nanoparticles. Before chemical treatment, the wetting contact angle of water droplets measured  $116^\circ$ , which significantly increased to  $158^\circ$  after chemical modification, indicating the attainment of superhydrophobic properties.

Characterization of the surface morphology of camel wool fibers was conducted through Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR). Moreover, a Contact Angle Meter was utilized to assess the surface's superhydrophobicity and water impermeability.

**Keywords:** Fiber surface, water contact angle, chemical modification, dip-coating



## Enhancing magnetic properties and Curie temperature of 4d and 5d transition metal and p-block element co-doped Fe<sub>2</sub>P alloys

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Permanent magnets play vital role in modern transitional technologies from electric motors to medical equipment. Iron phosphide (Fe<sub>2</sub>P) alloys exhibit excellent magnetic properties and are standout candidates to fill the gap magnets between hard ferrite and rare-earth based permanent magnets (PM). One of the major problems with Fe<sub>2</sub>P is the low Curie temperature (T<sub>c</sub>) compared with other PM materials. In this work, we investigated M<sub>0.04</sub>Fe<sub>2-x</sub>P<sub>y-1</sub>Z<sub>y</sub> (M = 4d and 5d heavy transition metals, and Z = p-block elements such as B, C, N for 2<sup>nd</sup> row, Al, Si and S for 3<sup>rd</sup> row and Ga, Ge, As and Se for 4<sup>th</sup> row) using the density functional theory (DFT) to determine if these doping compositions increase Curie temperature of the system. Our results show that Os 5d heavy transition metal doping enhances magneto-crystalline anisotropy up to 3.32 MJ/m<sup>3</sup>, 10% higher than for pristine Fe<sub>2</sub>P. We attribute this effect to the spin-orbit coupling of high nuclear charge and close to the half-filled electron configurations. Furthermore, our calculations suggest that doping with (M = Ru, Os, and Pt, Z = B group (B, Al, Ga) elements increases Curie temperature (T<sub>c</sub>), magnetic saturation (M<sub>s</sub>) and energy product (BH<sub>max</sub>) of M<sub>0.04</sub>Fe<sub>2-x</sub>P<sub>y-1</sub>Z<sub>y</sub> composition.

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## ***In vitro* cultivation and acclimatization to natural conditions of *Lycium ruthenicum* Murr**

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### Background

*Lycium ruthenicum* Murr., or wolfberry, is vital for sand migration and soil stabilization. Rich in proteins, polysaccharides, flavonoids, amino acids, and vitamins B1, B2, and C, it helps prevent diabetes, vision loss, lung diseases, and improves liver and kidney functions.<sup>[1]</sup>

For the initiation of *in vitro* cultures of wolfberry, shoot pieces, inoculated in culture medium Murashige-Skoog(MS), supplemented with hormones of different concentrations (IBA – Indole-3-butyric acid, GA – gibberellin acid, BAP – benzylaminopurine, NAA - naphthalene acetic acid) were used.

### Methods

For *in vitro* culture, seeds were sterilized using ethanol and sodium hypochlorite, then rinsed with sterile water. The sterilized seeds were planted in ½ MS medium with sucrose and agar, pH adjusted to 5.75-5.85, and cultured under controlled light and temperature conditions. 4 different hormones were used in 6 different variations.

### Results

*In vitro* regeneration of wolfberry shoots was successfully achieved using a nutrient medium containing IBA (0.5 mg/L) and GA (0.5 mg/L), while root regeneration was optimized using IBA (1.5 mg/L; 2.0 mg/L) and GA (0.5 mg/L) in a ½ MS nutrient medium. When 30-day-old micro-plants were transferred to an ex vitro environment, a soil mix of black soil, sand, and vermiculite (1:1:1) resulted in a viability rate of 100% (15 micro-plants).

### Conclusion

This study highlights the medicinal and economic potential of wolfberry, emphasizing the need for sustainable cultivation practices and the effective propagation of this valuable plant.

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## **Nanoceria-GO-intercalated multicellular spheroids revascularize and salvage critical ischemic limbs through anti-apoptotic and pro-angiogenic functions**

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Critical limb ischemia (CLI) is one of the most devastating peripheral arterial diseases. Cell therapy has been considered potential for the treatment of ischemic damages, including CLI. Compared to individual-cell delivery, multiple-cell delivery in the form of spheroids has often been shown better therapeutic capability and outcomes. Furthermore, engineering cells by combining with nanomaterials has proven to improve the therapeutic potential in CLI. We focused on the role of Nano ceria component in CeGO in terms of ROS scavenging and HIF1 $\alpha$ -activated pro-angiogenic capacity of multicellular spheroids. The intercalation of CeGO within HUVEC/MSC spheroids was shown to effectively scavenge environmental ROS, thus preserving cell survival and proliferative capacity (Ki67+ cells up-regulated) while concurrently reducing apoptotic signalings (BAX/p38/Cas3 down-regulated and Bcl2 up-regulated), which is helpful for securing the population of transplanted cells that can function to promote angiogenesis and tissue healing. On the other hand, the role of CeGO, particularly in the direct modulation of oxygen tension, was also proven which was mediated via APE/Ref-1 signaling pathway.

In this study, we demonstrated the potential of CeGO nano-microsheets as the multicellular delivery platform for CLI treatment. CeGO intercalated in HUVEC/MSC delivery is considered a potential nano-microplatform for CLI treatment, by scavenging excessive ROS and enhancing transplanted cell survival, while stimulating angiogenic events, which collectively help revascularization and tissue recovery, salvaging critical ischemic limbs.

Key words: Nano ceria, spheroids, CLI, angiogenesis



## Mechanical and liquid phase exfoliations of MoS<sub>2</sub>

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Two-dimensional layered material MoS<sub>2</sub> is an emerging material with wide-ranging applications in electronics, optoelectronics, energy conversion and storage. There are many methods for synthesizing continuous MoS<sub>2</sub> films that are capable of producing good quality MoS<sub>2</sub> layers. However, it is challenging to produce large-area MoS<sub>2</sub> films and large-area growth methods are needed to open the way for applications. This study focuses on the fabrication of large-area, atomically thin MoS<sub>2</sub> films using mechanical and LPE exfoliation techniques. Quantitative analysis of optical contrast, AFM, and combined resonant Raman spectroscopy was performed on few-layer MoS<sub>2</sub>, indicating a clear distinction between flakes with different numbers of layers.

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## Plant mediated synthesis of silver nanoparticles: their characteristic properties, antibacterial effect and their burn wound healing efficacy

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Green synthesis of nanoparticles has gained widespread attention due to their high stability, cost effectiveness, availability and low toxicity. One of the routes of green synthesis involves the utilization of plants' bioactive compounds to generate nanoparticles. The current study aims to develop silver nanoparticles (AgNP) with several plants, such as *Carduus crispus* (AgNP-C), *Rhodiola rosea* (AgNP-R) and *Campanula glomerata* (AgNP-G), and determine their characteristics, synthesis yield, antibacterial effects and burn wound healing efficacy. The silver nanoparticles synthesized with different plants exhibited distinct physical and chemical characteristics. And their characterization was assessed using UV-Vis spectroscopy, FTIR, Zeta potential, XRD, EDX, PCCS, AFM and SEM techniques. The results of our research indicated that manipulation of nanoparticle characteristics may be possible using plants specifically different plant organs. In addition, the biological and biomedical application of the synthesized AgNPs were studied by evaluating the effects of AgNP-loaded ointment on BALB/c mice's burn model. Our findings confirmed that AgNP-loaded ointment accelerated wound healing process through regulation of pro-inflammatory and anti-inflammatory gene expression, and the histological evaluation revealed the wound site treated with AgNP ointment had fewer mast cell infiltration. Moreover, the synthesized AgNPs inhibited both Gram-positive and Gram-negative bacteria at low concentrations while also exhibiting low toxicity effect. The findings suggest that the developed AgNP-loaded ointment has the potential to be applied in the field of biomedicine.

## Solid waste of tannery – opportunity of gelatin based organic fertilizer

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Mongolian agricultural area affected by erosion and the soil damage is increasing [1], so it must be supplemented with mineral and nutrient organic fertilizers [2]. For this purpose, this study was carried out to obtain gelatin based organic fertilizer from chrome free solid waste of the tannery.

The pretreatment of goat pelt was done by hydrochloric acid for 20 hours then for 3 months in lime solution. The gelatin was extracted at 60°C for 6 hours and dried. Prepared 4 different fertilisers: NK-1, NPK-2, NPK-3, NPK-4 based on gelatin with different ratio.

