Table of Contents

Part I Conference Schedule

Time: April 23-25, 2021
Location: Xi'an Grand Dynasty Culture Hotel
西安古都文化大酒店

Date	Time	Location: Lobby	
Apr. 23	**14:00-17:00**	**Registration**	
Date	**Time**	**Location: Taibaishan Room (太白山厅), 1st Floor**	**Location: Huashan Room (华山厅), 1st Floor**
Apr. 24	**08:30-12:00**	**Environmental Science** **Keynote Speech Session 1:** **Prof. Masaji Watanabe, Prof. Peimin PU, Prof. A. W. Jayawardena, Prof. Bill X. Hu, Dr. Gabor Harangozo** **Chair: TBD** **Group Photo & Coffee Break: 09:50-10:00**	**Chemistry Science** **Keynote Speech Session 1:** **Prof. Takashiro Akitsu, Prof. Ran Niu, Dr. Lalit M. Pandey, Dr. Kinjal J. Shah** **Chair: TBD** **Group Photo & Coffee Break: 09:50-10:20**
	12:00-13:30	**Lunch** Chinese Restaurant 中餐厅, 2nd Floor	
Date	**Time**	**Location: Taibaishan Room (太白山厅), 1st Floor**	**Location: Huashan Room (华山厅), 1st Floor**
Apr. 24	**14:00-18:00**	**Environmental Science** **Keynote Speech Session 2** **Dr. Lluís Miret-Pasto, Dr. Christopher M. A. Parlett, Prof. Baghdad Ouddane, Prof. Moshe Gophen, Dr. Dawen Li, Dr. Marek Wiśniewski** **Chair: TBD** **Group Photo & Coffee Break: 16:00-16:10**	**Chemistry Science** **Keynote Speech Session 2:** **Dr. Mirza Muhammad Faran Ashraf Baig, Prof. Ravinder Dachepalli, Dr. M. G. H. Zaidi, Prof. Yong Chen, Dr. Marini Andrea** **Chair: TBD** **Group Photo & Coffee Break: 16:00-16:20**
	18:00-19:30	**Dinner** Chinese Restaurant 中餐厅, 2nd Floor	
Date	**Time**	**Location: Huashan Room (华山厅), 1st Floor**	**Location: Huashan Room (华山厅), 1st Floor**
Apr. 25	**08:30-12:00**	**Environmental Science** **Keynote Speech Session 3** **Technical Session** **Dr. Mohd Anis Ganaie** **Chair: TBD** **Group Photo & Coffee Break: 09:30-09:50**	**Chemistry Science** **Keynote Speech Session 3** **Technical Session** **Prof. Vasudevanpillai Biju, Dr. Michael Badawi** **Chair: TBD** **Group Photo & Coffee Break: 09:50-10:00**
	12:00-13:30	**Lunch** Chinese Restaurant 中餐厅, 2nd Floor	

Part II Keynote Speech

Environmental Science: Keynote Speech Session 1

Keynote Speech 1: Study on change of topography in water area with field measurement [video]

Speaker: Prof. Masaji Watanabe, Okayama University, Japan
Time: 08:30-09:10, Saturday Morning, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Disastrous flood events in recent years include 2018 Japan floods (July 2018), Typhoon 19 (Hagibis, October 2019) and the following heavy rain event, and July 2020 heavy rain disaster. Such disastrous flood events are expected to occur more frequently as the climate change progresses, and it is indispensable to update information regarding water areas such as rivers, reservoirs, and coastal waters. This study demonstrates practical techniques to analyze underwater topography. Longitude and latitude components of ellipsoidal data recorded by a GPS receiver are projected to a rectangular coordinate system, and results are combined with vertical components including data recorded by an echo sounder unit so that tracks on an underwater floor are obtained. A mapping on a finite dimensional space of continuous functions over a triangular mesh is formulated, and its fixed point gives rise to an underwater floor that fits the tracks. Our techniques are illustrated with data obtained in measurement conducted in a reservoir called Kojima Lake located in Okayama Prefecture, Japan.

Keywords: underwater topography, RTK-GPS, echo sounder, triangular mesh, fixed point iteration

Keynote Speech 2: Water Structure & Water Quality/ Quantity Management

[video]

Speaker: Prof. Peimin PU, Nanjing Institute of Geography & Limnology, Academia Sinica & Taihu Laboratory for Lake Ecosystem Research, Academia Sinica, China
Time: 09:10-09:50, Saturday Morning, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

"What is the structure of water?" is the 46th issue among the 125 issues summarized by <SCIENCE> in 2005 as the most challenging issues in frontier basic sciences. The models for water (H_2O) molecule, liquid and solid states including snow and liquid water skin have been developed by authors of this paper. The water molecule is an equilateral triangular pyramid with 2 pairs of "+/-" electricity endpoints and edge length of 0.48017nm. The water ice structure has porosity of ≥2.28. The liquid water has the same structure of the solid ice, but there are 1/11 molecules leave from frame and get into the frame, being a "free water"; so the specific gravity of ice is 11/12. The conductivity of pure water is very low. The liquid water skin has 2 layers of special structure with porosity of 1. There are 1/1115 evaporated molecules from water surface may be negative ion. The thunder and lightning transfer the negative electricity return to earth surface like rainfall transfer the evaporated water molecule return to the earth surface. There are Zigzag Hexagon Tunnel-Vacancy Systems, where may store various substances, as "pollutants" (some of them are life supporting substances; the TDS and conductivity of polluted water increased with pollution state). The water has recycling characteristics in quality/ quantity and gas/ liquid/ solid state. We may remediate healthy aqua-ecosystem by high technology of **Physic- Ecological ENgineering-PEEN** using mainly solar energy, transforming pollutants into usable resources. In spacecraft we may recycle water quantity/ quality by using solar energy. The soft filter-wall-enclosures with sufficient vertical width for adapting variation of water level and wave-current are specially made up (like parachute) by synthetic fiber with floating up bar and lower anchored bar and might be easily assembled and anchored and adapting water level change and wave concussion at site for separating and filtering waters. All these construction in the catchment would be propitious to water level stable and decrease the possibility of drought and flood disasters. Various types of floating/suspending eco-islands for cultivating plants, including vegetable, feedstuff, flower, and snail, mussel, mollusk,. etc. Technology of Immobilized Nitrogen Cycling Bacteria-**INCB**, including 4 type bacteria and their carrier may accelerate decreasing nitrogen and COD in waters. "Jellyfish Engineering" may be used for collecting algae bloom by wind and transforming it into usable resources. Technology about planting, collecting, managing, and immediately drying water-hyacinth may be complexly used. Electric pulse+ photosensitization technology for decomposition of difficult decomposition chemicals using DC 24V and technology for quickly suppressing H_2S and increasing O_2 have been developed. We may develop **water body ecological agriculture**. By using dried water-hyacinth + wastewater+ vetiver grass+ management we may construct grass forest (much more quickly than tree forest) for suppressing sand blown by wind. System of DC 24V net may control fog and haze.

Underground channel reservoir without take off soil may decrease drought and flood disasters. Planting vetiver grass may use for decreasing water and soil loss and insect disease prevention.

Keywords: Water molecule structure, Water- ice and water surface structure, Production of negative ion in air, Water quality recycling & remediating healthy aqua-ecosystem, Controlling blue-algae bloom, water body ecological agriculture, Decreasing drought and flood disasters, Water and soil loss prevention

Keynote Speech 3: PARADIGM SHIFT FROM NATURAL INTELLIGENCE TO ARTIFICIAL INTELLIGENCE IN WATER RESOURCES MANAGEMENT [video]

Speaker: Dr. A. W. Jayawardena, Department of Civil Engineering of the University of Hong Kong, China
Time: 10:00-10:40, Saturday Morning, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

Water is essential for all form of life and food comes next. Management of the available water resources for direct consumption and for the production of food therefore goes as far back as one can trace the beginning of civilization. In the ancient times, this has been achieved through conventional wisdom, or natural intelligence, without much technological inputs. Community spirit, cultural values and in some cases religious and political guidance have helped to harness the available water resources for the benefit of not only human beings but also for all living things. Examples include the attempts to harness the waters of River Nile in Egypt, Tigris and Euphrates rivers in Mesopotamia, irrigation canals in India, China, Sri Lanka, Mexico, Grand Canal in China, underground canal systems (qanats) in Mesopotamia and the Roman aqueducts. The demand for water at that time has been mainly for domestic consumption, and for growing food.

Due to exponential explosion of population and the changing life styles in the modern world there are additional and sometimes conflicting demands for water. They include power generation, prevention of flooding, recreation, environmental conservation and sometimes for transportation. Managing the available resources which are dwindling in per capita quantity, as well as in quality, which fluctuate with time and space requires a more sophisticated approach. Artificial intelligence (AI) which has found many applications in science, engineering, medicine, and many other fields has the potential to optimize the use of this precious resource.

AI can be thought of as an electronic brain. Machine leaning, soft computing, statistical learning, artificial neural networks, fuzzy logic systems, support vector machines, deep learning, data mining etc. can be considered as sub-sets of AI. They all go through the stages of learning, reasoning and perception using external data and generally applicable to data rich theory weak situation. As such they are all data driven. In the context of water resources management, typical problems involve the prediction (or forecasting) of a dependent variable subject to a set of independent variables. In this

presentation, the application of artificial neural networks, support vector machines etc. for hydrological predictions will be illustrated.

Keynote Speech 4: Karst Groundwater Dynamics-Field Observation, Experiment and Modeling [video]

Speaker: Prof. Bill X. Hu, Institute of Groundwater and Earth Sciences, Jinan University, China
Time: 10:40-11:20, Saturday Morning, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Karst is a unique landscape containing caves and extensive underground water systems that is developed by dissolution in the carbonate rocks such as limestone and gypsum. Typical karst features are sinkholes and dolines on land surface, and the network of voids, caves and conduits below the surface, formed by the dissolution of the soluble carbonate rocks. The open and porous nature of a karst aquifer, combined with the dissolution of joints and fractures within the bedrocks over a geological time, evolve complex subsurface conduit systems. Compared to a porous medium, a karst aquifer is typically a dual-porosity system where groundwater and solutes move rapidly through conduits and water and solute exchanges between conduits and their porous media in a dual-permeability karst aquifer system. In the last 16 years, Dr. Bill Hu's groups used cave-divers, tracer tests, geophysical methods and well driving to extensively investigate two karst watersheds, Woodville Karst Plain (WKP) in USA and Maochun village in China and characterize the karst medium hydraulic properties. They conducted laboratory and field experiments to quantitatively study water and chemical exchanges between the conduits and the surrounding media. Based on the investigations and experiments, they developed a series of discrete-continuum hybrid numerical models to simulate regional groundwater and solute transport in the conduits and porous media in saturated and unsaturated karst media, and seawater intrusion through the subsurface conduit networks. The karst modeling established a framework for future developments, including, conduit evolution and contamination remediation.

