## PHYSICS & ENVIRONMENTAL SCIENCE

## Thermal conductivity of nanocrystalline silicon at high temperature

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#### ABSTRACT

Nanocrystalline silicon (nc-Si) is of interest for high temperature thermoelectric (TE) devices due to its low thermal conductivity. The temperature dependent phonon transport is the dominant mechanism of heat transfer in nc-Si film and it is greatly affected by nanocrystalline grain sizes. Specifically, phonons can be more effectively scattered by grain boundaries than by Umklapp phonon-phonon scattering, particularly so once the grain sizes become comparable or smaller than phonon wavelengths. We previously reported a record low thermal conductivity in nanocrystalline silicon (nc-Si) film prepared by plasma-enhanced chemical-vapor deposition (PECVD) from 80 to 300 K. In this work, we extended the thermal conductivity measurement of nc-Si up to 780 K by the differential 3 $\omega$  technique. Our results will be discussed through grain-size dependent phonon scattering at high temperature.

*Keywords:* Nanocrystalline thin films, thermal conductivity, grain boundary phonon scattering, thermoelectricity.

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### Structural and optical properties of cellulose nanocrystals fabricated using spray-drying process

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#### ABSTRACT

Cellulose nanocrystals (CNCs) are a type of nanomaterial that are derived from cellulose, which is the main structural component of plant cell walls. CNCs have a number of unique properties that make them attractive for a range of applications. They are exceptionally strong and stiff, with a tensile strength that is higher than many metals, and they are also biodegradable and renewable, making them environmentally friendly. Additionally, CNCs are transparent and have a high aspect ratio, which means they can form strong and lightweight composites with other materials. In this work, CNCs was prepared using spray-drying process in which CNC suspensions are first pumped through a nozzle. Plan-view scanning electron microscope (SEM) images combined with X-ray diffraction (XRD) data showed the presence of highly crystallized CNCs with needle–like morphological structure. The diameter and length of CNCs were measured to be 80-110 nm, 500–700 nm, respectively. The UV-Vis spectroscopy revealed that the reflectance of CNCs gradually decreased with increasing wavelength. Furthermore, from UV-Vis reflectance spectra, the energy bandgap of CNCs was calculated to be 2.03 eV.

*Keywords:* Cellulose nanocrystals, Spray-drying process, XRD, SEM, Energy bandgap.

## The phonon dispersion of graphene

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#### ABSTRACT

In frame of De Launay model we calculated phonon dispersion of graphene in  $\Gamma M$  direction using radial and tangential force constants for first four neighbor atoms. Calculated phonon dispersion is in satisfactory agreement with experimental phonon spectra of graphite. In long wave approximation we estimated elastic modulus of graphene in comparison with experimental results for graphite and carbon nanotube.

*Keywords:* De Launay model, phonon spectra of graphene, crystal structure, dynamical matrix, radial force constant, tangential force constant, elastic constant.

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# Plasmonic nanofocusing for tip-enhanced nanospectroscopy

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#### ABSTRACT

Nanofocusing of optical energy has played a critical role in tip-enhanced nanospectroscopy over the past several decades, serving the growing demand for breaking the diffraction limit of light. By utilizing a plasmonic tip, a highly localized enhanced electric field can be formed to act as an excitation source, generating a spectral signal from the sample.

In traditional approaches, laser light illuminates the tip apex via an objective lens, resulting in not only a near-field hot spot but also a far-field light spot. Unfortunately, the latter produces background noise that overwhelms faint spectral signals. We deliberately engineered a radial vector field in an optical fiber, which evolved into surface plasmonic polaritons (SPPs) on a conical metal-coated tapering tip. This allowed us to nanofocus the light energy on the tip apex, thereby overcoming the background noise issue associated with traditional approaches. In this presentation, we will showcase our methodology for manipulating light and demonstrate the fantastic results of our spectroscopic experiments.

*Keywords:* Surface plasmon polaritons, nanofocusing, tip-enhanced nanospectroscopy, radial polarized beam, raman spectroscopy.

### Pressure consistency for binary hard-sphere mixtures from an integral equation approach

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#### ABSTRACT

The site-site Ornstein-Zernike equation combined with the Verlet-modified bridge function has been applied to the binary hard sphere mixtures and pressure consistency has been tested. An equation of state has been computed for a packing fraction of 0.49, and the diameter ratios of spheres of 0.3 and 0.6, and several values of a mole fraction of a larger component. An excess chemical potential for each component has been obtained as well. Our findings for thermodynamic properties are in good agreement with available data in literature.