The yield of acid-treated skin gelatines were 8.2%, alkali-treated skin gelatines 8.4% and the pH of acid-treated and alkali-treated skin gelatines were 3 and 7 respectively. SEM-EDS analysis showed surface-morphology and content of elements. Thermogravimetric analysis was used to characterize the thermal stability of the gelatines. Those gelatins showed a weight loss (54-58%) in the temperature range between 269°C-499°C. FTIR spectra for gelatin extracted from acid and alkali treated skins showed -O-H, -C-H, C=O, -NH-, O=C=C stretching. For fertilisers, 8 gr of 4 deifferent fertilezers in 4 kg of soil and planted chinese cabbage in fertilised soil. Determined plant growth height and leaf area by 1 and 2 weeks after. After 14 days of plantation NPK-4 organic fertiliser was given the best results, height was 43 mm, leaf area was 236 mm<sup>2</sup>.

By the results of the experiments, NK-1 and NPK-4 have low polyacrylamide, thus can release N, P, K needed to plants through the soil for develop plant nutrition. It gives the opportunity to produce organic fertilizer with gelatin from tannery solid wastes, thus it will increse usage of wastes and decrease environmental pollution due to tannery wastes.

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## Characteristics and effects of hair products containing Mongolian natural mineral zeolites

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Hair and scalp diseases are currently one of the most vibrant and rapidly evolving fields in dermatology. With advances in technology, many treatments have been proposed for seborrheic dermatitis, atopic dermatitis, and psoriasis. However, due to the recurrent nature of these diseases, scientists are also looking for routine treatments. One of the easiest and most effective methods is the use of hair treatment products. Shampoo, conditioner, hair mask. These preparations are safe to use daily and provide nutrients and other essential vitamins to your hair and scalp. The uniqueness is that all products in the set contain zeolites, rich in clinoptilolite. Topical application of clinoptilolite has been shown to be effective in treating skin ulcers, reduce healing time for wounds and surgical incisions, and have several benefits in the treatment of psoriasis. The clinoptilolite contents in shampoo, conditioner, and mask of this set were 1.71%, 1.02%, 2.64 %, respectively, and heavy metals levels measured in all product samples were within the permissible limits for cosmetics. Here, we investigated the effects of zeolite containing hair care products on human scalp parameters. A total of 36 people (control group n=16, experimental group n=20) living in Ulaanbaatar, aged between 15 and 55, were subjected to the measurement of scalp parameters and scalp disease symptoms (participants have seborrheic dermatitis, atopic dermatitis, and psoriasis) before and after using the product. Participants in the experimental group were involved in 30 days of treatment with the “Zeolite” set product. Before and after treatment, scalp pH, moisture, and oil content were analyzed at five different scalp sites using the Khazaka Courage instrument. As a result of using the “Zeolite” set product for 30 days, participants' hair density increased by 0.8-1.6 times in occipital, parietal and frontal regions, whereas scalp oil decreased in temporal, parietal and frontal regions, indicating improved condition of the scalp. Furthermore, some common symptoms such as itching, dryness, and dandruff decreased by 33.3%, 26.7%, and 29.8%, respectively. Research results suggest that the potential effects of zeolite may reduce symptoms of scalp diseases and improve hair and scalp properties through the effects of clinoptilolite.



Key word: Scalp, Zeolite, Clinoptilolite, Hair care products



## **Analysis for germination activity and salinity stress resistance on some mongolian pasture plants**

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Mongolia, located on the Central Asian plateau, has a harsh continental climate. There is a huge variation in air temperature not only between winter and summer but also between day and night. The weather is unstable and changes several times, even in one day, and the air is dry, and the wind is strong. The total amount of precipitation is very low, with short summers and long winters. Mongolian wild plants are believed to have certainly adapted to external environmental stresses such as heat, cold, drought, strong sunlight, salinity, poor soil, and the impact on livestock and other animals. In other words, we consider Mongolia's natural and climatic conditions to be a living and valuable research object, not artificial, to discover plants resistant to abiotic and biotic environmental stress. This research is not only cognitively significant in explaining plants' environmental adaptability and the role of plants in ecosystems from the point of view of genomics but is also important in discovering the benefits of limited natural plant resources and contributing to social and economic development.

Here, we started the germination tests on 73 pasture plants collected from the Tuv, Dornogovi, Uvs, and Selenge provinces of Mongolia. As a result, 32 species germinated within 7 days, and notably, six species germinated within the first 24 hours. Among them, three plant species demonstrated the fastest germination rates and the ability to germinate at vernalization stage. To reveal salinity stress tolerance on the fastest germinated plants, plants were treated with NaCl for 3 weeks, and plant biomass and malondialdehyde (MDA) content were measured. Four plant species showed high tolerance against salt stress with increasing biomass and a low concentration of MDA content. In addition, according to increasing concentration of NaCl, *Chloris virgata* showed salty crystals on the leaf surface. Further, more detailed exploration will be needed.



## Isolation, purification, and antioxidant activity evaluation of polysaccharides from cynanchum thesiodes (Freyn).K.Schum

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This study aimed to isolate and purify polysaccharide components from *Cynanchum thesiodes*, a natural plant, and to investigate their structural analysis and antioxidant activities. Crude polysaccharide was extracted from *Cynanchum thesiodes* using the hot water extraction and alcohol precipitation method. Protein removal was conducted using the Sevag method, followed by decolorization with H<sub>2</sub>O<sub>2</sub> [1].

The total sugar content was determined by the phenol-sulfuric acid method, and molecular weight and monosaccharide composition were analyzed. Polysaccharides with homogeneous molecular mass were purified by ion exchange chromatography and gel chromatography for further structural analysis and biological assay [2]. Finally, the scavenging abilities of DPPH, superoxide anion, and hydroxyl radicals of polysaccharides were measured to evaluate their antioxidant capacities [3].

Results: The total sugar content of crude polysaccharides from *Cynanchum thesiodes* was found to be 33.16±0.27%, mainly consisting of rhamnose, arabinose, galactose, glucose, mannose, and galacturonic acid. Four fractions, CTST-W, CTST-0.2M, CTST-0.5M, and CTST-1.0M, were separated by DEAE 52 ion exchange column with yields of 9.79%, 5.44%, 3.04%, and 0.09%, respectively. Water fraction CTST-W was further purified by gel chromatography and yielded one homogeneous polysaccharide, CTST-W2 fraction (Mw=9862 Da). Antioxidant capacity showed that CTST and its fractions (CTST-W, CTST-0.2M, CTST-0.5M, and CTST-1.0M) had certain DPPH, superoxide anion, and hydroxyl radicals scavenging abilities, in a dose-dependent manner.

Conclusion: This study provides a theoretical basis for further research on the isolation, purification, structural analysis, and biological activity of *Cynanchum thesiodes* polysaccharides. It aims to boost the application of *Cynanchum thesiodes* in medicine and functional foods, and promote the development and application expansion of natural plant polysaccharides.

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## An amount that determines the particle size of fortified calcite

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Calcium is mostly found in nature as calcium carbonate, and it is considered to be abundant and bioactive. Calcium carbonate is composed of calcium (Ca), carbon (C), and oxygen (O) and occurs naturally in mammalian bones, teeth, calcite, limestone, marble, or shells. Among them, calcite is used in traditional medicine as part of many types of medicines. Therefore, in our research, we experimented with adding calcite, a mineral raw material used in traditional medicine, to the nanoscale using one of the main methods of nanotechnology, the top down method.

In the previous study, the physical and chemical analysis of the samples collected from 19 points in Mongolia was carried out. Among them, samples with a high calcium content and a good transition from calcium carbonate to calcium oxide were selected based on the calcite samples before and after taming.

The samples were milled with zirconium balls at different speeds of 50, 350, and 500 rpm to decrease particle size. The samples milled with a ball mill were soaked in 0.25% milk. After fortified, the samples were thoroughly dried and analyzed by XRD, AFM, and PCCS to determine the particle size. The crystallization size was 27.8-36.35 nm by the XRD. The particle size was 18.79-65.93 nm by the AFM. By PCCS, the particle size was 8973.06 nm, 5528.26 nm, 2883.49 nm, and 1961.9 nm, respectively.

From the above results, the amount of crystallization increases with the increase of rotation speed, but the amount of crystallization of the sample milled at 500 rpm rotation speed decreases. Also, according to the results of the measurement, the calcite samples were modified to uniform calcium hydroxide. Using a ball mill, the selected samples were subjected to decrease particle size at different rotation speeds, and the nanoscale was determined for each sample, and the samples with 350 rpm were selected as suitable for use.

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## Enhancing intrinsic magnetic properties of ThMn<sub>12</sub>-type Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>11.5</sub>Ti<sub>0.5</sub> through interstitial B, N, and C elements

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The SmFe<sub>11</sub>Ti alloy has been recognized as a possible contender for high-performance permanent magnets thanks to its high energy density product and saturation magnetization. The early transition metal Ti stabilizes the SmFe<sub>12</sub> phase but significantly reduces its permanent magnet performance, thus needs to be minimized. In this presentation, we report the effects of interstitial boron (B), nitrogen (N), and carbon (C) elements on the intrinsic permanent magnetic properties of ThMn<sub>12</sub>-type Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>11.5</sub>Ti<sub>0.5</sub> compound using density functional theory and Monte Carlo simulations. It is demonstrated that the presence of all interstitial elements considered (B, N, and C) substantially improves the permanent magnetic properties of Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>11.5</sub>Ti<sub>0.5</sub> phase while maintaining the structural stability. These results will also be discussed and analyzed in comparison with experimental results.