Keynote Speech 5: Lessons learned from the ecological footprint as an indicator of sustainable development with a special focus on urban areas [video]

Speaker: Dr. Gabor Harangozo, Institute of Business Economics at Corvinus University of Budapest, Hungary
Time: 11:20-12:00, Saturday Morning, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Seeking for a better understanding of human development in relationship to the carrying capacity of the Earth, the ecological footprint indicator has gained considerable attention in both academic and educational literature recently. As an indicator illustrating the use of humanity's natural resources in territorial units, provides a good overview of the ecological constraints at global, national level, or even regarding smaller regional units.
In addition to its simplicity to interpret it at the level of different stakeholders, an additional advantage is that the basic data are available for almost all countries (National Footprint Accounts), which also provides an opportunity to compare individual countries and track the development of the indicator over time. The more widespread, consumption-oriented version of the indicator illustrates the environmental impacts of international trade in a new light. For example, China as a major global exporter country performs much better if we allocate the ecological footprint associated with exported products at consuming countries (while, of course, the opposite is true for imported products).
The ecological footprint indicator is also very useful to address the environmental impacts of urbanization in the age of the dominance of metropolitan areas. In many continents, emerging mega cities and suburban areas reshape the countries and raise new challenges for policy makers.
The series of research presented here cover the timeframe between 2000 and 2020. Data for the Budapest Metropolitan Region are used as the basis of the calculation, but lessons learned can be generalized to other urban regions as well. Multi method ecological footprint calculations are used (both bottom-up and top-down, with using household consumption data and national input-output accounts).
Results show that the biggest contributors of the urban ecological footprint are the carbon and the crop footprint (in terms of ecological footprint categories). In terms of consumption habits of citizens the major contributors to the ecological footprint are food consumption, transportation and household energy use. However, there are significant differences in this respect between central areas (where higher income levels and demand for services are responsible for a bigger ecological footprint) and suburbs (where heating and commuting are even more dominant).
The impacts of the Covid pandemic on the ecological footprint of urban areas are yet to become clear. Lockdowns result temporarily lower transportation based footprint, but increase it through household level energy consumption. The future greening of economy and urban lifestyles may have significant positive potential in this field.

Keywords: ecological footprint, urbanization, sustainable development.

Environmental Science: Keynote Speech Session 2

Keynote Speech 6: Eco-certificates and eco-labels as a way to advance towards the sustainability of the seas [video]

Speaker: Dr. Lluís Miret-Pastor, Polytechnic University of Valencia, Spain
Time: 14:00-14:40, Saturday Afternoon, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Fishing worldwide is facing growing and diverse environmental problems, one of the main ones being the overexploitation of fishing grounds. In order to face this problem, in recent years, different eco-labels and environmental certificates have emerged with the declared objective of guaranteeing that the fish we consume comes from fisheries with sustainable production methods. In recent years these certificates have had a great growth, partly due to a greater environmental awareness of customers, but also because numerous retailers, wholesalers, restaurant chains, etc. force their suppliers to supply them with fish from certified fisheries.
Certification has become a powerful competitive weapon for fisheries and the fishing industry, as well as an important tool on the path to the sustainability of seas and oceans. In any case, eco-labels are not without criticism. In the first place, because they have also become a profitable business and today there is a huge variety of eco-labels and certification standards, even for fish products exclusively, which makes their identification difficult. There are also criticisms of its bureaucracy and its price, criticism of its use as entry barriers to certain markets or doubts about its true environmental effectiveness. In any case, fisheries certification is a growing trend and is expanding to other products such as aquaculture.

Keynote Speech 7: Shedding light on heterogeneous catalyst systems for selective oxidation reactions. [video]

Speaker: Dr. Christopher M. A. Parlett, University of Manchester, UK
Time: 14:40-15:20, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Chemical manufacturing has relied heavily on the exploitation of crude oil feedstock, with heterogeneous catalysis playing a key role through underpinning 90% of chemical production. Growing concerns over the accessibility of fossil fuel

reserves, and the impact of their utilisation on climate change, is driving research into alternative sustainable fuels and chemicals via novel catalytic routes. Identifying structure-activity correlations in conjunction with operando measurements enables a detailed interrogation of a catalytic material, which when combined offers the potential to gain a significant advancement in the understanding of a catalytic process. I will give examples of how synchrotron x-ray spectroscopic techniques have enabled this strategy to be employed for the development of catalyst systems for selective oxidation reactions. 5-hydroxymethylfurane, derivable from non-edible cellulosic biomass, represents an interesting platform molecule with multiple potential applications. Its controlled oxidation to 2,5-Furandicarboxylic acid, a potential bio-plastic monomer, over solid base supported Au nanoparticles has revealed an interesting correlation between NP size and basicity of the reaction media, with the degree of progress through the multistep oxidation highly dependent on the two. The selective oxidation of allylic alcohols, to either their aldehyde or carboxylic acid derivatives, reflects selective chemical transformations for fine chemical production. Operando spectroscopic measurements have shown the critical role of surface oxide on supported Pd nanoparticles for selective aldehyde production, whereas the employment of Pt as the active site yields at a catalyst capable of high selectivity towards the carboxylic acid (when starting from the aldehyde). Coupling these two active species within a single hierarchical support architecture, via active site compartmentalisation within distinct pore domains, permits the one-pot selective oxidation catalytic cascade of the alcohol to its carboxylic acid. This, therefore, reflects an alternative strategy for multistep oxidations, which has the potential to be tuned for a wide array of reactions.

Keynote Speech 8: Behavior of metal contaminants in aquatic system [video]

Speaker: Prof. Baghdad Ouddane, University of Lille, France
Time: 15:20-16:00, Saturday Afternoon, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Trace metals are considered as serious pollutants in our natural environment because of their persistence, toxicity and bioaccumulation effects. Their presence in irregular contents in waters, sediments, suspended particles and soils could reveal the incidence of anthropogenic sources. Intensive exploitation by industrial activities in densely populated areas often results in the introduction of potentially hazardous levels of metals into aquatic ecosystem because of large amounts of wastes discharged from neighbouring mines and/or smelters along the banks. Trace metals tend to be trapped in the aquatic medium and are concentrated in sediments. Their releases into overlaying waters through sediment resuspension or by organism degradation, desorption from in-place sediments primes to an increased bioavailability, and thereby disturb the aquatic ecosystem. The loading of rivers with toxic metals is now of increasing importance because these aquatic reservoirs become more and more sources of drinking water. Our recent studies on anthropogenic metals present in the case of highly populated and greatly industrialized region of Northern France were focused on some sites like the Seine, the Deûle and the Lys rivers system. A focus will be done on mercury contamination in such area; mercury is a toxic

element, widely distributed in the environment and is present in the aquatic systems. It exists in a different chemical species with a wide range of properties and its toxicological and ecotoxicological effect are strongly dependent on the chemical form present. Inorganic mercury Hg (II) is the main form of Hg in waters and sediment samples, which can be naturally converted to much more toxic form methylmercury (MeHg) by bacterial activity (SBR). MeHg is accumulated by aquatic organisms and is known to be bio amplified along the food chain, and poses a threat to humans consuming fish. Knowledge of the concentration, transport and speciation of this compound in aquatic ecosystems is needed to predict the potential impact on human and aquatic life. Functionality and the relationship between metal and biogeochemical parameters will be presented and discussed. Various factors control the transformation of mercury species. Dissolved organic carbon, sulphate, sulphides, pH, temperature, microorganisms are all dependent factors ruling mercury methylation. Methylmercury degradation is photochemically induced in which this mechanism of degradation is mostly dominant at surface waters. Sulphides, organic matter, fine/coarse fraction, Fe/Mn oxyhydroxides, mercury partition coefficient between aqueous and solid phases and resuspension activities mainly control mercury mobility. Recent developments in Hg isotopic tracers have provided new experimental tools to measure the reactivity and dynamics of mercury including different transformations (methylation, demethylation, reduction…). Thus, different mechanisms of mercury biogeochemical cycle and rates of Hg transformation can identified. This allows better understanding of the predominating factors regulating mercury transformation and mobility.

Keynote Speech 9: The Impact of Climate Change on Inland Waters: The Lake Kinneret (Israel) Case Study [video]

Speaker: Prof. Moshe Gophen, MIGAL-Scientific Research Institute, Israel
Time: 16:10-16:50, Saturday Afternoon, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Regional (Lake Kinneret Watershed) changes of climate conditions indicates air and water temperature increase, decline in rainfall, and diminishing river discharges resulting lower lake water level. Consequent reduction in nitrogen input and therefore decline of Nitrogen availability in the Kinneret Epilimnion whilst that of Phosphorus was slightly elevated resulting decline of the Epilimnetic TN/TP mass ratio. Such a trend of change is favored by Cyanbacteria. As a result of temperature elevation and nitrogen deficiency, the biomass of Nitrogen required Peridinium spp domination was replaced by Cyanobacterial biomass enhancement. Cyanobacteria have a deterioration effect on water quality when their biomass is high. Cyanobacteria were found also to be toxic to human beings, livestock, and to freshwater invertebrates. Microcystis bloom and scum formation are a globally known factor deteriorating water quality. Cyanobacteria are ubiquitous in inland aquatic ecosystems, especially lakes and reservoirs. Among filamentous and non-filamentous Cyanobacteria there are about 30 toxic compound – producing species. The diversity, density, toxicity and longevity of Cyanobacteria are influenced by temperature, water mass

motion, thermal structure, light intensity, chemical conditions, such as nutrient availability and allelopathic relations, and grazing by fish, zooplankton, and large invertebrates. Freshwater bodies became globally more Eutrophic due to climate changes which enhanced water scarcity and consequently increase in human consumption. Therefore, global and regional climate change conditions enforced susceptibility of drinking water sources to Cyanobacteria blooms.