*Keywords:* Site-site Ornstein-Zernike, hard-sphere, pressure consistency, excess chemical potential.

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### Photoionization cross section of a hydrogenic impurity in a piezoelectric core-shell nanowire

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#### ABSTRACT

The photoionization cross section of a hydrogenic impurity in a piezoelectric core-shell nanowire is investigated by a variational method combined with a finite-difference algorithm. The quantum Stark effect induced by the piezoelectric field, the quantum confinement effect due to structural dimension and the electron-impurity coulombic interaction are taken into account for analyzing the photoionization properties of different types of electronic intersubband transitions. Two types of optical transitions, i.e., the transition from the impurity ground state to the unbound electron ground state and the transition between the impurity states, are involved in our numerical calculation. The PCS shows an obvious resonant peak for each optical transition, especially from the impurity high-energy states in core-shell NWs. The peak position and intensity are more sensitive to core radius than impurity position. The quantum Stark effect plays a more important role in the variation of PCS when the impurity is located at the core region but becomes less influential when the impurity moves to the shell layer. Our method can be easily applied in other low-dimensional nanostructures.

*Keywords: Photoionization cross section, impurity, piezoelectric polarization, coreshell nanowire.* 

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## Lightning recording system design and lightning signals recorded from Mongolia

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#### ABSTRACT

Low-intensity lightning is not recorded in Mongolia due to the number of lightning stations and distance from stations. Consequently, the authors of this work have successfully developed a lightning signal receiver to have its own lightning location system based on the time of arrival method (ToA). We recreated a second-order bandpass filter containing high-pass and low-pass filters in the electromagnetic region of very low frequencies (VLF) to record lightning signals. The relative frequency response of the filter is more than 50% from 1.0 kHz to 50 kHz and less than 5.0% in the outer region of 0.8 kHz to 200 kHz, indicating it works according to the filter principle. The analog signal from the filter is converted to digital by the microcontroller's ADC, which checks for permanent lightning flashes. If a signal higher than the base level or trigger point is received, it is assumed to be lightning, and the waveform is stored on the SD card for 5 ms. The "Atmel SAM3X8E ARM Cortex-M3 CPU" processor performs these storage and transfer processes. A lightning signal is recorded successfully at the National University of Mongolia. Lightning in July. Therefore, the protection and prevention of lightning require a clear understanding of local lightning and related lightning incidents.

Keywords: Lightning, amplifier, propagation, distribution, distance.

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### Magnetron sputter deposition of calcium

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#### ABSTRACT

Sputter deposition of high reactivity metals such as calcium require some special preconditions, and hence less literature data is available on the influence of the deposition on the film growth. Nevertheless, calcium is an important alkali-earth element in many compounds such as mechanoluminescent materials, but it has also received considerable attention in metallic form in for example polymer light-emitting diodes (LEDs) as the electron injection contact due to its low work-function. In this work, calcium thin films were successfully synthesized by pulsed DC magnetron sputtering at room temperature. Due to its high reactivity with air, the calcium target was mounted on a magnetron using a glove box under a slight positive pressure of argon. To protect the calcium film from ambient air, a thin copper layer was deposited on both sides of the calcium film. X-ray diffraction (XRD), Fourier transform infrared (FTIR), and Scanning electron microscope (SEM) were used to confirm the crystal phase. We also studied the chemical stability of the calcium thin film. Long term exposure of the film to ambient conditions were performed. As for future work also CaO can be of importance the reactive sputtering behaviour of Ca was studied in detail.

Keywords: Calcium thin film, magnetron sputtering.

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## Stray grain susceptibility during laser remelting/cladding process in Ni-based single crystal superalloys

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#### ABSTRACT

Due to their excellent resistance to mechanical and chemical degradation, Ni-based Singlecrystal superalloys are high-temperature materials used in gas-turbine engines. However, because of their extremely harsh service condition, Ni-based SX superalloys are often subjected to cracking failure, bringing enormous risks to the service safety of aircraft. Laser cladding, as one typical additive manufacturing technology, has been used to repair the cracked superalloy components. During the repair process, one key point is to suppress the stray grain formation to guarantee that the repaired part keeps the same orientation as that in the substrate. Thus, the factors that influence the stray grain susceptibility should be studied.