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## Epitaxial growth of SmFe<sub>12</sub> films by molecular beam epitaxy

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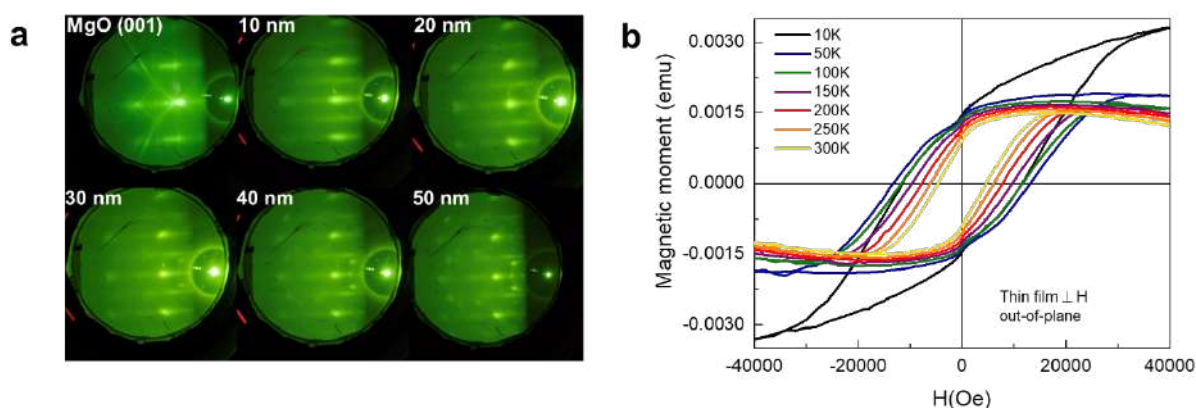
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Although inherently unstable in bulk form, SmFe<sub>12</sub> has garnered significant attention as a potential candidate for the next generation of permanent magnets. Herein, we report the first epitaxial growth of SmFe<sub>12</sub> films using Molecular Beam Epitaxy (MBE), exploring various flux ratios of Sm and Fe to optimize their magnetic and structural properties for high-performance applications.

SmFe<sub>12</sub> thin films were grown on the cleaned MgO (001) substrates (lattice mismatch ~1%) at temperatures of 200° C, 300° C, and 400° C. By controlling the power of effusion cells containing Sm (99.9%) and Fe (99.99%), we achieved various Fe/Sm flux ratios (1, 3, 6, 9, 10.5, and 12).



**Fig. 1.** (a) Evolution of RHEED patterns for 50 nm SmFe<sub>12</sub> films epitaxially grown on MgO (001) substrates. (b) Out-of-plane magnetization at different temperatures

Analysis of RHEED patterns (Fig. 1a) revealed a clear progression in the film growth: up to 20 nm thickness, only iron diffraction lines were observed, indicating the dominance of  $\alpha$ -Fe.



Beyond this threshold, the appearance of dots signified the initiation of the  $\text{SmFe}_{12}$  phase. The coercivity of the out-of-plane magnetization decreased from 1.3 T to 0.46 T as the temperature increased to room temperature (Fig. 1b).

The research is funded by Office of Naval Research and Office of Naval Research Global of the US Department of Defense Grant N62909-22-1-2045.



## **Mineralogical analysis of copper concentrate and tailings from the ore flotation process of a copper molybdenum porphyry deposit**

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Copper-molybdenum porphyry deposits represent significant sources of copper and molybdenum. Therefore, investigating the mineralogical characteristics of porphyry ores and the mineral composition of copper concentrates offers advantages in enhancing metal recovery and optimizing further processing of copper concentrates and by-products. This research aims to analyze the chemical composition of the 'Erdenetin-Ovoo' copper-molybdenum porphyry deposit, along with the morphology and intergranular features of key copper and molybdenum minerals. The study also explores mineral composition in relation to beneficiation technology and product quality. Furthermore, it investigates the chemical composition and structure of minerals in rocks and concentrates, assesses the liberation degree of chalcopyrite minerals in copper concentrates and by-products, and examines mineral associations and grain relationships. Future research directions include expanding studies on copper concentrates and by-products, investigating the production and properties of anode copper and cement copper, and exploring opportunities for production expansion.



## Development of electrospun scaffolds containing nanohydroxyapatite for bone regeneration

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Bone regeneration is a critical area of biomedical research, necessitating advancements in tissue engineering to address bone defects and injuries effectively [1]. Electrospun nanofibers have emerged as promising scaffolds due to their high surface area, porosity, and biomimetic properties resembling the extracellular matrix [2]. This study investigates the impact of nanohydroxyapatite (nHAp) concentrations (1%, 2%, and 3%) incorporated into polycaprolactone (PCL) electrospun nanofibers on bone regeneration acceleration. Methods involved electrospinning PCL solutions containing varying nHAp concentrations, followed by characterization using scanning electron microscopy (SEM) to assess fiber morphology. Moreover, we confirmed the cytocompatibility of these membranes in culture with bone-marrow mesenchymal stem cells (BM-MSCs). Functional assessments included Alizarin Red staining to evaluate mineralization and osteocalcin (OCN) immunofluorescence imaging to quantify osteogenic differentiation. Results indicate that increasing nHAp concentration enhances the structural integrity and bioactivity of electrospun nanofibers, promoting osteogenic differentiation and accelerating bone regeneration processes. SEM analysis reveals uniform fiber morphology across all concentrations, with increasing nHAp showing enhanced surface roughness and mineral deposition. Alizarin Red staining confirms enhanced mineralization in higher nHAp concentrations, while OCN immunofluorescence demonstrates elevated osteogenic marker expression. In conclusion, electrospun nanofibers containing higher nHA concentrations exhibit improved potential for bone regeneration applications.

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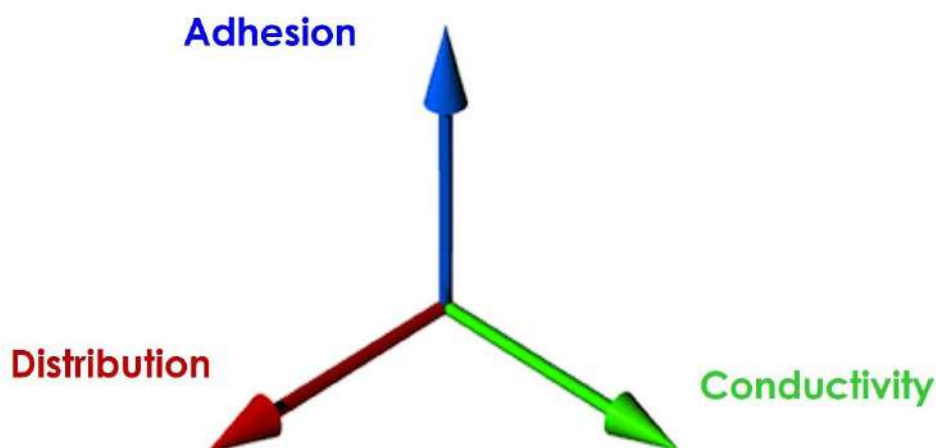
## Influence of long-chain alkyl groups in graft binders on carbon agent distribution for high-capacity anodes in lithium-ion batteries

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A small amount of the conductive carbon agent in lithium-ion battery formulations significantly impacts the rate capability performance of battery. However, the distribution of the conductive carbon material presents in the electrode slurry due to its hydrophobic and inert characteristics. To overcome this problem, the use of dispersant agent was proposed during the electrode fabrication process.

In this study, the *grafting* of adhesive acrylamide monomer and a long-chain alkyl (LCA) monomer onto carboxymethyl cellulose is applied to binder to improve the distribution of the carbon agent in a high-capacity anode. The LCA group in the graft copolymer binder exhibits good dispersibility of the carbon agent and an improved conductive matrix compared to the binder with no LCA monomer. This may be explained by CH- $\pi$  integration between the LCA group in graft polymer and carbon agent. The high-capacity anode with the LCA-introduced graft binder is examined in the slurry level for rheology and dispersion stability, at the electrode sheet level for electrical resistance, adhesion strength, and at coin-cell level for various electrochemical performance including charge/discharge performance.



**Keywords:** Silicon oxide; Graphite; Carbon agent distribution, long-chain alkyl monomer; Acrylamide; Graft copolymer



## Single-cell mass cytometry for the nanotoxicity studies: interaction between the peripheral blood mononuclear cell and nanoparticles

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Single-cell mass cytometry, also known as cytometry by time-of-flight (CyTOF), is a cutting-edge technology for multi-parametric cell analysis in a single-cell mode using metal-tagged cellular markers. This technique minimizes signal overlap and allows for the use of up to 50 metal isotope labels, surpassing the limitations of fluorescence-based flow cytometry. CyTOF can phenotype and profile immune cells by simultaneously detecting heterogeneous immune cell populations. Over the past decade, this technique has become prominent in biological and medical research due to its ability to generate high-dimensional, single-cell data. This capability enables deep profiling of diverse immune cells, monitoring disease progression or recovery, and conducting high-resolution analyses of cytokine expression and signaling responses.