Keynote Speech 10: Photonic Annealing for Manufacturing of Perovskite Solar Cells [video]

Speaker: Dr. Dawen Li, Department of Electrical and Computer Engineering, The University of Alabama, Tuscaloosa, Alabama, USA
Time: 16:50-17:30, Saturday Afternoon, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Hybrid perovskite solar cells (PVSCs) have attracted extensive attention due to rapid progress in power-conversion efficiency (champion efficiency ~25.5%) and device fabrication from solution processes, which is fully compatible with low-cost roll-to-roll (R2R) printing. However, large-scale R2R manufacturing is currently limited by their lengthy annealing times from traditional hotplate heating. Thus, developing an alternative annealing technique is essential to realize mass-production of high-performance PVSCs through high-speed printing. In this seminar presentation, I will talk about rapid photonic annealing to make high-performance perovskite solar cells. We demonstrated that infrared lamp, rapid thermal processing (RTP), UV-LEDs can be employed to anneal perovskite active layer and achieve high-performance solar cells in a much short time (tens of seconds) as compared to hotplate annealing with comparable or better performance. These novel technology developments, particularly layer-specific UV-LED annealing, will pave the way to realize large-scale manufacturing of high-performance fully flexible perovskite solar panels through cost-effective R2R printing.

Keynote Speech 11: Glowing gases for green chemistry – mechanistic viewpoint of catalytic processes under non-thermal plasma [video]

Speaker: Dr. Marek Wiśniewski, Nicolaus Copernicus University in Toruń, Poland
Time: 17:30-18:10, Saturday Afternoon, April 24, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

The low temperature plasmas are extremely complex systems and processes being performed under these conditions usually involve a "great zoo" of different charged and uncharged species which can all contribute to the properties of the resulting products. Despite great advancements in the field of plasma based processes, the details involved in this "plasma production process" are still far from being understood. The non-thermal plasmas are nowadays widely used for a variety of different applications ranging from the VOC removal, CO_2 reduction, etching of microstructures and the deposition of thin films to the modification of surfaces and the synthesis of novel materials. The flexibility of plasma based processes and in particular the possibility to combine different kinds of plasma based processes make them an ideal tool for the fabrication of nanocomposite materials and catalysts.

On the other hand we can observe the "water paradox"–our planet is full of this compound, however drinking water starts to be rare. Thus we need to start use water (not-tap-water) as a reagent. New technologies treating water as a source of hydrogen are required.

Also, the "Oil Crisis" has stimulated research on new energy sources as substitutes for fossil fuel. Hydrogen is an excellent energy source and one of the most important raw materials, used in large scale in many industrial processes such as ammonia synthesis, methanol synthesis, CO hydrogenation, metallurgy, and many petrochemical reactions. Current methods for hydrogen production still include steam reforming of methane, the water gas shift reaction, and electrolysis of water.

H_2O splitting (actually co-splitting) is the key step of reactions utilized in many environmental-friendly processes. Two most important are: so called "artificial photosynthesis" (CO_2/H_2O), "nitrogen fixation" (N_2/H_2O). However, there are some inconveniences: water molecules are very stable. Their decomposition is a strongly endothermic reaction (AG°= 229 kJ/mol). Thus, external energy such as thermal, light, or electric energy are needed.

Low temperature plasma (LTP) can perfectly function as sources of energy suitable for water splitting, thus solving the catalysis society challenge: the production of hydrocarbons from water and CO_2 in low energy consumption systems.

Also, the N_2 fixation reaction is one of the most important chemical processes in nature as it is essential for both human beings and the planet's ecosystem. NH_3 is the main product of N_2 fixation and nowadays is the most widely produced chemical, with an annual production of over 200 million tons. Nearly 80% of synthetic NH_3 is consumed as a raw material in industry for the synthesis of fertilizers.

The main objective of the presentation will be to answer the questions: (i) is it possible to control the overall catalytic activity and selectivity to most wanted product: hydrogen, hydrocarbons, ammonia, urea?; (ii) how the main parameters affected the mechanism of the process?; (iii) are surface structures, in form of: C=O, C–O, and C–OH for CO2/H2O, and C=N, C–N and –NCO (–CNO), when N_2 is incorporated into the reaction zone, the main intermediates of the processes?

Environmental Science: Keynote Speech Session 3

Keynote Speech 12: TBD [video]

Speaker: Dr. Mohd Anis Ganaie, Government of Jammu and Kashmir, India
Time: 08:30-09:10, Sunday Morning, April 25, 2021
Location: Taibaishan Room (太白山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
TBD

Chemistry Science: Keynote Speech Session 1

Keynote Speech 1: Photophysical and chiroptical properties of hybrid materials of chiral azo-Schiff base metal complexes [video]

Speaker: Prof. Takashiro Akitsu, Tokyo University of Science, Japan
Time: 08:30-09:10, Saturday Morning, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Herein we have originally designed chiral azo-salen Mn(II) and Zn(II) complexes for interacting silver nanoparticles (AgNPs) exhibiting localized surface plasmon resonance (LSPR). Understanding excited state and reaction intermediate during light irradiation to return to ground state may be important for such composite systems. Therefore, we investigated such optical properties for systems using time-resolved luminescence and transient absorption measurements. DMSO solutions of the four newly prepared and characterized complexes (MMn, MZn, CMn, and CZn) and ethanol solutions of the composite materials of each complex with AgNPs were served for optical measurements. The time-correlated single photon counting (TCSPC), the streak camera which is much shorter period of time than TCSPC and transient absorption measurement, was performed for the eight samples. The fluorescence lifetime of the sole complexes and the composite materials with AgNPs was derived from curve-fitting analysis of luminescence decay curves of TCSPC. Lifetime of the composite systems with AgNPs was longer than that of the corresponding sole metal complexes for three cases. It was revealed that composite systems may go through three reaction intermediates during relaxation from excited state to ground state.

Keywords: Schiff base metal complexes, azobenzene, silver nanoparticles, fluorescence lifetime

Keynote Speech 2: Self-assembly and modular microswimming [video]

Speaker: Prof. Ran Niu, Huazhong University of Science and Technology
Time: 09:10-9:50, Saturday Morning, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Micro-/nanoswimmers (also called motors) have attracted significant interest due to their suitability for applications in biomedical engineering and environmental remediation. Typical biological and artificial micro-swimmers use non-reciprocal motion (e.g. flagellae) or phoretic propulsion (e.g. driven by chemical reactions) [1]. We here present a complementary

approach to micro-swimming by combining several non-active parts to self-organize into a self-propelling complex. Our modular phoretic micro-swimmer consists of an ion exchange resin (IEX) particle (being the fuel reservoir) and a charged colloidal particle (CP, acting as gearing), both settled to a charged substrate and hydro-dynamically coupled by an electro-osmotic solvent flow along the substrate (acting as a motor), which is caused by the gradient generated by the IEX [2,3]. Combining experiment, theory and simulation, we systematically characterize the self-assembly and swimming performance of this complex as a function of system parameters and understand the underlying mechanisms [4-6]. We further show how the moving direction and speed of this complex can be controlled for potential applications.

Reference

[1] V. Yadav, W. Duan, P. J. Butler, and A. Sen, Annu. Rev. Biophys. 44, 77 (2015).
[2] A. Reinmüller, H. J. Schöpe, and T. Palberg, Langmuir 29, 1738 (2013).
[3] R. Niu, D. Botin, J. Weber, A. Reinmüller, T. Palberg. Langmuir 33, 3450−3457 (2017).
[4] R. Niu, T. Palberg, T. Speck. Physical Review Letters 119, 028001 (2017).
[5] R. Niu, A. Fisher, T. Palberg, T. Speck. ACS Nano 12, 10932−10938 (2018).
[6] R. Niu, P. Kreissl, A. T. Brown, G. Rempfer, D. Botin, C. Holm, T. Palberg, J. de Graaf. Soft Matter 3, 1505−1518 (2017).

Keynote Speech 3: Surface engineering of Ti_6Al_4V by forming hybrid self-assembled monolayers and its effect on collagen-I adsorption, osteoblast adhesion and integrin expression [video]

Speaker: Dr. Lalit M. Pandey, Department of Biosciences and Bioengineering, IIT Guwahati, India
Time: 10:20-11:00, Saturday Morning, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

This study focused on the surface engineering of Ti_6Al_4V by forming self-assembled monolayers (SAMs) towards improving bio-interfaces interactions [1]. Adsorption of adhesive protein collagen-I (Col-I) and subsequently on osteoblast adhesion and integrin expression were studied on the engineered surfaces. The moderate hydrophobic Ti_6Al_4V surfaces ($\theta = 78 \pm 3^\circ$) were prepared by forming hybrid self-assembled monolayers (SAMs), which contain both hydrophobic and hydrophilic moieties on the same SAM molecule. The experimental adsorbed amounts of Col-1 were compared with the predicted ones using the Gibbs equation, which were overestimated but linearly related. Secondary structure and morphology analyses of adsorbed Col-I revealed globular morphology with significant change only in helical content. Cell-surface interactions on hybrid surface pre-adsorbed with Col-1 exhibited better cell adhesion (~100%) and

spreading area (1127 μm2) as compared to cells adhered to hybrid surface without (adhesion of 69% and cell area of 509 μm2) and with (adhesion of 94% and cell area of 908 μm2) fetal bovine serum (FBS) in cell culture media. It was observed that higher expression of α 1 and α 2 integrins on surfaces with pre-adsorbed Col-I and were correlated with the increase in nuclei area indicating α 1 and α 2 mediated cell adhesion promoted the cell proliferation. Overall, cell-surface interactions were improved on hybrid surfaces with pre-adsorbed Col-I, which designated the surface engineered Ti_6Al_4V as potential implant biomaterials.

Reference

1. Hasan, A. and L.M. Pandey, Surface modification of Ti_6Al_4V by forming hybrid self-assembled monolayers and its effect on collagen-I adsorption, osteoblast adhesion and integrin expression. Applied Surface Science, 2020. 505: p. 144611..

Keynote Speech 4: Removal of Cd(II) ions from bioretention system by soil wettability [video]

Speaker: Dr. Kinjal J. Shah, Nanjing Tech University, China
Time: 11:00-11:40, Saturday Morning, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

This study aims to identify the role of wettability on the heavy metal immobilization in the bio-retention system. In general, agricultural soils get wetted easily by water and thereafter evaporates water into the atmosphere due to atmospheric conditions such as sunlight, wind, temperature, and humidity. To lower the water loss, a layer of silane modify soil was laid on the ordinary hydrophilic soil. This system amazingly decreased the loss of water from the soil. The potential of hydrophobic soil for the removal of Cd(II) ions from the bioretention system was investigated. The effects of pH, mixing ratio, layer thickness were studied. In addition, the growth of the plant was analyzed. It was found that the length of roots, shoots, and the number of leaves and branches, etc. were significantly increased with the use of hydrophobic soil in comparison to hydrophilic soil with similar bioretention systems. Such a practical application can decrease water consumption and also help to prevent the distribution of heavy metals in the plant system. From the investigation, it is concluded that hydrophobic soil could be useful energy, environmentally friendly, and economically affordable tool for removal of Cd(II) ions from the bioretention system.