Substrate orientation plays a key role in the stray grain formation. In this work, our recent results of substrate orientation-dependent stray grain susceptibilities during the laser remelting/cladding were presented. The substrate orientation has been adjusted either by altering the orientation via rotations around different crystallographic axes or by varying laser scanning directions on the different crystallographic planes. The orientation shows a drastic effect on the stray grain susceptibility. Our results can provide an in-depth insight into the underlying mechanism on suppressing stray grains by the substrate orientation in single crystal superalloys.

Keywords: Ni-based Single-crystal superalloys, crystallographic axes.

## Aerodynamic Forces Acting on Circular and Rectangular Cylinders using the Entropic Lattice Boltzmann Method

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#### ABSTRACT

The Lattice Boltzmann Method (LBM) is a simple and accurate algorithm to implement the Boltzmann equation on a rectangular lattice to simulate gas/liquid flows. In this work, we studied the dependence of the drag and lift coefficients and the Strouhal number of the rectangular cylinder and circular on the Reynolds number, using the entropic lattice Boltzmann method. Calculations made for the low Mach number Ma < 0.1 and the computational grid has the size of 500x181 and 1140x181. We calculated drug and lift coefficients and the Strouhal number for rectangular cylinder using entropic lattice Boltzmann method and two dimensional D2Q9 model for the stationary flow (Re =0.1, 1, 10, 100, 200, 300).

*Keywords:* Circular, rectangular cylinders, entropic lattice Boltzmann method, drag, lift.

# Synchronization of time-delay interacting cavitation oscillators near the liquid free surface

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#### ABSTRACT

The dynamics of cavitation near the liquid-free surface is of increasing interest due to applications in 3D printing. For widespread applications of high-frequency ultrasonic cavitation in sonochemistry, gene and drug delivery to cells by sonoporation, we need synchronized high-amplitude cavitation oscillations. Chaotic oscillations and the inhibitory nature of bubble interaction make synchronization difficult. We show that chaotically oscillating bubbles can be synchronized with indirect coupling via waves reflected from the free surface of the liquid for a limited range of delay. We have demonstrated the robustness of the synchronization to external disturbances.

Keywords: Cavitation, interaction, synchronization.

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## Estimation of average particle size and standard deviation on scanning electron microscopy images through Fourier transformation

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#### ABSTRACT

Measuring the size distribution of particles in Scanning Electron Microscopy (SEM) images is crucial for material science research, but can be a time-consuming process. This study proposes a method for estimating particle size and standard deviation through Fourier transformation of SEM images. Although Fourier transformation is commonly used for estimating particle size from x-ray diffraction patterns and light scattering, its application to SEM images has been rarely discussed. The proposed approach involves digitally processing SEM images using Fourier transformation to obtain a power spectrum plot. The power spectrum plot is then analysed to determine the particle size distribution. The effectiveness of this approach is demonstrated through its application to SEM images with both single and varying particle sizes. This study presents a quick and efficient method for estimating particle size and standard deviation in SEM images using Fourier transformation.

*Keywords:* Fourier transformation, scanning electron microscopy, Particle size distribution, image processing.

## Managing end-of-life electric vehicles and their batteries in the Global South: risks and challenges

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#### ABSTRACT

The shift from internal combustion vehicles to electric vehicles is essential to reduce carbon emissions from road transportation and mitigating the effects of climate change. However, as the transition is still in its early stages, it is important to consider not just its environmental benefits but also its potential drawbacks. The current number of electric vehicles (EV) has been projected by researchers to rise from 2.4 million in 2020 to 81 million in 2050. This poses a risk of resource depletion, due to a drastic increase in resource pressure for rare earth metals such as lithium and cobalt and urges the world to establish reuse and recovery routes for End-of-Life (EoL) EVs and their batteries.

However, managing EoL EVs and their batteries is more challenging than managing fossilfueled cars due to the large amounts of hazardous chemicals they contain. Therefore, the paper discusses important topics for understanding the potential risks associated with the transition to electric mobility, including international used vehicle trade flows, waste management challenges for end-of-life battery electric vehicles and their lithium-ion batteries, environmental and human health impacts of disposing of these batteries, and policies and regulations related to the electric vehicle life cycle.