In this study, understanding the nanotoxicity and biomolecular interactions between upconversion nanoparticles (UCNPs) and human immune cells is crucial before UCNPs can be utilized as diagnostic or therapeutic tools. CyTOF enables the detailed characterization of these complex interactions and the safety of UCNPs. We investigated NaYF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> UCNPs with 20 nm core size on 12 immune cell populations including monocytes, B cells, dendritic cells, natural killer cells, CD4 T and CD8T cells, interrogating 14 surface markers. Our findings revealed that UCNPs have a higher affinity for phagocytic cells like monocytes and dendritic cells than for other immune cell types due to cell type dependent heterogeneity as well as incubation time dependence. In addition, the toxicity of NaYF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> UCNPs with low concentrations (from 0.5 to 2 ppm) was analyzed where the major cell types showed similar cell viability in control and UCNP-treated samples. Furthermore, this study provides a framework for the use of CyTOF by describing an innovative approach for analyzing the effects of nanomaterials on different human immune cells.



## Effect of different ball sizes on particle size variation and grinding kinetic of calcite powder using a planetary ball mill with DEM simulation

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The effect of variation of ball sizes on the grinding kinetics of calcite powder was studied and ball-to-ball and ball-to-wall collision of shear energy and ball impaction was calculated through a DEM simulation. Also, as the ball size decreases, the contact number increases and the effect on the powder increases, so we chose 0.3 mm and 3 mm zirconia balls in this study. The calcite powder particle morphology and size were characterized by scanning electron microscopy (SEM) and particle size analyzer (PSA). The grinding kinetics was calculated by Tanaka's equation for ultrafine grinding based on particle size changes of calcite powder using a planetary ball mill. This study showed that grinding kinetic parameters could be different for variation rotation speed and ball sizes. The effects of ball size and particle size on the grinding kinetic were quantitatively confirmed.

Keywords: ball size, grinding kinetic, calcite powder, particle size, ball impaction.





## Enhancing the extraction of rare earth elements (rees) from coal ash through acid-leaching

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Rare earth elements (REEs) are crucial for various renewable and clean technologies. As the global gap between their supply and demand widens, the feasibility of recovering REEs from secondary sources increases. Our study focused on coal, fly ash from coal mining deposits in Mongolia, and thermal power plants.

We analyzed rare earth elements (REEs) and other chemical elements in coal samples from the deposit using the inductively coupled plasma-mass spectrometry (ICP-OES) technique and conducted acid-leaching experiments on coal ashes. Additionally, we characterized the mineralogy of coal and fly ash using TESCAN Integrated Mineral Analyzer (TIMA) and X-ray diffractometer (XRD).

Sieve analysis of coal ashes was conducted, determining a P80 of 150  $\mu\text{m}$  through dry sieve testing and 26  $\mu\text{m}$  through wet sieve testing.

Two acid leaching methods were conducted: direct acid leaching and acid leaching with alkaline pretreatment. We achieved a metal recovery rate of 44.4% with direct acid leaching and 62.6% with acid leaching preceded by alkaline pretreatment. This process also resulted in an increased amount of REEs recovered.

**Keywords:** Rare Earth Elements, fly ash, coal combustion by-products, acid leaching, alkaline pre-treatment

## **Effect of ball powder ratio variation on particle size distribution and morphology evolution of calcite powder using a planetary ball mill**

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The particle size distribution and particle morphology evolution of calcite powders were studied as a function of ball to powder ratio. The calcite powders were milled using a planetary ball mill with different ball-to-powder ratios of 20:1 and 40:1 under the same experimental conditions. The influence of the ball-to-powder ratio on particle size changes and morphological evolution of the milled calcite powders has been examined by a particle size analyzer (PSA) and scanning electron microscopy (SEM). The particle size and morphology evolution of calcite powder changed as ball size and BPR varied. Compared with the samples with a BPR of 20:1 and 40:1 under the same experimental conditions, the calcite powders with a BPR of 40:1 experienced it was de-agglomerated, fabricated finer and uniform powders, and particle size decreased. The result has been concluded as the increased frequency and intensity of particle and ball collisions.

**Keywords:** ball-to-powder ratio (BPR), calcite powder, particle size, particle morphology, ball size.



## Some results of the technological study to obtain innovative products from the raw materials of mongolian medicine

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**Background:** Mongolia imports 89.4% of necessary medicines, which shows the need to increase the number of domestic medicines.

**Methods:** The powdering degree and absorption coefficient of plant raw materials were defined by I.A.Muraviev and Yu.G.Pshukov ' s method, moisture was defined by the Mongolian Pharmacopoeia method, and the flowability was determined by I.A.Muraviev ' s method.

**Result:** The extractives amount was  $32.58 \pm 0.52\%$  in 1mm powdered root of *Glycyrrhiza uralensis*,  $31.51 \pm 0.49\%$  in the fruit of *Rosa acicularis*, and  $55.26 \pm 0.74\%$  in the root of *Inula helenium*;  $34.45 \pm 0.55\%$  in 2mm powdered root of *Glycyrrhiza uralensis*,  $32.15 \pm 0.85\%$  in the fruit of *Rosa acicularis*, and  $32.15 \pm 0.85\%$  in the root of *Inula helenium*;  $32.81 \pm 0.19\%$  was found in 3mm powdered root of *Glycyrrhiza uralensis*,  $31.66 \pm 0.34\%$  in the fruit of *Rosa acicularis*, and  $55.82 \pm 0.18\%$  in the root of *Inula helenium*. The internal absorption coefficient (IAC) is  $1.778 \pm 0.03$ , the complete absorption coefficient (CAC) is  $3.815 \pm 0.09$  for the root of *Glycyrrhiza uralensis*, the IAC is  $1.69 \pm 0.01$ , the CAC is  $3.3336 \pm 0.07$  for the root of *Inula helenium*, the IAC is  $1.2945 \pm 0.01$ , and the CAC is  $2.008 \pm 0.002$  for the fruit of *Rosa acicularis*. The granules moisture were  $1.31 \pm 0.78\%$  for 1<sup>st</sup> model,  $1.91 \pm 0.87\%$  for 2<sup>nd</sup> model,  $1.45 \pm 0.39\%$  for 3<sup>rd</sup> model, and  $1.35 \pm 0.64\%$  for 4<sup>th</sup> model. The granules of each model were wholly dissolved in 200 ml of hot water in 5 minutes. The flowability of granules is  $4.3 \pm 0.3$  g/sec for the 1<sup>st</sup> model,  $3.75 \pm 0.59$  g/sec for the 2<sup>nd</sup> model,  $3.36 \pm 0.41$  g/sec for the 3<sup>rd</sup> model, and  $2.5 \pm 0.1$  g/sec for the 4<sup>th</sup> model.

**Conclusion:** The suitable size of the raw material is 2mm. The absorption coefficient was 1.8 for the root of *Glycyrrhiza uralensis*, 1.3 for the fruit of *Rosa acicularis*, and 1.7 for the root of *Inula helenium*. The granules of the 1st model meet the requirements of technological parameters and quality indicators.

**Keywords:** *Glycyrrhiza uralensis*, *Rosa acicularis*, *inula helenium*, granules



## **Biosynthesis of silver nanoparticles with antimicrobial activity using novel yeast strains**

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Yeast strains from Mongolian plants were identified as *Candida tropicalis*, *Candida norvegensis*, and *Kloeckera apiculata*. These strains produced silver nanoparticles at 30°C in 24 hours. The AgNPs were characterized using NIR spectroscopy, Dynamic Light Scattering (DLS), and Fourier Transform Infrared (FTIR) analysis. Characterization showed nanoparticles with 54.9 - 108.2nm size and specific chemical markers. FTIR analysis indicated the presence of biomolecules responsible for AgNPs synthesis, evidenced by particular stretching vibrations at 3425.9-3208.1  $\text{cm}^{-1}$ , 1641.5-1638.1  $\text{cm}^{-1}$ , and 2125.6-2108.4 $\text{cm}^{-1}$ . AgNPs demonstrated strong antibacterial effects, particularly against *Staphylococcus aureus* and *Escherichia coli*.