Chemistry Science: Keynote Speech Session 2

Keynote Speech 5: A DNA Nanodevice Simultaneously Activating the EGFR and Integrin for Enhancing Cytoskeletal Activity and Cancer Cell Treatmen [video]

Speaker: Dr. Mirza Muhammad Faran Ashraf Baig, The University of Hong Kong, China
Time: 14:00-14:40, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Cell-surface receptors (e.g., EGFR and integ-rin) and their interactions play determining roles in signal transduction and cytoskeletal activation, which affect cell attachment/detachment, invasion, motility, metastasis (intra-cellular), and cell − cell signaling. For instance, the interactions between the EGFR and integrin (α 6 β 4) may cause increased mechanical force and shear stress via enhanced cytoskeleton activation. Here, we design a DNA nanodevice (DNA-ND) that can simultaneously target the EGFR and integrin receptors on the caveolae. The piconewton (pN) forces in response to the EGFR − integrin coactivation can be sensed upon the unfolding of the DNA hairpin structure on the side arm of the device via changes of the fluorescence and plasmonic signals. We find that simultaneous activation of EGFR − integrin receptors causes enhanced signal transduction, contractions of the cells, and initiation of the biochemical pathways, thus resulting in a change of the cell division and endocytosis/exocytosis processes that affect the cell proliferation/apoptosis. The DNA-ND further enables us to visualize the cointernalization and degradation of the receptors by lysosomes, providing a novel approach toward bioimaging and mechano-pharmacology.

Keywords: Cell surface receptors, EGFR and integrin, caveolae, cytoskeleton, pN forces, DNA nanodevice (DNA-ND)

Keynote Speech 6: Pearls of Pediatric Non-alcoholic Fatty Liver Disease [video]

Speaker: Prof. Ravinder Dachepalli, Osmania University, Telangana, India
Time: 14:40-15:20, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract

Synthesis of Cobalt-Erbium nano-ferrites with formulation CoErxFe2-xO4 (x = 0 0.005, 0.010, 0.015, 0.020, 0.025, and 0.030) using technique of citrate-gel auto-combustion was done. Characterization of prepared powders was done by using XRD, EDS, FESEM, VSM, FTIR Spectroscopy, DC resistivity and dielectric properties respectively. XRD Rietveld Analysis, SEM, TEM and EDAX analysis were taken up in studying spectral, structural, magnetic and electrical properties. XRD pattern of CEF nano particles confirm single phase cubic spinal structure. The structural variables given by lattice constant (a), lattice volume (v), average crystallite size (D) and X-ray density(dx), Bulk density (d), porosity (p), percentage of pore space (P%), surface area (s), strain (ε), dislocation density (δ), along with ionic radii, bond length and hoping length were calculated. SEM and TEM results reveal homogeneous nature of particles accompanied by clusters having no impurity pickup. TEM analysis gives information about particle size of nanocrystalline ferrite while EDAX analysis confirm elemental composition. Emergence of two arch shaped frequency bands (v1andv2) that represent vibrations at tetrahedral site (A) and octahedral site (B) was indicated by spectra of FTIR. The samples electrical resistivity (DC) was measured between 300C -6000C with Two probe method. Dielectric parameters were studied at room temperature between 1Hz to 8MHz frequency range. XRD Rietveld analysis confirm crystallite size lying between 20.84nm-14.40nm while SEM analysis indicate formation of agglomerates and TEM analysis indicate particle size ranging between 24nm-16 nm. DC Electrical measurements indicate continuous decrease in resistivity with increasing temperature while increasing doping decreases curie temperature. Magnetization measurements indicated increasing Er3+ content in cobalt ferrites decreases magnetization from 60emu/g to 42emu/g while coercivity decreases to (18990) as compared to CoFe2O4(18998) in cobalt ferrites with doping. The present study investigates the effect of different compositions of Er3+ replaced for Fe on structure, dielectric, magnetic properties and electrical resistivity of cobalt ferrites.

Keynote Speech 7: Magnetic Polymer Nanocomposites Derived through Dispersion of Siliconized Ferrofluid into Epoxy Resin in Supercritical Carbon Dioxide [video]

Speaker: Dr. M. G. H. Zaidi, G. B. Pant University of Agriculture & Technology, India
Time: 15:20-16:00, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Magnetic polymer nanocomposites (MPNs) are of immense importance in biotechnology1-5, stealth 6, inductive, capacitive materials, microwave absorbers7, electrical8 and electronic applications9. Physical properties and applications of MPNs are governed by qualitative dispersion of nanomagnetic materials and their interfacial adhesion with polymer matrix. However, inherent agglomerations among magnetic nanoparticles makes difficult in achieving the MPNs with uniform dispersion and physical properties1-9. The present lecture shall demonstrate a method of preparation of MPNs through dispersion of siliconized ferrofluid (FF) into epoxy resin (ER) in supercritical carbon dioxide (SCC), followed by curing with triethylene tetramine. SCC is the family member of supercritical fluids that is economically produced through operating carbon dioxide above critical temperature and pressure10-11. Due to pressure tunable density, diffusivity and solvating properties, SCC facilitates the enhanced dispersion of FF into ER that on curing with polyamines delivers MPNs. Dispersion of FF into ER was found progressive with pressure of SCC ranging 1200 to 1600 psi at 90 oC over 1hr. Dispersion of FF into epoxy matrix was revealed through diverse analytical methods based on microscopy, quantitative ultraviolet spectra, X-ray diffraction, magnetometry, laser induced break down spectra and DC conductivity measurement. MPNs synthesized through the present methods have shown improved impact, dispersion, DC conductivity, compressive strength, hardness, resistance against wear and thermal degradation with simultaneous reduction in their tensile behavior over cured epoxy. The proposed method of synthesis of MPNs offers a clean and scalable alternative to ultrasonication or mechanical mixing methods employed for dispersion of magnetic nanoparticles into ER to achieve the MPNs8.

Keynote Speech 8: Environmenatal chemistry of dissolved organic matter

Speaker: Prof. Yong Chen, Huazhong University of Science and Technology
Time: 16:20-17:00, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
TBD

Keynote Speech 9: Pump driven choerence: evidence of an excitonic insulator transition or normal charge migration effects? [video]

Speaker: Dr. Marini Andrea, Division of Ultrafast Processes in Materials (FLASHit); Istituto di Struttura della Materia (ISM); National Research Council (CNR)
Time: 17:00-17:40, Saturday Afternoon, April 24, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
TBD

Chemistry Science: Keynote Speech Session 3

Keynote Speech 10: TBD [video]

Speaker: Prof. Vasudevanpillai Biju, Hokkaido University, Japan
Time: 08:30-09:10, Sunday Morning, April 25, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
TBD

Keynote Speech 11: Use of ab initio modeling for the design of nanomaterials in environmental and catalytic applications [video]

Speaker: Dr. Michael Badawi, Université de Lorraine, France
Time: 09:10-09:50, Sunday Morning, April 25, 2021
Location: Huashan Room (华山厅), 1st Floor, Xi'an Grand Dynasty Culture Hotel

Abstract
Nowadays the degree of sophistication of atomistic simulations based on density functional theory (DFT) can be very high and "numerical experiments" can be realized [1-5]. Combining different atomistic simulation techniques such as ab initio molecular dynamics with advanced method such many-body schemes to take into account non-local dispersion forces, one can accurately predict adsorption enthalpies of molecules in nanoporous materials. This allows a fast screening of a large number of formulations to design efficient and selective adsorbents with optimized properties for various applications. The use of atomics simulations also helps to understand at a molecular level the interactions between molecules and materials. We will give some applications of these modeling tools for the selective capture of radioactive iodine in case of nuclear severe accident [1-4] and for the production of biofuels from biomass waste [5,6]. Surface or catalytic reaction mechanisms can be also computed to identify the key steps in a specific process [4,5]. In close connection with experiments, the use of ab initio modeling open the path to an integrated approach for the development of optimized nanomaterials and processes in the fields of catalysis and environment.

Keywords: Density Functional Theory, Ab initio Molecular Dynamics, zeolites, adsorption, catalysis, biomass, nuclear safety

Reference
[1] S. Chibani, M. Chebbi, S. Lebègue, Bučko, M. Badawi, J. Chem. Phys. 144 (2016) 244705.
[2] M. Chebbi, S. Chibani, J.-F. Paul, L. Cantrel, M. Badawi, Micropor. Mesopor. Mater. 239 (2017) 111.
[3] H. Jabraoui, E. P. Hessou, S. Chibani, L. Cantrel, S. Lebègue, M. Badawi, Appl. Surf. Sci. 485 (2019) 56.
[4] T. Bučko, S. Chibani, J.-F. Paul, L. Cantrel, M. Badawi, Phys. Chem. Chem. Phys. 19 (2017) 27530.
[5] M. Badawi et al., Journal of Catalysis 282 (2011) 155-164.
[6] Y. Berro, S. Gueddida, S. Lebègue, A. Pasc, ⋯, M. Badawi, Appl. Surf. Sci. 494 (2019) 721.