*Keywords: E-mobility, electric vehicles, waste management, circular economy, lithium-ion batteries, used vehicles trade.* 

## Effects of main inorganic salts on aggregation and sedimentation of endogenous fine loess particles in groundwater over Guanzhong plain, China

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#### ABSTRACT

The aggregation and sedimentation of fine soil particles is critical to their transport and cotransport with adsorbed contaminants in groundwater environment. Numerous studies were conducted on engineered particles, and few were on endogenous fine particles. In the present study, Chinese loess was sampled from Xi'an, China, as well as NaF, NaNO<sub>3</sub> and Cu(NO<sub>3</sub>)<sub>2</sub> were selected as inorganic salts, and then batch tests were conducted to explore the effects of the main inorganic salts in the aggregation and sedimentation of endogenous fine loess particles in groundwater. The results show that the endogenous fine loess particles with 1.1 um, 1.9 µm and 3.4 µm median particle sizes, which are extracted from the Chinese loess, inherit almost the mineral composition of their parent loess matrix as well as metallic oxides but Na<sub>2</sub>O, indicating the minerals containing Na<sub>2</sub>O are likely to dissolution, and have high zeta potentials ( $\zeta$ ) as -14.6  $\pm$  0.25 mV, -13.9  $\pm$  0.23 mV and -3.19  $\pm$  0.16 mV, showing their relatively good dispersivity in the study systems, and their sedimentation rates are kept stable over 40-hour reaction. Both results of tests and theoretical calculation confirm that the critical coagulation concentrations (CCCs) for Cu (II) and Na (I) are 0.1mmol/L and 50 mmol/L, which are bigger than their concentrations in the groundwater over Guanzhong plain, respectively, implying these fine loess particles released from the loess are likely to be dispersive and suspended and then transport in groundwater. The results of the multi-factor tests showed that, particle size, salt type (NaF, NaNO3 and Cu (NO3)2) and salt concentration (1 mmol/L, 5 mmol/L and 10 mmol/L) are the key influent factors and interact with each other, resulting that their relative magnitudes were changed in the tests progresses, whose performance is that the role of salt concentration got big as well as the role of salt type got small. So, the dispersion and suspension of these particles get strengthen along the groundwater flow path, which is conducive to the cotransport of the particles with adsorbed contaminants in groundwater environment. The results could deepen understanding for aggregation mechanisms of fine soil particles and further help in predicting their environmental behaviours.

*Keywords:* Endogenous fine loess particles, main inorganic salts, Aggregation and sedimentation, Groundwater, Guanzhong plain, China.

## Prediction of reaeration and deoxygenation rate constant in Selbe river, Mongolia: Dissolved oxygen and BOD assimilative capacity of the river

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#### ABSTRACT

Most hydrological research works on Rivers in Mongolia, were conducting water quality analysis, particularly inorganic components. This study is the first time considering the dissolved oxygen (DO) and BOD assimilative capacity of the river. Mass balance of DO in river and stream interplays between deoxygenation and reaeration rate constant to predict its purification capacity. The purification system is used the classic Streeter-Phelps model which is modified, to describe the critical oxygen deficiency and critical time or distance of the river. In this study, the deoxygenation rate  $(k_1)$  and the reaeration rate  $(k_2)$  constants were determined on the Selbe river, Ulaanbaatar, Mongolia. The mean  $k_1$  was calculated using two models, namely the Thomas slope and first-order function methods. The results showed that the firstorder function model was more suitable for describing  $k_1$ , which is  $0.1070 \pm 0.0236$  and 0.2465 $\pm$  0.0543 respectively in 10 and e of logarithm base because the sampling standard deviation of the model we used is more reliable than the Thomas method. The mean  $k_2$  was estimated by 8 models out of 22 different available models. Jha's model resulted more reasonable because there had the lowest sampling standard deviation compared with other models. Accordingly, the mean  $k_2$  in the Selbe river was found  $3.91 \pm 1.009$ . As a result of using  $k_1$ and k2, there has been found 4.0 mg/L of critical oxygen deficit, 0.75 d of critical time, and 20 km of the longest distance using the purification model for steady-state conditions and zero initial oxygen deficit because non-point pollution sources occurred in most sampling points. With limited available data on hydrology in Mongolia, there is not able to compare with prior study analysis to this study. Furthermore, we should continue to produce the data.

*Keywords:* BOD, dissolved oxygen, deoxygenation rate, reaeration rate, critical time, deficit oxygen.

## Research of non-balanced dynamics of pasture ecosystems in Mongolia

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#### ABSTRACT

Mongolia's traditional pastoralism produces 40 percent of the gross national product and 80 percent of the agricultural product. For this reason, it is the main sector of our economy that provides the population with food, consumer goods, and raw materials for industry. Due to the distribution of precipitation and thermal fluctuations, the huge change in pasture productivity is a process of determination. Mongolia has a negative climate against the mainland and low rainfall. In the southern Gobi desert, 50-100 mm per year and 300 - 350 mm of precipitation falls in the mountainous region of the north.