## Rare-earth free permanent magnet –transition 3d metal and Si doped iron phosphide ( $\text{Fe}_2\text{P}$ )

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Due to the inherent structural instability, rising costs and limited availability of rare earth (RE) compounds, search of alternative permanent magnetic materials free of RE has become one of the most pressing fields of research. Iron phosphide ( $\text{Fe}_2\text{P}$ ) in hexagonal structure has attracted attention for permanent magnetic applications due to its large uniaxial magneto-crystalline anisotropy. The goal of this research is to investigate effects of alloying substitutions on its Curie temperature, the main limitation of  $\text{Fe}_2\text{P}$  alloys for permanent magnet application, while retaining its high magneto-crystalline anisotropy. In this poster, we will review the properties that make a material good permanent magnet, including saturation magnetization, uniaxial magneto-crystalline anisotropy, maximum energy density product, Curie temperature, and thermodynamic stability. In addition, we present our approach to designing new rare-earth free permanent magnets that are comparable to  $\text{Nd}_2\text{Fe}_{14}\text{B}$  in performance. Finally, we discuss initial findings from our density-functional theory calculations on Fe-P-Mn, Fe-P-Si, and Fe-P-Mn-Si alloys.

### Acknowledgements

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## Theoretical study of rare earth element doped $\text{SmFe}_{12}$ compound

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$\text{SmFe}_{12}$  is considered one of the most promising compounds for permanent magnet research since the discovery of the  $\text{Nd}_2\text{Fe}_{14}\text{B}$  compound. However, its bulk structure is known to be unstable [1]. Recent theoretical and experimental studies have demonstrated that doping  $\text{SmFe}_{12}$  with small amounts of Ti and V atoms can stabilize the compound [2-3]. While Ti and V are effective stabilization elements, they have been found to negatively impact the magnetic properties. To address this issue, we aim to enhance the magnetic properties by doping the compound with rare earth elements. In this study, we have selected commercially available and cost-effective elements such as La, Ga, Ce, and Dy. Using the VASP software and employing the density functional theory (DFT) method, we have investigated the potential of these doping elements to improve the stability and magnetic properties of  $\text{SmFe}_{12}$ .

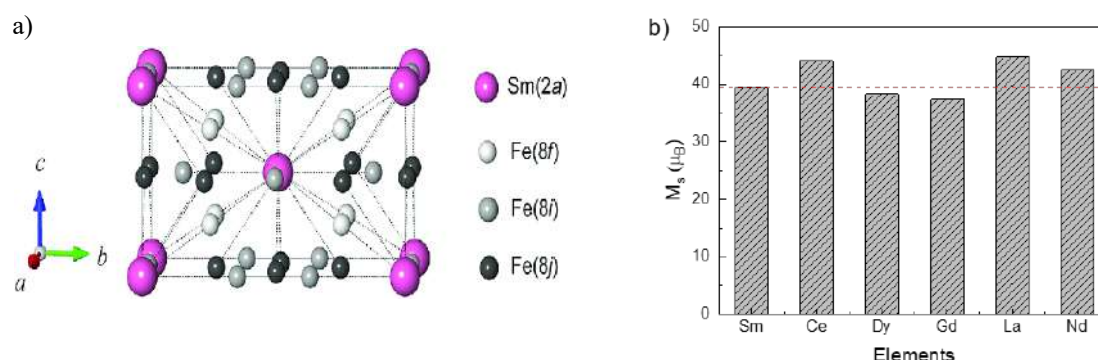


Figure 1.  $\text{SmFe}_{12}$  crystal structure and total magnetization dependence with dope elements

From the results, dopes other than Gd atoms increased the total magnetic moment of the system and value of  $K_u$  when Ce doped was higher than  $\text{SmFe}_{12}$ .

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## Structural optimization of FeCo alloys by doping elements

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Although FeCo alloys exhibit relatively high saturation magnetization ( $M_s$ ) and Curie temperature ( $T_c$ ), their low coercivity ( $H_c$ ) makes them unsuitable for use as permanent magnets. Herein, we report on Ti doped FeCo to optimize their structural properties for high-performance applications. The aim of this study is to investigate how doping with Ti can induce tetragonality in the FeCo lattice, potentially enhancing the anisotropy and improving the magnetic properties of the alloy.

The compounds were synthesized using the Spark Plasma Sintering (SPS-Labox 650F) technique. The fabrication process involved high-purity powders: Co (99.98 wt.%), Fe (99.95 wt.%), and Ti (99.95 wt.%). The precursor powders were prepared using a planetary ball mill (KGB-0.2) for 6, 12, and 24 hours in an inert Ar gas atmosphere, maintaining a ball-to-powder mass ratio of 10:1. The sintering process was conducted at 1123 K, applying a pressure of 50 MPa for 20 minutes. Phase and crystalline structure were explored using X-ray diffraction (XRD, Shimadzu XRD-7000) analysis with Co-K $\alpha$  radiation ( $\lambda = 1.789 \text{ \AA}$ ).

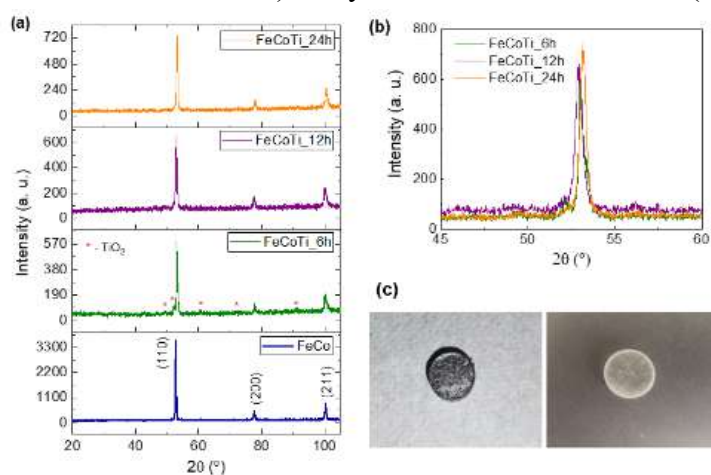


Fig. 1. (a) XRD patterns of pure and Ti-doped FeCo alloys. (b) Zoomed-in view of the FeCo (110) peak. (c) XRD patterns of the prepared Ti and B doped FeCo alloys.



Analysis of the XRD patterns (Fig. 1a) revealed a single phase of FeCo with a Pm-3m crystal structure, corresponding to JCPDS No.: 49-1567. Upon doping with Ti, additional peaks corresponding to TiO<sub>2</sub> were observed. However, the intensity of these secondary phase peaks decreased and the crystallinity of FeCo increased with longer milling times, as seen in Fig. 1b.

The research is funded by Office of Naval Research and Office of Naval Research Global of the US Department of Defense Grant N62909-22-1-2045.





## Phytochemical screening of the forage plants and its importance for livestock animals in mongolia, artemisia sieversiana and chloris virgata as examples

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### Objective

In Mongolia, plants play a crucial role as traditional medicinal resources and fodder for livestock. Livestock animals can obtain approximately 90% of their feed from pasture throughout the year. However, Mongolian rangelands experience extreme temperatures, ranging from -40°C in winter to +40°C in summer, making it difficult to maintain consistent feed availability year-round. Additionally, around 80% of Mongolia's agricultural sector focuses on animal husbandry, serving as the primary livelihood for about one-third of the population. Understanding native plants from a phytochemical perspective is essential for finding affordable ways to increase livestock production, thereby highlighting the critical role of livestock and plants in the country's economy and sustenance. Therefore, our team have focused on various forage plants, and we would like to introduce *Artemisia sieversiana* and *Chloris virgata* that are considered to play a distinctive role as pasture for animals under certain conditions

### Experimental

We collected *Artemisia sieversiana* at the beginning of spring and *Chloris virgata* in the winter season. After collecting the samples, we prepared crude extracts using an acetone-water (4:1) mixture and utilized spectroscopic methods for purification. The compounds were then isolated through repeated fractionation using HPLC. The chemical structures of the purified compounds were determined using spectroscopic data using NMR and MS and physical properties.

### Result and discussion

In our research, we have isolated several novel and bioactive compounds from *Artemisia sieversiana* and *Chloris virgata*, which are important and widely distributed forage plants. Specifically, some flavonoids and lignans from *A. sieversiana* demonstrated trypanocidal activities. Notably, our findings indicate a possibility that we can combat infectious diseases using native natural resources. The investigations for chemical constituents of *Chloris virgata* were also repeated, and major components such as flavonoid C-glycosides were obtained. The focus was on a flavonoid triclin, which was also identified as a common component of *Artemisia sieversiana* and *Chloris virgata*. Of course, triclin is commonly found in grasses, but the next step in our research is to investigate the specific effects of these various compounds in plants on animals in Mongolia.