Part III Technical Sessions

Environmental Science: Keynote Speech Session 3 & Technical Session

Session Chair: TBD

Location: Huashan Room (华山厅), 1st Floor 08:30-12:00, April 25, 2021

Time	Paper Title	Author	Affiliation
08:30-09:10	TBD	Dr. Mohd Anis Ganaie	Government of Jammu and Kashmir, India
09:10-09:30	MicroRNA-382-5p is involved in pulmonary inflammation induced by fine particulate matter exposure.	You Fu	Southeast University, China
09:30-09:50	**Group photo & Coffee Break**		
09:50-10:10	Comprehensive evaluation of flood and flood in the Yellow River Basin based on gray correlation analysis	Han Mo	Postgraduate of Sichuan University, China
10:10-10:30	Impact of partially covered vegetation on the lateral velocity distribution of open channel flow	Xiaonan TANG	Xi'an Jiaotong-Liverpool University, China
10:30-10:50	Structural design of a bionic anti-clogging drip irrigation emitter based on shark dorsal fin	Caixiang Wei	Xi'an Jiaotong University, China
10:50-11:10	Novel and legacy flame retardants in paired human fingernails and indoor dust samples	Yi Chen	Nanjing University, China
11:10-11:30	Photocatalytic Degradation of Ammonia gas by Cu2O/{001}TiO2 and its mechanism analysis.	Jiaming Zhu	Chongqing Academy of Animal Sciences, China
11:30-11:50	The implication of Iron Nanoparticles to Human Exposure Through Radish by Enhancing the Nutrients	Noman Shakoor	College of resources and environmental science, China Agriculture University
11:50-12:10	Bio-interaction of nano and bulk Rare earth oxides in soil system: Biochemical, genetic, and histopathological effects on *Eisenia fetida*	Muhammad Adeel	College of resources and environmental science, China Agriculture University

poster	Numerical simulation and characteristic analysis of migration of uranium and sulfate in situ leaching	Haibo Li	School of Environmental studies, China University of Geosciences, China
poster	Fitting of water requirement and yield of winter wheat in north china plain based on artificial neural network	Weibing Jia	Xi'an Jiaotong University, China
poster	The molecular initiation events and signaling pathways of thyroid hormone disrupting effects of TDCPP and BDCPP	Ying Xu	College of Water Sciences, Beijing Normal University, China

Chemistry Science: Keynote Speech Session 3 & Technical Session

Session Chair: TBD

Location: Huashan Room (华山厅), 1st Floor 08:30-12:00, April 25, 2021

Time	Paper Title	Author	Affiliation
08:30-09:10	TBD	Prof. Vasudevanpillai Biju	Hokkaido University, Japan
09:10-09:50	Use of ab initio modeling for the design of nanomaterials in environmental and catalytic applications	Dr. Michael Badawi	Université de Lorraine, France
09:50-10:00	**Group photo & Coffee Break**		
10:00-10:20	CO_2/CaO-responsive behavior of amine emulsion and its application in oil-based drilling fluid	Yanjun Ren	Southwest Petroleum University, China
10:20-10:40	Folding Graphene into a Chern Insulator with Light Irradiation	Gan Zhao	University of Science and Technology of China
10:40-11:00	Mechanistic Insights into the Visible-Light-Promoted Radical Coupling Reactions within the Electron Donor-Acceptor Complex	Lishuang Ma	China University of Petroleum (East China), China
11:00-11:20	Reducing anionic surfactant adsorption using polyacrylate as sacrificial agent	Zilong Liu	China University of Petroleum (Beijing), China
11:20-11:40	Highly conductivity and biocompatibility conducting polymer/PEDOT:PSS hydrogels for bioelectronic devices	Taotao Yang	Huazhong University of Science and Technology, China
11:40-12:00	Black-Phosphorus-Incorporated Hydrogel as a Conductive and Biodegradable Platform for Spinal cord repair	Chao Xu	Huazhong University of Science and Technology, China
poster	Two-Dimensional Quadrupole Topological Insulator in γ-Graphyne	Bing Liu	University of Science and Technology of China

poster	Facile fabrication of carbon nanotubes/CoNiFe layered double hydroxide hybrid material for high-performance asymmetric supercapacitors	Hongjuan Li	Northwest A&F University, China
poster	Polymorphs and pharmacokinetics of an antipsychotic drug candidate	Chao Hao	Huazhong University of Science and Technology, China

Part IV Technical Sessions Abstracts

ID: CECE2021_20000

Title: Up-regulation of miR-297 mediates aluminum oxide nanoparticle-induced lung inflammation through activation of Notch pathway.

Name: Jie Xu
Affiliation: Southeast University, China
Email: 1282107044@qq.com

Abstract

Exposure to Aluminum oxide nanoparticles (AlO NPs) has been associated with pulmonary inflammation in recent years; however, the underlying mechanism that causes adverse effects remains unclear. In the present study, we characterized microRNA (miRNA) expression profiling in human bronchial epithelial (HBE) cells exposed to AlO NPs by miRNA microarray. Among the differentially expressed miRNAs, miR-297, a homologous miRNA in Homo sapiens and Mus musculus, was significantly up-regulated following exposure to AlO NPs, compared with that in control. On combined bioinformatic analysis, proteomics analysis, and mRNA microarray, NF-κB-activating protein (NKAP) was found to be a target gene of miR-297 and it was significantly down-regulated in AlO NPs-exposed HBE cells and murine lungs, compared with that in control. Meanwhile, inflammatory cytokines, including IL-1β and TNF-α, were significantly increased in bronchoalveolar lavage fluid (BALF) from mice exposed to AlO NPs. Then we set up a mouse model with intranasal instillation of antagomiR-297 to further confirm that inhibition of miR-297 expression can rescue pulmonary inflammation via Notch pathway suppression. Collectively, our findings suggested that up-regulation of miR-297 expression was an upstream driver of Notch pathway activation, which might be the underlying mechanism involved in lung inflammation induced by exposure to AlO NPs.

ID: CECE2021_20001

Title: MicroRNA-382-5p is involved in pulmonary inflammation induced by fine particulate matter exposure.

Name: You Fu
Affiliation: Southeast University, China
Email: 1282107044@qq.com

Abstract

Exposure to atmospheric particulate matter (PM) has been related to the increasing incidence and mortality of pulmonary diseases, where microRNAs (miRNAs) play significant roles in these biological and pathological processes. In the present study, we found that miR-382-5p played an anti-inflammatory role in pulmonary inflammation induced by fine particulate matter (PM2.5) or diesel exhaust particles (DEPs) in vitro and in vivo. The expression level of miR-382-5p was downregulated, while its target gene, namely CXCL12, was elevated in HBE cells after exposure to PM2.5 or DEPs. Mechanistically, PM2.5 or DEPs exposure increased CXCL12/MMP9 expression via miR-382-5p inhibition, subsequently triggered pulmonary inflammation. Furthermore, antagonizing the function of CXCL12 significantly reduced the expression of MMP9 and local inflammation induced by PM2.5 or DEPs. PM2.5 or DEPs caused apoptosis and G1 phase arrest could be partially restored by overexpression of miR-382-5p and antagonism of CXCL12. In a murine model, enhanced miR-382-5p expression effectively reduced expression levels of CXCL12, MMP9 and inflammatory cytokines, hereby protected lung tissues against PM2.5 or DEPs-induced lesions. Collectively, the miR-382-5p/CXCL12/MMP9 pathway may provide a mechanism, which mediates inflammatory response to PM2.5 or DEPs exposure.

ID: CHWM2021_20000

Title: Comprehensive evaluation of flood and flood in the Yellow River Basin based on gray correlation analysis

Name: Han Mo

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Abstract

Due to the concentrated rainfall and serious soil erosion in July and August in the Yellow River Basin, the flood discharge is not timely leading to serious floods. Therefore, a reasonable assessment of the flood-affected areas, advance arrangements for the deployment of the Yellow River basin flood disaster prevention and control plays a decisive role. For this purpose, this paper proposes a level assessment method based on the flood which analyzes three factors related to flooding disaster (disaster impact range, social index, and property index) through the gray correlation analysis method, to evaluate the level of flood disaster. Different from the traditional assessment method, which evaluates the nature of flood from the perspective of indicators such as frequency, duration, and magnitude, or indirect factors such as rainfall and soil loss, this paper conducts qualitative calculation of macro-scale indicators from the perspective of post-disaster losses in previous years. This study provides a new way of thinking and method for the classification of the flood disaster, which has certain practical application value under the condition of conforming to its own use.

ID: CHWM2021_20002

Title: Impact of partially covered vegetation on the lateral velocity distribution of open channel flow

Name: Xiaonan TANG

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Abstract

The vegetation affects the flow process and water environment, thus drawing increasing attention to river environment management. Previous research is mainly focused on flow through vegetation in a channel with fully covered sin-gle-layer vegetation. However, in natural rivers, different heights' vegetation often co-exists along one or two sides of a river. This paper experimentally stud-ies how the flow velocity distribution is affected by the two different-layered vegetation allocated along two sides of an open-channel. The vegetation was simulated by dowels of two heights, 10 cm and 20 cm, and arranged in a parallel pattern along two sides of a flume under partially submerged conditions. The velocities along a cross-section were measured by Acoustic Doppler Velocimetry (ADV). The results of lateral velocity distribution show that a strong shear layer exists between vegetation and non-vegetation zones, indicating the retarding effect of vegetation. Meanwhile, as the flow depth increases, the relative veloc-ity in the free flow zone decreases compared with that in the vegetated region, indicating that vegetation resistance to the flow decreases as increasing depth under the same vegetation configuration. These fi ndings would help understand the role of multi-layered vegetation in the riparian management.

ID: CHWM2021_20009

Title: Structural design of a bionic anti-clogging drip irrigation emitter based on shark dorsal fin

Name: Caixiang Wei

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Abstract

Due to the poor anti-clogging performance of the common drip irrigation emit-ters, this paper designed a new bionic flow channel in the emitter based on the shape of shark dorsal fin. After preliminary structural design, the computational fluid dynamics (CFD) simulation showed that the bionic emitter exhibited supe-rior anti-clogging performance and reasonable hydraulic performance. The pas-sage rate of particles

of the bionic emitter in simulation reached 96.3% which was 37.6% higher than 70% of traditional emitter, and the discharge exponent reached 0.4995 which was close to traditional emitter. Physical experiments were consistent with the CFD results, which confirmed the correctness of simu-lation. After a short cycle anti-clogging performance experiment, the bionic emitter still maintained 96.09% of the initial flow rate.

ID: CHWM2021_20010

Title: Fitting of water requirement and yield of winter wheat in north china plain based on artificial neural network

Name: Weibing Jia

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Abstract

The fitting of water requirement and yield during the growth period of winter wheat can improve yield effectively and improve irrigation water use efficiency with a certain amount of resource input. This paper selects the irrigation amount, precipitation and yield of winter wheat at the Wuqiao Scientific Observation and Experimental Station. Fitting the water requirement and yield of winter wheat based on three types of artificial neural networks. This paper uses support vector machine (SVM), thought evolution algorithm to optimize BP neural network (MAE-BP) and generalized re-gression neural network (GRNN) to fit the water requirement and yield of two crops. The SVM is the model with the highest fitting accuracy among the three models, the RMSE, MAE, NS and R2 between predictive value and true value are 7.45 kg/ hectares, 213.64 kg/ hectares,0.8086,0.9409 respectively.

ID: CHWM2021_20008

Title: Numerical simulation and characteristic analysis of migration of uranium and sulfate in situ leaching

Name: Haibo Li

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Abstract

Uranium extraction by in-situ leaching is realized by a set of pumping and injecting holes, that is, the leaching solution is injected into the ore-bearing aquifer through the pumping hole, and then the leaching solution is pumped to the surface for treatment to recover the natural uranium. However, due to the complexity of geological conditions, groundwater dynamics and the influence of pollutant dispersion, it is inevitable that a small amount of leaching solution will flow outside the well site. Therefore, it is necessary to predict and evaluate the environmental impact of wells leaching solution on groundwater. In this study, the generalized model was established and the numerical solution was carried out to simulate the hydrodynamic flow field and solute dispersion field. GMS 3D groundwater migration software was used in this evaluation. At the fifth year of the end of the test, the longest migration distance of uranium was about 43.2m, and the distance beyond 43.2m was basically at the background level. At the 15th year after the end of the test, the longest migration distance of uranium was about 47.0m, and the distance beyond 47.0m was basically at the background level.SO42- At the fifth year of the end of the experiment, the maximum migration distance of SO42- was about 52.2m, and the distance beyond 52.2m was basically at the background level; at the 15th year after the end of the experiment, the maximum migration distance of SO42- was about 57.3m, and the distance beyond 57.3m was basically at the background level. Due to the depth of the ore aquifer and the relative stability of the top and bottom of the ore aquifer, there is little possibility of groundwater from the ore aquifer flowing over to the submarine or other confined aquifer at this distance,

with little impact on the environment and no additional exposure dose to the public.

ID: CECE2021_20002

Title: The molecular initiation events and signaling pathways of thyroid hormone disrupting effects of TDCPP and BDCPP

Name: Ying Xu

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Abstract

The typical organophosphate tri(1,3-dichloropropyl) phosphate (TDCPP) and its metabolite bis(1,3-dichloro-2-propyl) phosphate (BDCPP) have potential damage effects on the thyroid system of human and animal. However, the research on the molecular mechanism of thyroid hormone disrupting effect is not in-depth. This study focuses on the molecular initiation events (MIE) and signaling pathways of thyroid hormone disrupting effects of TDCPP and BDCPP. Based on rat pituitary tumor (GH3) cell, the binding affinity of TDCPP and BDCPP to thyroid hormone membrane receptor, integrin αvβ3, was determined by radioligand competitive binding assay. The results showed that the RIC20 values of TDCPP and BDCPP were 4.58×10-7 and 6.64×10-6 mol/L, respectively. Molecular docking simulation results suggested that both TDCPP and BDCPP had strong binding ability with integrin αvβ3, and the binding energy were -55.68 and -48.09 kcal/mol, respectively. The results of two methods confirmed the strong binding affinity of TDCPP and BDCPP for integrin αvβ3.Real-time PCR also supported the supposition that, after binding to integrin αvβ3, TDCPP and BDCPP might induce the activation of the extracellular signal-regulated protein kinase (ERK1/2) signal transduction pathway. In conclusion, the results of this study confirmed that the binding of TDCPP and BDCPP to membrane receptor integrin αvβ3 might be one of new MIEs of their thyroid hormone disrupting effects, and the activation of ERK1/2 signaling pathway might be involved in thyroid hormone disrupting effects. This study provides a new idea to the thyroid hormone disrupting effects of TDCPP and BDCPP.

ID: ICN2021_20000

Title: Regulation of colorectal cancer metastasis by synthesizing HIF1α-AS2 specific nano lipoplexes.

Name: Jie Xu

Affiliation: Southeast University, China

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Abstract

Long non-coding RNAs (lncRNAs) play a vital role in tumor regulation. Metastasis is the most important factor affecting the prognosis of colorectal cancer (CRC). Here, we identified a lncRNA HIF1α-AS2, which was gradually upregulated following the adjacent-adenoma-CRC. In addition, HIF1α-AS2 promoted progression and metastasis in CRC cells both in vitro and in vivo. Mechanistically, HIF1α-AS2 enhanced transcription factors HIF1α expression by competitively adsorbing the microRNAs miR-18a/b-5p and miR-20a-5p. Meanwhile, HIF1α transcriptionally activated RMRP by directly binding to its promoter region. Moreover, RMRP enhanced the metastasis capacity of CRC through RMRP-IGF2R complex to enhance the expression of IFG2. Importantly, pegylated cationic liposomes was constructed for the efficient entrapment of HIF1α-AS2 siRNA (nano lipoplexes)，which significantly inhibited hepatic and pulmonary metastasis in a CRC xenograft mouse model. Overall, these findings revealed that HIF1α-AS2 may be a potential target in halting CRC metastasis, HIF1α-AS2 specific nano lipoplexes can effectively inhibit the metastasis of colorectal cancer.

ID: CIC2021_20000

Title: CO2/CaO-responsive behavior of amine emulsion and its application in oil-based drilling fluid

Name: Yanjun Ren

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Abstract

An amine emulsion was treated with green and cheap CO2 and CaO as stimulus source. After investigating the responsive behaviors of the amine emulsion, an oil-based drilling fluid was formed and its properties were valued. The results showed that the amine emulsion inversed from water-in-oil state to oil-in-water state readily and its rheology underwent a cosine-like transition via induction by CO2. These CO2 responsive behaviors could be reversed by CaO. Several oil-based drilling fluids were prepared based on the amine emulsion. They had oil-water volume ratios of 50:50~70:30, densities of 1.5~2.0g/cm3 and heat resistance of 160 ℃, and performed well in rheology and filtration. Their filter cake and oily cutting could be readily cleaned up using CO2 bubbling, and the useless solid phase with low density could be removed efficiently via reducing the viscosity of emulsion by CO2, and the residual emulsion phase could be returned to the original state which could be reused to prepare drilling fluid. The mechanisms involved were revealed using fourier transform infrared spectroscopy (FT-IR) and particle size distribution analysis. Results indicated that CO2/CaO induced the reversible conversion between amine emulsifiers and their salts, followed by the reversible regulation of the hydrophilic-lipophilic balance of amine emulsifiers and the reversible increase-decrease of the emulsion particles' size, which finally caused the controllable-reversion of type and rheology of amine emulsion and its feasible application on the clean-up and recycling of oil-based drilling fluids and the removal of useless solid phase with low density.

ID: CPC2021_20005

Title: Folding Graphene into a Chern Insulator with Light Irradiation

Name: Gan Zhao

Affiliation: Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China

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Abstract

Recently, the precise folding of flexible graphene is reported experimentally[1], demonstrating an efficient approach to manipulate its electronic and optoelectronic properties. Here, we propose a light-induced high-Chern-number Chern insulator (CI) in the folded graphene. Along both armchair and zigzag folding directions, we demonstrate that there are two-handedness-dependent chiral interface states localized at the curved region. Physically, they can be attributed to the light-induced mass-term inversion across the folded graphene. Most remarkably, by rationally designing the folding processes, 2D and 3D CIs are also realizable in a single-wall carbon nanotube and periodic folded graphene, respectively, illustrating a high tunability of the folding degree of freedom. We envision that this intriguing form of "foldtronics" will provide a new platform for investigating the topological state in 2D materials to draw immediate experimental attention.

[1] Chen H, Zhang X L, Zhang Y Y, et al. Atomically precise, custom-design origami graphene nanostructures. Science, 365(6457), 1036-1040 (2019).

ID: ISP2021_20000

Title: Mechanistic Insights into the Visible-Light-Promoted Radical Coupling Reactions within the Electron Donor-Acceptor Complex

Name: Lishuang Ma

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Abstract

The association of an electron-poor donor with an electron-rich acceptor can bring about an electron do-nor-acceptor (EDA) complex, which usually extend the absorption to visible light range through the in-termolecular charge transfer excited states, facilitating various of catalyst-free photochemical transfor-mations under mild visible-light conditions. However, a number of fundamental questions are still ambig-uous, such as the origin of visible light absorption, the photochemical and photophysical properties of the EDA complex, as well as the detail mechanism of the radical coupling pathways mediated by EDA com-plex. Herein, multiconfigurational ab initio calculations have been carried out to provide mechanism in-sights into radical coupling reactions within the EDA complexes. Our calculations results reveal that broadening spectra of EDA complex originates from the strong coupling among σD-πA* excitations ac-companied with an intermolecular electron transfer. The subsequent photoinduced C-I bond cleavage was found occur in the triplet state, which is accessible through a fast intersystem crossing (ISC) process that controlled by the strong spin−orbit coupling resulting from the heavy iodine atom. Moreover, the compu-tational results show that the radical-radical coupling and radical chain propagation processes can coexist thermodynamically, which is the key factor that determine the efficiency of the photochemical reactions induced by EDA complexes.

ID: CPC2021_20004

Title: Two-Dimensional Quadrupole Topological Insulator in γ-Graphyne

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Abstract

Two-dimensional quadrupole topological insulator (2D QTI), as a new class of second-order topological phases[1], has been experimentally confirmed in various artificial systems recently. However, its realization in electronic materials has seldom been reported. In this work, we predict that the experimentally synthesized γ-graphyne is a large-gap (~ 0.2 eV) 2D QTI. Three characterized features for 2D QTI are simultaneously observed in γ-graphyne: quantized finite bulk quadrupole moment, gapped topological edge states, and in-gap topological corner states. Intriguingly, we found that gapped topological edge states exist on armchair edge with C≡C (but not C-C) termination, and in-gap topological corner states exist at corner with 120° (but not 60°) termination, which can be explained by different edge-hopping textures and corner chiral charges. Moreover, the robustness of in-gap topological corner states is further identified by varying edge-disorder and system-size calculations. Our results demonstrate a realistic electronic material for large-gap 2D QTI, which is expected to draw immediate experimental attention.

ID: CIC2021_20003

Title: Facile fabrication of carbon nanotubes/CoNiFe layered double hydroxide hybrid material for high-performance asymmetric supercapacitors

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Abstract

A novel hybrid electrode material based on

CoNiFe-LDH and CNTs was prepared by a facile one-step homogeneous precipitation approach for supercapacitors. The CNTs/CoNiFe-LDH hybrid electrode exhibited significantly enhanced specific capacitance (1045 F g − 1 at 1 A g − 1) and high capacitance retention of 73% even at a high current density of 20 A g − 1. Additionally, the asymmetric supercapacitor based on CNTs/CoNiFe-LDH as positive electrode and activated carbon as negative electrode was manufactured and it exhibited a specific capacitance of 95.6 F g−1 at 1 A g−1 and a high energy density of 29.9 W h kg − 1. More importantly, this device showed long-term cycling stability, with 85.0% capacity retention after 3000 cycles at 15 A g−1. Two asymmetric supercapacitors connected in series were able to light up a red LED indicator. This strategy fabricated an excellent hybrid electrode material, which will be one of the promising candidates as electrode materials for supercapacitors.