## Research on the possibility of reducing the soil lead pollution by using microorganisms

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In Ulaanbaatar City's soil, the main polluters of the surface soil are lead, chromium, and other heavy metals from industrial and mining activities, electric power stations, sewage, and vehicle emissions. Organisms that live in environments polluted by heavy metals do the mechanisms of adaptation to survive. Some microorganisms are not only resistant to metal but also can accumulate it in their cells or detoxify it by reacting with its metabolic products. The purpose of the work was to identify bacteria which can resist to the action of lead salts and to determine their some activity. In 18 city soil samples, lead was found at 5.9-5132 mg/kg, and 3 points exceeded the maximum permissible level. Resistant bacteria isolates to varying concentrations of heavy metals such as lead, zinc, ferric, copper, chromium, and cadmium were determined by agar dilution method. Lead-resistant bacteria were isolated on medium with PbCl<sub>2</sub>. There were four strains can resist to 9 mM of concentration of Lead, to 2 mM of Zinc and to 2 mM of Chromium, can tolerate 1 mM of Iron. The DNA product was amplified by PCR using primers 27F (5'-AGAGTTTGATCCTGGCTCAG-3') and 1492R (5'-TACGGYTACCTTGTTACGACTT-3'). In liquid media our strain *B.thuringiensis MN01* able to reduce the lead concentration up to 46 % within 1 month. Consortium bacteria has been determined in laboratory conditions that it was active to reduce the concentration of 1 mM of lead to 0 mM after 1 month. Two bacteria was *B.cereus* and one was *S.paucimobilis*.



## **Fabrication of P3HT-Based Red Electroluminescent Diodes and Their Optical and Morphological Studies on Polymer Thin Films**

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This study investigates the fabrication and characterization of a red electroluminescent (EL) device utilizing a combination of poly(3-hexylthiophene) (P3HT) and tris(8-hydroxyquinolino)aluminum (Alq3) in an ITO/P3HT/Alq3/LiF:Al structure. P3HT was selected for its strong red photoluminescence properties, and Alq3 was incorporated to facilitate efficient electron transport. The device exhibited electroluminescence initiation at a threshold voltage of 2.5V. Spectral analysis revealed a peak emission wavelength at 656 nm, closely matching the photoluminescence spectrum of P3HT, confirming that the red light emission originates from the P3HT layer.

The combination of P3HT and Alq3 in the device structure enhances charge carrier injection and recombination, resulting in efficient red light emission. These findings highlight the potential of P3HT and Alq3 for high-performance red light-emitting applications and provide valuable insights for the design and optimization of red organic light-emitting diodes (OLEDs).

**Keywords:** *Organic electronics, Electroluminescence, Photoluminescence, Red electroluminescent device*

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## **Improving The Electrical Characteristics of Pentacene Organic Field Effect Transistors with Low-Cost Copper Electrodes by Self-Assembled Monolayer Modification**

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This work explored the possibility to tune the properties of the metal-semiconductor interface in organic field-effect transistors (OFETs) through insertion of 2,3,4,5,6-Pentafluorothiophenol (PFBT) and octadecyl phosphonic acid (ODPA) self-assembled monolayer on the metal-organic and dielectric organic interface of OFET respectively. The interfaces were modified with their respective self-assembled monolayers (SAMs) through immersion method and the modified surfaces were characterized with contact-angle measurements and atomic force microscopy measurements. Then, OFETs employing pentacene semiconductor with and without modified electrodes were fabricated and among them, the devices with PFBT modification demonstrated a superior operational parameter as opposed to as-prepared OFETs in terms of in saturation field-effect mobility going from 0.0002 to 0.0254 cm<sup>2</sup> V s<sup>-1</sup>, and improvement in threshold voltage and on/off-current ratio.

Keywords: Organic field effect transistor, self-assembled monolayer, contact engineering

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## **Intrinsic room-temperature ferromagnetism in two-dimensional MoSe<sub>2</sub> monolayer**

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Developing two-dimensional (2D) magnetic semiconductors that exhibit room-temperature ferromagnetism is a major challenge in materials science and is crucial for advancing next-generation spintronic devices. In this study, we employ density-functional theory (DFT), Monte Carlo (MC), and molecular dynamic (MD) simulations to systematically investigate the intrinsic magnetic properties induced by natural defects, specifically Mo vacancies, in MoSe<sub>2</sub>. Our findings reveal that these vacancies result in ferromagnetism, with up to 4  $\mu\text{B}$  per local site of neighboring atoms. By controlling the inter-vacancy distances, we can manipulate the magnetic moments, thereby driving a phase transition from a non-magnetic to a ferromagnetic state at room temperature. Theoretical calculations reveal that the ferromagnetic exchange interactions between Mo-Mo and Mo-Se atoms are enhanced with increasing distance between Mo vacancies. Additionally, we explore the impact of magnetic impurities, such as Fe and Co atoms, on the ferromagnetic properties of MoSe<sub>2</sub> monolayers. The introduction of these impurities enhances the magnetic characteristics, particularly leading to higher Curie temperatures ( $T_c$ ) of up to 500 K due to the strong exchange interaction between Fe-Fe atoms. Achieving intrinsic room-temperature ferromagnetism in these materials addresses a significant challenge in materials science and opens new avenues for advanced spintronic applications.

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## Fe-Ni based alloys as rare-earth free gap permanent magnets

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$L1_0$ -ordered FeNi phase has potential as a rare-earth free permanent magnet due to its large magnetization and high Curie temperature. However, low long-range crystal ordering and weak magnetocrystalline anisotropy ( $K_u$ ) impede its practical use in a technologically relevant permanent magnet. Employing density functional and Monte Carlo simulations, we demonstrate the substantial improvements on structural and thermal stability, disorder-order phase transition, and intrinsic permanent magnetic properties of Fe–Ni structures. We propose that this is achievable through the complementary elemental substitutions by metal elements (M) and interstitial doping with  $2p$  elements.  $\text{Fe}_{1-x}\text{M}_x\text{Ni}$  with simple metal (M = Ga and Al) and metalloid (M = Ge and Si) elemental substitutions at  $x = 0.5$  are broadly known as Heusler ( $L2_1$ ) structures with no permanent magnet characteristics. On the contrary, we find that for  $x = 0-0.5$ ,  $L1_0$ -type structure is energetically favored over the Heusler-type structures. The predicted structures exhibit  $K_u$  values up to approximately  $2.1 \text{ MJ/m}^3$ , which is roughly three times that of FeNi phase ( $0.68 \text{ MJ/m}^3$ ), where the absolute value of  $K_u$  depends on the degree of  $L1_0$  crystal ordering. Interstitial doping with B elevates  $K_u$  further up to a maximum value of  $3.9 \text{ MJ/m}^3$  (at 0 K), leading to room-temperature intrinsic permanent magnetic properties, including maximum energy density product  $(BH)_{\text{max}}$ , anisotropy field  $\mu_0 H_a$ , and hardness parameter  $\kappa$ , comparable to the widely investigated MnBi and MnAl permanent magnets. These results may serve as a guideline in designing Fe–Ni based rare-earth free gap permanent magnetic materials that were previously overlooked.

The research is funded by the Office of Naval Research and the Office of Naval Research Global of the US Department of Defense Grants N62909-22-1-2045.



## Production of light hydrocarbons (C<sub>2</sub>-C<sub>4</sub>) by hydrogenation of CO<sub>2</sub> using Co-K/γ-Al<sub>2</sub>O<sub>3</sub> catalysts with additional metal promoters (Ba, La, Ce) and combined supports (Y<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>)

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This study investigates the conversion of CO<sub>2</sub> to C<sub>2</sub>-C<sub>4</sub> hydrocarbons using Co-K/γ-Al<sub>2</sub>O<sub>3</sub> catalysts in Fischer-Tropsch synthesis (FT-CO<sub>2</sub>). The research focused on evaluating the effects of various promoters and supports on CO<sub>2</sub> conversion efficiency and C<sub>2</sub>-C<sub>4</sub> selectivity. Specifically, the catalysts were modified with 1% of the promoters Ba, La, and Ce, and supported on 10% Y<sub>2</sub>O<sub>3</sub> and 10% TiO<sub>2</sub>. These modifications aimed to enhance the catalytic properties and performance of the Co-K/γ-Al<sub>2</sub>O<sub>3</sub> system.

Catalysts were prepared using the impregnation method, and their structural and chemical properties were thoroughly characterized by X-ray diffraction (XRD), temperature-programmed hydrogen reduction (TPR), and CO<sub>2</sub> desorption techniques [1]. The primary objective was to determine how these modifications influence the interaction between the metal and the support, thereby affecting the active site formation and CO<sub>2</sub> activation processes.

The catalyst was mixed with inert SiC in a 1:4 weight ratio to prevent from overheating due to exothermic reaction, and Fischer-Tropsch catalytic activity was conducted at 350°C. The hydrogenation of CO<sub>2</sub> was performed using a syngas mixture with H<sub>2</sub>/CO<sub>2</sub>=3:1 at a pressure of 0.3 MPa and a flow rate of 50 ml·min<sup>-1</sup>, GHSV=3000 h<sup>-1</sup>. Gas products were in situ analyzed using a YL-GC6100 gas chromatograph.