Keywords: layered double hydroxides, carbon nanotubes, electrode materials, supercapacitor

ID: CEMC2021_20000

Title: Photocatalytic Degradation of Ammonia gas by Cu2O/{001}TiO2 and its mechanism analysis

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Abstract

A heterogeneous composite catalyst Cu2O/{001}TiO2 was successfully prepared by the impregnation-reduction method. With ammonia as the target pollutant, the degradation performance and degradation mechanism analysis of the prepared composite catalyst were investigated, providing technology for the application of photocatalysis technology in ammonia treatment reference. The catalysts were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), specific surface area (BET), fluorescence spectrum (PL) and UV-VIS DRS. The results showed: compared with the single {001}TiO2 catalyst, the composite catalyst has enhanced absorption in the visible light range, reduced band gap width, and enhanced photoelectron-hole separation capability.When the composite ratio was 1:10, the specific surface area of the catalyst was the largest and the ammonia removal efficiency was the highest. In the whole reaction process, surface adsorbed water and associated hydroxyl radical participate in the ammonia degradation reaction, and finally form free hydroxyl radical and NO3-.

Keywords: Cu2O/{001}TiO2; Composite catalyst; Photocatalytic; Ammonia; Mechanis

ID: CIC2021_20001

Title: Reducing anionic surfactant adsorption using polyacrylate as sacrificial agent

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Abstract

Adsorption behavior of surfactants to reservoir rock surfaces is an important issue in oil recovery, especially in the process of alkaline surfactant flooding. However, the loss of surfactant by adsorption onto the rock surface makes surfactant economically less feasible. In this study, we investigated polyacrylate as a sacrificial agent in the reduction of anionic surfactant adsorption with focus on calcite surfaces by using quartz crystal microbalance with dissipation monitoring. The results demonstrated that the adsorption of the anionic surfactant alcohol alkoxy sulfate (AAS) followed a Langmuir adsorption isotherm, and the adsorbed amount reached saturation above its critical micelle concentration. Compared to AAS adsorption, adsorption of polyacrylate was a much slower process. Experimental results combined with density functional theory calculations indicated that calcium cation bridging was important for anionic surfactant and polyacrylate adsorption to calcite surfaces. To effectively reduce the amount of

surfactant adsorption, it was needed to preflush with polyacrylate, rather than by a simultaneous injection. Preflushing with 30 ppm polyacrylate gave a reduction of AAS adsorption of 30% under high salinity conditions, compared to 8% under low salinity conditions. On different mineral surfaces, polyacrylate reduced the AAS adsorption in the order of alumina > calcite > silica. These results offer important insights into mitigating surfactant adsorption using polyacrylate as sacrificial agent and contribute to improved flooding strategies with reduced surfactant loss.

ID: CECE2021_20005

Title: Novel and legacy flame retardants in paired human fingernails and indoor dust samples

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Abstract

The widespread use of flame retardants (FRs) in various commercial and household products resulted in their accumulation in indoor dust, which may further induce human exposure. Fingernails were used as a non-invasive biomarker for FRs. However, little is known about FR occurrence in human fingernails and the association of FRs between paired human fingernail and indoor dust, which may provide new insight for understanding exposure pathways to FR compounds. In this study, the occurrence of 8 polybrominated diphenyl ethers (PBDEs), 5 alternative flame retardants (AFRs), and 7 organophosphate flame retardants (OPFRs), was determined in 50 pairs of human fingernail and indoor dust samples. The concentrations in indoor dust were 71.1-4035 ng/g, 48.5-3915 ng/g, and 331-6362 ng/g for PBDEs, AFRs, and OPFRs. The levels in fingernail were 9.79-242 ng/g, 17.7-926 ng/g, and 58.0-590 ng/g for PBDEs, AFRs, and OPFRs. Male fingernail showed significantly ($p<0.05$) higher Σ8PBDE concentrations than female fingernails, while no significant gender differences were observed for AFRs and OPFRs. Lower ratios of BDE209 to Σ8PBDE and DBDPE to Σ5AFRs were found in fingernails than in dust. Due to their relatively rapid in vivo debromination, BDE 209 and DBDPE in fingernails were most likely from external sources rather than internal exposure (such as through blood circulation). Similar composition profiles between fingernail and dust were observed for PBDEs (excluding BDE209), AFRs (excluding DBDPE), and OPFRs, indicating that indoor dust may be a significant source for these FRs in human fingernails. Significant correlations between fingernail and dust were observed for BDE 47 ($p<0.01$; $r=0.50$), TBPH ($p<0.01$; $r=0.37$) and TBOEP ($p<0.01$; $r=0.53$). Results in this study provided information about contamination levels and exposure sources of FRs, which is important for long-term biomonitoring and health risk assessment of FRs.

Keywords: fingernail, indoor dust, organophosphate flame retardants, polybrominated diphenyl ethers, alternative flame retardants

ID: ICN2021_20001

Title: Highly conductivity and biocompatibility conducting polymer/PEDOT: PSS hydrogels for bioelectronic devices

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Abstract

In order to solve the biocompatibility problem of polyaniline/phytic acid conductive hydrogel, we have found a material with high conductivity and high biocompatibility, PEDOT:PSS, as the cross-linking of the preparation of conductive hydrogel to replace crosslinking agents with poor biocompatibility, such as phytic acid, amino trimethylene phosphonic acid, folic acid, copper phthalocyanine and ferric phthalocyanine. This method has a certain versatility. Using PEDOT:PSS as a crosslinking agent can not only prepare PAni/PEDOT:PSS and PPy/PEDOT:PSS two conductive polymer hydrogels, but also can be used to

prepare a new type of polymer Indole amino (PIn-X-NH2) conductive polymer hydrogel (PIn-X-NH2/PEDOT:PSS; X=4, 5, 6, 7), this type of hydrogel has never been reported before. The experimental results show that the conductive polymer/PEDOT:PSS hydrogel prepared by this method has good biocompatibility, and the conductivity is also greatly improved. Compared with the traditional conductive polymer/phytic acid hydrogel, the conductivity of the polymer/PEDOT:PSS hydrogel is increased by nearly 10 times. Based on the conductive polymer/PEDOT:PSS hydrogel platform, we constructed an in-situ cell electrochemical sensor for the detection of active molecules dopamine and hydrogen peroxide released by cells, and showed excellent electrochemical sensing performance.

Keywords: Conducting polymer hydrogels, In-situ cell electrochemical sensor

ID: ICN2021_20002

Title: Black-Phosphorus-Incorporated Hydrogel as a Conductive and Biodegradable Platform for Spinal cord repair

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Abstract

Conductive hydrogel scaffolds have important applications for electroactive tissue repairs. However, the development of conductive hydrogel scaffolds tends to incorporate nonbiodegradable conductive nanomaterials that will remain in the human body as foreign matters. Herein, a biodegradable conductive hybrid hydrogel is demonstrated based on the integration of black phosphorus (BP) nanosheets into the hydrogel matrix. To address the challenge of applying BP nanosheets in tissue engineering due to its intrinsic instability, a polydopamine (PDA) modification method is developed to improve the stability. Moreover, PDA modification also enhances interfacial bonding between pristine BP nanosheets and the hydrogel matrix. The incorporation of polydopamine-modified black phosphorous (BP@PDA) nanosheets into the gelatin methacryloyl (GelMA) hydrogels significantly enhances the electrical conductivity of the hydrogels and improves the cell migration of neural stem cells (NSCs) within the 3D scaffolds. On the basis of the gene expression and protein level assessments, the BP@PDA incorporated GelMA scaffold can significantly accelerated the differentiation of NSCs into neurons in vitro. Furthermore, the biohybrid hydrogel can activate endogenous NSC neurogenesis in the lesion area, resulting in significant recovery of locomotor function. This strategy of integrating biodegradable conductive BP nanomaterials within a biocompatible hydrogel provides a new insight into the design of biomaterials for broad application in spinal cord injury (SCI) therapy.

Keywords: black phosphorus, biodegradable, Nanocomposite hydrogel, neural stem cells, spinal cord injury

ID: ICN2021_02001

Title: Polymorphs and pharmacokinetics of an antipsychotic drug candidate

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Abstract

A potent antipsychotic drug candidate, 7-(4-(4-(6-fluorobenzo[d]-isoxazol-3-yl)-piperidin-1-yl) butoxy)-4-methyl-8-chloro -2H-chromen-2-one mesylate(CY611), with good in vitro and in vivo antipsychotic effects was investigated for preformulation evaluation by crystallography methods. Three anhydrous polymorphs(Form I - III), a monohydrate(Form IV), and a NMP solvate(Form V) were discovered and characterized by powder X-ray diffraction, thermal analysis, attenuated total

reflection-fourier transform infrared spectroscopy and scanning electron microscopy. Form I, monohydrate Form IV, and a NMP solvate Form V of the drug candidate were isolated, and their structures were determined by single crystal X-ray diffraction. IDR and relative stability experiment were performed. Although Form II has the fastest release rate in water, it easy transformed to monohydrate which has the lowest release rate. In vivo pharmacokinetic study showed that the Form III has the highest bioavailability at 35.4%. Considering the balance between the physicochemical properties, bioavailability and manufacturability of the available polymorphs, Form III may be the optimal form candidate for the eventual formulation.

ID: CECE2021_20102

Title: The implication of Iron Nanoparticles to Human Exposure Through Radish by Enhancing the Nutrients

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Abstract

Iron (Fe) scarcity is a pervasive nutritional disorder affecting human health and interest in producing vegetables enriched with this Fe-based nanoparticle (NPs) as a dietary source of Fe. Owing to high nutritional value and improved bioaccessibility of essential elements, red radish is promising target for enrichment. In this study, an attempt was made to evaluate the effects of three types of Fe based NPs on (i) the red radish physiology, (ii) Fe bioaccumulation, (iii) the nutritional quality and (iv) the essential amino acids content at 10, 50, 100, 200 and 500 mg kg-1 concentration level. The growing of red radish in the presence of Fe based NPs a significant increase in the Fe concentration in leaves and radish fruit, additionally highest accumulation observed with exposure of Fe_3O_4 (53-58%) and FeO(OH) (37-48%) at 100 and 200 mg kg-1 as compared to control. Application of Fe_3O_4 and FeO(OH) at 100 and 200 mg kg-1 significantly increased (37-58%) the daily intake of Fe content with consumption of treated red radish. Nutritional quality (zinc, total nitrogen, crude protein and VC content) of red radish significantly increased (37%, 66%, 67% 48%) with concentration level. Whereas, non-significant effects were reported in γ -Fe_3O_4 treatments at various (10, 50, 100, 200 and 500 mg kg-1) level. To date, our study revealed that radish grown in the presence of Fe_3O_4 and FeO(OH) NPs at 100 and 200 mg kg-1 proved to be the most suitable for enrichment with Fe content as they accumulated considerable amounts of Fe content in fruit, increased the nutritional quality and dietary intake.