Among the catalysts tested, the Co-K-1Ce/γ-Al<sub>2</sub>O<sub>3</sub> catalyst exhibited the highest performance at an operational temperature of 350°C. It achieved a remarkable CO<sub>2</sub> conversion rate of 44.90%, a C<sub>2</sub>-C<sub>4</sub> hydrocarbon yield of 14.91%, and a selectivity of 37.17% towards C<sub>2</sub>-C<sub>4</sub> hydrocarbons. The study found that the interaction between the cobalt metal and the alumina support was significantly enhanced by the addition of cerium, which increased the number of active sites and facilitated CO<sub>2</sub> activation [2].

In contrast, the use of Y<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> supports primarily boosted CO yield through the reverse-water gas shift reaction, but did not substantially enhance the FT-CO<sub>2</sub> synthesis. This indicates that while these supports can aid in certain reaction pathways, they do not significantly impact the overall performance in producing C<sub>2</sub>-C<sub>4</sub> hydrocarbons.



Ultimately, the addition of cerium emerged as the most effective promoter for enhancing the catalytic activity of the Co-K/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> system. Meanwhile, the Y<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> supports had limited impact on the FT-CO<sub>2</sub> synthesis performance, proving the importance of promoter selection in catalyst design for efficient CO<sub>2</sub> conversion.

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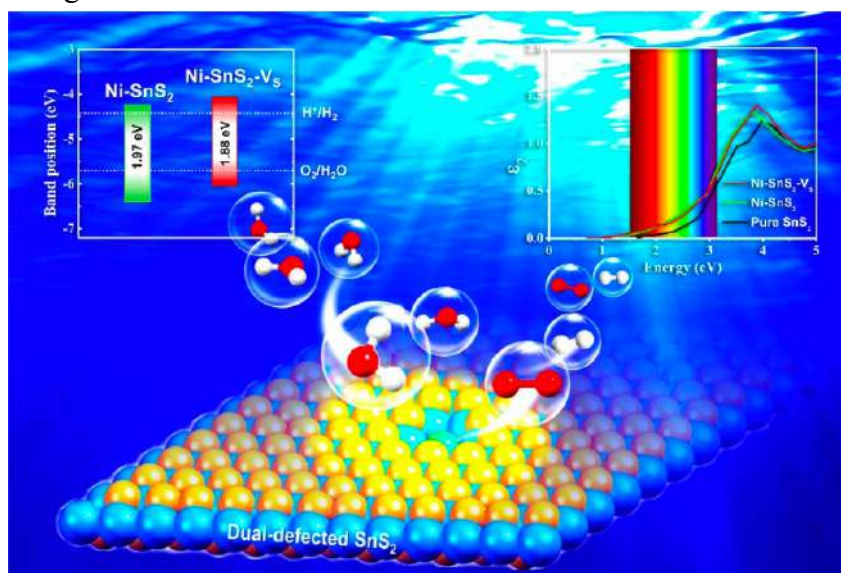
# Dual-defective SnS<sub>2</sub>: a promising 2D photocatalyst semiconductor for overall water splitting toward hydrogen fuel

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Solar-to-hydrogen fuel conversion through photocatalytic water splitting is a promising green pathway for achieving carbon-neutral and net-zero targets worldwide. In this regard, designing efficient photocatalytic materials that can split water into oxygen and hydrogen is essential. Using quantum-mechanical first-principles calculations, we demonstrate that the dual-defective SnS<sub>2</sub> (Ni-SnS<sub>2</sub>-V<sub>S</sub>), incorporating both nickel doping and sulfur vacancy, becomes a promising 2D photocatalyst semiconductor compared with pure SnS<sub>2</sub>.<sup>1-2</sup> In particular, the Ni-SnS<sub>2</sub>-V<sub>S</sub> monolayer not only displays suitable band alignment that perfectly overcomes the redox potentials for overall water splitting, but also exhibits enhanced photocatalytic activity, spatial carrier separation, and a broadened optical absorption spectrum. Therefore, the dual-defective SnS<sub>2</sub> can serve as an efficient photocatalyst for overall water splitting to produce hydrogen fuel. Remarkably, the dual-defect method can be an effective strategy to enhance the optoelectronic and catalytic behaviors of 2D materials, offering atomic-scale guidance in the development of solar-fuel generation.



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## Research on possibility to obtain fuel product from animal fat oil

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According to the results of the 2022 livestock census, our country has 71.3 million animals, and it is believed that one sheep can produce an average of 3-4 kg of fat. Also, we noticed that a lot of animal fat is discarded during the meat preparation and production, and most families separate the outer fat of meat when cooking. It is thrown away with garbage and pollutes the environment. This waste fat can be used to produce biodiesel fuel to replace imported products. Biodiesel can be obtained from waste fat oil by transesterification reaction, and biodiesel is released at upper phase. On the other hand, biodiesel (BD) can be produced from waste vegetable oil and mixed with commercial diesel fuel at a ratio of up to 20% by volume if it meets the requirements of biodiesel standards. We are working with the goal of processing this raw material and creating a technology for the production of products for fuel, including the possibility of obtaining biodiesel by transesterification reaction.

In this study, sheep tail fat (STF), yak visceral fat (YVF), goat visceral fat (GVF), mutton soup oil (MSO), and industrial oil (IO) were used as samples. Based on the chemical properties of each sample STF and GVF were low acid number (<3.0). The upper phase was isolated with a yield of 100% and 94.5% by one-step transesterification of those 2 samples. In the other 3 samples with a high acid number, two-step re-esterification was carried out, and the upper phase was successfully isolated from YVF and IO with yields of 90.1% and 103%, respectively. Unfortunately, the reaction wasn't complete and did not isolate the upper phase from the sample of MSO. This sample was probably polymerized during cooking. It was confirmed that a product with a low amount of the specific gravity, kinematic viscosity, and freezing temperature was obtained from the original sample, during the determining the chemical and technical properties of the biodiesel (upper phase) and fat oil samples. For example, density of the GVF and the biodiesel obtained from GVF were 0.936 g/cm<sup>3</sup>, 0.884 g/cm<sup>3</sup>, kinematic viscosity were 42.9 mm<sup>2</sup>/s, 9.66 mm<sup>2</sup>/s, and the freezing temperature was reduced from 33.5°C to 22.8°C, respectively. Optimum conditions were determined for each sample by varying the reaction time and rotation speed, respectively, to obtain the biodiesel in maximum yield. The chemical and technical



parameters of the obtained biodiesel were determined. Also, biodiesel was distilled under vacuum pressure to determine the content of gasoline and diesel fractions.

**Keywords:** Animal fat oil, biodiesel, upper phase, transesterification, reaction time, rotation speed



## Smart biomaterials and bioresponsive materials

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In this document, we present the run down preparation of our research about can adjustable color change nanomaterials. This research is based on the study of material strength and nanoparticle changes in the materials.



## **Nitrate pollution and its sources in ground and surface waters of central Mongolia**

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This research utilized isotope analysis to identify the sources of nitrates in groundwater and surface waters in Central Mongolia. We selected 34 water samples with previously noted high nitrate concentrations, including lake (n=2), well (n=17), and river and spring samples (n=15).

Nitrate isotope analysis indicated that nitrates in Ishgent Lake were mixed with ammonia from rainfall, while contamination in some groundwater in Ulaanbaatar's Ger district was likely due to unsanitary pit latrines. Bacteriological analysis revealed the presence of intestinal pathogens in some samples.

Out of the 34 samples, 21 were found to pose a high risk of causing non-cancerous diseases in adults and children due to their nitrate levels. Since most of these waters are used for drinking purposes, it is essential to implement measures to reduce nitrate levels, eliminate water pollution sources, and prevent the poisoning of the population.



## Green synthesis and characterization of silver nanoparticles using *Dracocephalum foetidum* aqueous extract and evaluation of their antibacterial and antioxidant activities

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A simple, effective and rapid approach for the green synthesis of silver nanoparticles (Df-AgNPs) using aqueous extract of *Dracocephalum foetidum* and its in vitro antioxidant and antibacterial activities were investigated in this study. Df-AgNPs were featured by UV-visible, Fourier-transform infrared spectroscopy, scanning electron microscopy (SEM), and powdered X-ray diffraction (XRD) analyses. The maximum absorption peak was detected at 420 nm. The average size of Df-AgNPs was  $19.99 \pm 6.30$  nm and their spherical shape was determined by SEM spectral analysis. Df-AgNPs have the potential of  $-52.19$  mV which indicated the stability of nanoparticles as well as repulsion among the particles. Df-AgNPs were found to be very stable and they did not exhibit sedimentation for over 6 months. Antioxidant activities of Df-AgNPs and the extract were investigated by the DPPH•, ABTS•+ and FRAP assays. The Df-AgNP was found a excellent antioxidant and exhibited a highly biocidal activity against four test pathogens when compared to aqueous extracts from the *D. foetidum*. The results obtained indicate that an aqueous extract of *D. foetidum* is suitable for synthesizing stable silver nanoparticles, which act as excellent antioxidants and better antimicrobial agents.

**Keywords:** *Dracocephalum foetidum*, aqueous extract, silver nanoparticle, green synthesis, antioxidant, antibacterial activity

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## **A Correlation between ore mineralogical composition at different depths and bond work index for the Erdenetiin Ovoo Cu-Mo porphyry deposit, Mongolia**

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The Erdenetiin Ovoo Cu-Mo porphyry deposit in Mongolia is the nation's largest copper mine. This study investigates the grinding properties of biotite granodiorite (BGDP) and granodiorite (GDIR) rock alteration with depth, focusing on their mineral composition correlation. Bond Work Index (BWI) tests were applied to Cu-Mo porphyry ore from the Erdenet Mining Corporation. Samples were collected from 10 composites at 5 depth levels (~90 m intervals) between 1175 m and 725 m. Analytical and mineralogical characterizations of BGDP and GDIR ores were performed using X-ray fluorescence (XRF) and X-ray diffractometer (XRD) methods. The chemical data indicated that Cu and Mo percentages in both BGDP and GDIR decreased with depth. XRD data on mineral composition were used to set up a BWI estimation model, showing a linear correlation with measured BWI. The results revealed strong correlations between major mineral phases and BWI values, integrating ore hardness and mineralogical data.



## **Towards mineralogical characterization of the flotation products using automated mineral liberation analysis at the “Erdenetiin ovoo” Cu-Mo porphyry deposit, Mongolia**

**Batmunkh Tumen-Ayush**

The flotation process is used to extract copper-molybdenum sulfide minerals from ore. The selection of the flotation technology scheme largely depends on factors such as the composition of sulfide ore in the ore body, grain size, and characteristics of the ore mineral association. The chemical and mineralogical analysis of flotation products was collected from the “Erdenetiin Ovoo” Cu-Mo Porphyry Deposit (Erdenet Mining Corporation SOE, Mongolia). Erdenetiin Ovoo is the largest porphyry copper-molybdenum deposit in Mongolia. The aim of this study was to demonstrate the occurrence mechanism of copper minerals in flotation tailing using the fully automated TIMA (Tescan Integrated Mineral Analyzer). The chemical analysis of the flotation products (feed, concentrates and tailings) sample was conducted by X-ray fluorescence, and the mineralogical composition of the flotation feed sample was characterized using X-ray diffraction. The copper content of the flotation tailing was 0.024%. Mineralogical characterization results showed that almost all copper minerals occurred within coarse gangue particles, the primary and secondary copper minerals were accumulated in the size fractions less than 150  $\mu\text{m}$  and 13.5  $\mu\text{m}$ , respectively. The finest grain size distribution was observed in secondary copper particles of size -19  $\mu\text{m}$ . Chalcopyrite was the main copper-bearing mineral and it was closely associated with K-feldspar and silicate in the flotation tailings. The flotation tailing sample still contained 24.1wt% liberated primary copper (chalcopyrite) and 24.13wt% secondary copper due to their extremely fine grain size particle. The mineral map derived from TIMA analysis revealed that copper minerals mainly occurred as finely disseminated and fully enclosed structures within gangue minerals. The information obtained from this research has the potential to provide valuable insights into the recovery of residual copper from flotation tailings.





## Surface and Porosity Characteristics of Mesoporous Silica Synthesized from Sodium Silicate

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In this research work, the results of obtaining mesoporous silica oxide nanoparticles with high surface area by sol-gel method and precipitation method with surfactants and their surface and physicochemical properties were compared.

When mesoporous silica oxide was extracted from sodium silicate and analyzed by surface area and porosity analyzer, the material obtained by sol-gel method had a surface area of 128.7  $\text{m}^2\cdot\text{g}^{-1}$ , a pore diameter of 15.5 nm, and a pore volume of 0.8  $\text{cm}^3\cdot\text{g}^{-1}$ . The obtained material obtained using cetyltrimethylammonium bromide (CTAB) surfactant has a surface area of 422.8  $\text{m}^2\cdot\text{g}^{-1}$ , a pore diameter of 3.6 nm, and a pore volume of 0.5  $\text{cm}^3\cdot\text{g}^{-1}$ , respectively. It was determined that mesoporous silica oxide was synthesized by the above methods. When measuring the zeta potential, the colloidal solution has good stability, and the high purity according to X-ray diffractometer and infrared spectrometer analysis shows that it is suitable for use as an absorbent material for organic pollution and heavy metals.

Keywords: Mesoporous silica oxide, High surface area nanomaterial, Gas adsorption



## Controlled growth of tmds films using Atmospheric pressure chemical vapor deposition

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Transition metal chalcogenides (TMDs) show significant promise for next-generation advanced optics and electronic devices, driven by recent advancements. A comprehensive understanding of the growth kinetics of these materials is essential for the development of lab-on-chip devices. This study focuses on the growth of mono- and multi-layered WS<sub>2</sub>, a prominent TMD, using the NaCl-promoted atmospheric pressure chemical vapor deposition technique on SiO<sub>2</sub>/Si substrates. The experiment was conducted in a three-temperature zone furnace CVD system with a diameter of 40 mm of the quartz tube. It was operated under atmospheric pressure and hydrogen-free conditions, The growth process was systematically explored by varying parameters such as crystal growth temperature, nucleation time, and catalyst concentrations. Atomic force microscopy (AFM) and Raman spectroscopy identified mono-, few-, and multi-layer WS<sub>2</sub>. Increasing substrate temperature and deposition time induced screw dislocations, forming three-dimensional spiral step edges (0.7 nm to 3 nm heights) in hexagonal and triangular patterns. Dominant Raman peaks at 419 cm<sup>-1</sup> and 349 cm<sup>-1</sup> indicate precise control over mono and layered TMD formation. By examining the frequency differences between the E<sub>2g</sub> and A<sub>1g</sub> modes, we identified the sample thickness. We observed that as the reaction time increased from 3 to 50 minutes, the frequency difference of the peaks at 350 cm<sup>-1</sup> (E<sub>2g</sub>) and 420 cm<sup>-1</sup> (A<sub>1g</sub>) increased from 66.5 to 69.8 cm<sup>-1</sup>. Simultaneously, the peak intensity ratio increased from 1.6 to 4.4. Based on these observations, monolayers and bilayers are predominant in our samples. Additionally, we noticed that the size of the flakes decreases with decreasing reaction time. Therefore, reaction time is a critical parameter affecting the thickness and size of WS<sub>2</sub>. The Raman analysis results of the effect of the NaCl weight ratio on WS<sub>2</sub> growth confirmed that NaCl can promote growth in the



synthesis. We observed induced screw dislocations in the form of hexagonal and triangular patterns at higher temperatures ( $>1020^{\circ}\text{C}$ ) and longer deposition times ( $> 25$  min).



## **A study on improving the activity of ciprofloxacin using silver/silica core-shell (Ag@MSNs) nanoparticles**

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The global consumption of antibiotics has seen a significant rise, reaching 40.2 billion defined daily doses in 2018, a 46% increase since 2000. However, ineffective pathogen clearance and antimicrobial resistance have driven the emergence of multidrug-resistant (MDR) bacteria, posing severe threats to global health and necessitating new antibiotic therapies. Despite this urgency, the discovery of novel antibiotics has stagnated due to high costs and technical challenges. As an alternative, nanoparticles (NPs) have emerged as promising antimicrobial agents. Silver nanoparticles (AgNPs), in particular, exhibit potent antibacterial activity through mechanisms such as controlled silver ion release, increased bacterial membrane permeability, and reactive oxygen species (ROS) production.

However, silver nanoparticles face challenges such as tissue accumulation, potential toxicity, poor dispersion in biological systems, and susceptibility to degradation. These limitations can be addressed by forming a core/shell structure with mesoporous silica nanoparticles. In this study, silver-silica core/shell nanoparticles were synthesized using a reduction method, a sol-gel technique, and the self-assembly properties of CTAB surfactant. The synthesized nanoparticles underwent optical characterization using a UV-visible spectrophotometer, and size analysis through scanning electron microscopy (SEM), photon cross-correlation microscopy, and atomic force microscopy (AFM). Structural analysis was performed using infrared (IR) spectroscopy and X-ray diffraction (XRD).

IR spectroscopy revealed peaks at 964.92 and 1064.62  $\text{cm}^{-1}$ , corresponding to symmetric and asymmetric vibrations of silicon oxide bonds, while a peak at 798.77  $\text{cm}^{-1}$  was attributed to metal oxide bonds between silver and oxide, indicating the presence of silver nanoparticles in the core. SEM analysis determined the size of the silver-silica core/shell nanoparticles to be approximately 100 nm. Antibacterial activity was evaluated for silver-silica mesoporous nanoparticles loaded with the antibiotic ciprofloxacin against gram-positive bacteria (*Staphylococcus aureus* and *Micrococcus luteus*) and gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*). Results showed a sixfold increase in the bacterial inhibition zone for gram-positive bacteria and a



twofold increase for gram-negative bacteria compared to ciprofloxacin alone, demonstrating enhanced antimicrobial efficacy.