ID: CECE2021_20103

Title: Bio-interaction of nano and bulk Rare earth oxides in soil system: Biochemical, genetic, and histopathological effects on *Eisenia fetida*

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Abstract

The enormous application of rare earth elements (REEs) in electronic industries cause their inevitable release into the environment; however, its effects on soil biota remain largely unaddressed. We investigated the *E. fetida* detoxification potential of nano and bulk La_2O_3 and Yb_2O_3 and their potential impact on biochemical and genetic markers at various concentrations levels. We found that earthworms bioremediate 3-15% La_2O_3 and Yb_2O_3 contaminated soil at low and medium levels, while this potential was limited at higher levels. Nano and bulk La_2O_3 and Yb_2O_3 treatment induced neurotoxicity in earthworm by inhibiting acetylcholinesterase by 49-65% and 22-36% at 500 and 1000 mg kg-1, respectively. Nano La_2O_3 proved to be highly detrimental, mainly through oxidative stress and subsequent failure of antioxidant system. Nano La_2O_3 and Yb_2O_3 at 100 mg kg-1 significantly down-regulated the expression of

annetocin mRNA in the parental and progeny earthworms by 50% and 20%, which is crucial for earthworm reproduction. Similarly, expression level of heat shock protein 70 (HSP70) and metallothionein was significantly upregulated in both generations at medium exposure level. Histological observations showed that nano REEs at 200 mg kg-1 induced drastic changes in the intestinal epithelium and typhlosole of *E. fetida*. To date, our results enhance the understanding of interaction between REEs and earthworms.

ID: CIC2021_20002

Title: Determination of N-acylpyrrolidines by GC-MS/MS using surfactants containing adjacent binary hydroxyl groups

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Abstract

Gas chromatography (GC) is widely used in chemical analysis for its capacity of separating compounds in complex matrix. However, a common problem in GC applications is that susceptible analytes would adsorb or degrade at the active sites (silanol groups and metal ions) on surface of GC flow path (injection port, column and detector), resulting analyte losses and peak tailing. Generally, susceptible analytes contain active groups, such as hydroxyl, carbonyl, ester, amino, amide, unsaturated bond, heteroatom, etc. Analyte protectants were defined as compounds that strongly interact with active sites in GC system, thus decreasing degradation, adsorption, or both of coinjected analytes. A mixture of ethylglycerol, gulonolactone, and sorbitol was previously found to be the most effective in minimizing losses of susceptible analytes and significantly improving their peak shapes.

In this study, a gas chromatography tandem mass spectrometry(GC-MS/MS) method was developed to simultaneously determine nine N-acylpyrrolidines, including N-formylpyrrolidine, N-acetylpyrrolidine, N-propionylpyrrolidine, N-butyrylpyrrolidine, N-isobutyrylpyrrolidine, N-isovalerylpyrrolidine, N-crotonylpyrrolidine, N-decanoylpyrrolidine, N-myristoylpyrrolidine. Due to the active amide groups, N-acylpyrrolidines at trace level gave poor peak shapes, thus had higher detection limits, and were more prone to interferences. Combination of surfactants that contain adjacent binary hydroxyl groups was added to matrix-free calibration standard of N-acylpyrrolidines, inducing effective response enhancement in the whole analyte elution range. Adjacent binary hydroxyls are on the end of used surfactant molecule, which could connect with silanol groups and metal ions respectively in the form of hydrogen bonds and coordination bonds, while alkanes chain is on the other end which could reduce the free energy on the surface of GC flow path. Therefore, when the surfactants entered GC system, they could quickly occupy internal active sites. The volatility (retention time coverage) of analyte protectant was another key factor in the enhancement effect. Combination of alkanol surfactants with different numbers of carbon atoms covered the entire volatility range of GC-amenable analytes, thus could serve as a very effective additive to generally improve responses (peak shapes and intensities) of analytes.

Keywords: N-acylpyrrolidines; Analyte protectant; Alkanol surfactant

Part V Instructions for Presentations

Oral Presentation

Devices Provided by the Conference Organizing Committee:

- Laptops (with MS-office & Adobe Reader)
- Projectors & Screen
- Laser pointer

Materials Provided by the Presenters:

- PowerPoint or PDF files

Duration of each Presentation:

- Regular Oral Session: 10-15 Minutes of Oral Presentation
- Keynote Speech: 40-45 Minutes of Keynote Speech

Poster Presentation

Materials Provided by the Conference Organizing Committee:

- X Racks & Base Fabric Canvases (60cm×160cm, see the figure below)
- Adhesive Tapes or Clamps

Materials Provided by the Presenters:

- Home-made Posters

Requirement for the Posters:

- Material: not limited, can be posted on the Canvases
- Size: smaller than 60cm×160cm
- Content: for demonstration of the presenter's paper

Part VI Hotel Information

About Hotel

The Grand Dynasty Culture Hotel (西安古都文化大酒店) is ideally located in the city center near several major Xi'an attractions. All 464 guestrooms in this Xi'an hotel feature modern amenities including large screen TV's, mini-bars and 24-hour room service. The hotel's restaurant serves a variety of Asian and Western delicacies, and a bar/lounge caters for after dinner drinks. Conference rooms at the business center are equipped with audiovisual facilities as well as all necessary amenities for an efficient office environment away from home. In terms of recreation, the hotel offers a fully-equipped gymnasium and a tennis court for active guests, along with an indoor swimming pool, steam room and sauna for guests seeking something a little more relaxed.

Address: No.172 Lianhu Road, Lianhu District, Xi'an, China

陕西省西安市莲湖区莲湖路172号

Post code: 710002

Tel: +86-029-87216868

How to Get to the Hotel

Xi'an Xianyang International Airport: 34.15km

咸阳国际机场：全程约34.15公里，打车费约95元

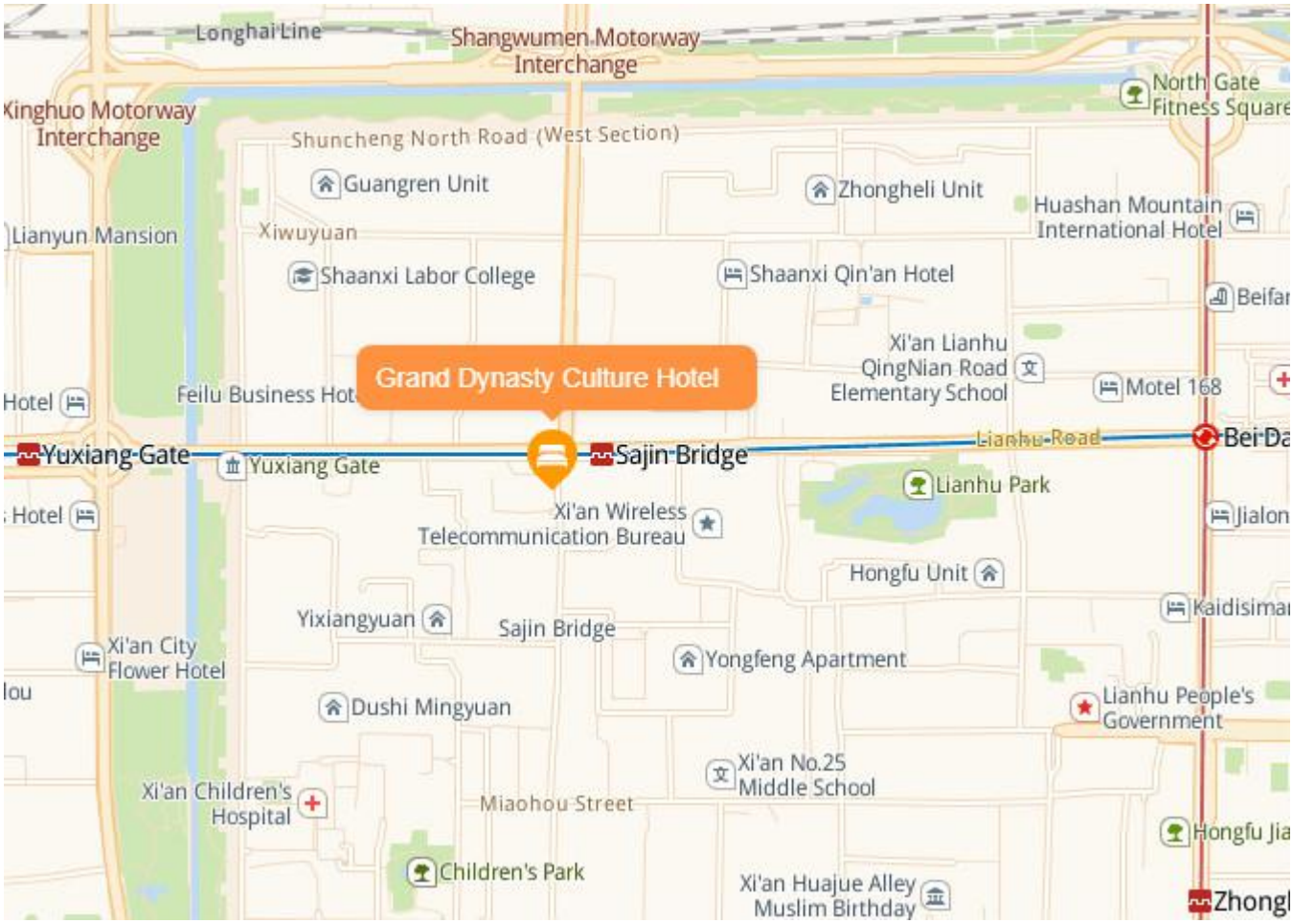
Xi'an Railway Station: 3.75km

西安火车站：全程约3.75公里，打车费约11元

Line 1 Metro Station Sajinqiao: 0.24km

For authors who do not understand Chinese, please show the following info to the driver if you take a taxi:

请送我到：陕西省西安市莲湖区莲湖路172号　西安古都文化大酒店



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