*Keywords:* Non-balanced dynamic, pasture of ecosystem, coefficient of evolution, loss of livestock.

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## Impact of integrated home insulation and heating solutions in Mongolia on air quality and health

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#### ABSTRACT

Air pollution in large regional centers of our country is increasing and reaches a level that adversely affects the health of the population. It is highly recommended to control the presence of mechanical impurities (PM<sub>2.5</sub>, PM<sub>10</sub>), chemical (CO, CO<sub>2</sub>, NO<sub>2</sub>, VOC), and biological (bacteria, fungi, etc.) pollutants in indoor air. The majority of the population of provincial centers in Mongolia reside in their own gers and houses, providing their own sources of heat and preparing food and drinks in traditional ways on fire. In order to increase the quality of indoor air in gers, nearly 600 households in Bayankhongor province, Gobi-Altai province, and Bayanzurkh district of Ulaanbaatar city use the Cooking, Heating, and Insulation package (CHIP). This study aims to determine the impact of indoor air quality of gers with CHIP on maternal and child health. Data in this study is collected by quantitative (questions, measurements) and qualitative (observation, interviews) methods using instantaneous and reflective survey models. Indoor air measurements are taken. A total of 200 households in Bayankhongor and Gobi-Altai provinces using CHIP and 100 households with fireplaces to determine the level of microclimate parameters of indoor pollutants PM<sub>2.5</sub>, PM<sub>10</sub>, CO, and CO<sub>2</sub> once a month, 7 days 24 hours a day. 1,108,624 numerical data of microclimate indicators taken from 700 measurements in the premises of households using fire and CHIP packages were analyzed. A questionnaire collects the heights of children aged 0-2 years and the health and development indicators of 18-month-old children. Information on diseases of family members for 2020-2021 are collected from the Ministry of Health and medical records, information on cardiovascular, primary hypertension, and respiratory diseases.

Integrated solutions for thermal insulation and heating of houses in Mongolia improve indoor air quality, conditions, and health impact consequently.

Keywords: CHIP package, indoor air quality, health impact, PM2.5, CO.

## Assessment of indoor environmental conditions in schools in Ulaanbaatar, Mongolia

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#### ABSTRACT

Overcrowding in classrooms, which is caused by a lack of educational facilities, worsens indoor air quality and acts as a main cause of respiratory diseases among children and adults. Therefore, it is essential to measure and assess the indoor air quality where children spend extended periods of time such as at schools. In this study, four schools with old buildings and four schools with new buildings in Bayanzurkh, Sukhbaatar, Khan-Uul, and Chingeltei districts of Ulaanbaatar, were selected. PM10 and PM2.5, CO2, air temperature, humidity, and microbiological count from chosen classrooms were measured and evaluated against the national standard MNS4585:2016. The measurements reveal that the 24-hour average PM2.5 concentrations was 64.3 (95% CI: 64.1-64.5) µg/m3, which was 4.3 and 1.3 times higher than the WHO guideline value and the national standard, respectively. The 24-hour average PM10 concentration was 85.3 (95 % CI: 85.1-85.6) µg/m3, which is 1.9 times higher than WHO guideline value. In schools with old buildings, the 24-hour average PM2.5 concentrations was 5.6 and 1.7 times higher than the the WHO guideline value and the national standard, respectively; the average PM10 concentration was 2.8 and 1.3 times higher than the WHO guideline value and the national standard. The air temperature and CO2 concentration in classrooms meet the national standard. However, the average relative humidity in all schools is 24.2±6.5%, which is 14-16% lower than the MNS4585:2016. According to the measurements conducted in schools in this study, the indoor air quality of the schools with new and old buildings was similarly poor, therefore a variety of steps is needed to improve the indoor environmental condition.

*Keywords:* School indoor environment, indoor air, measurements, PM2.5, PM10, CO.

## Satellite based estimation of landcover change and soil degradation in Urgamal, Durvoljin, Erdenekhairkhan Soums of Zavkhan province

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#### ABSTRACT

In recent years, the warming process observed throughout Mongolia, quantitative changes in pastoralism, and chaotic mining activities have become factors that accelerate the process of desertification. Therefore, the purpose of the research work is to scientifically evaluate the process of desertification under the combined influence of nature, society, and economy, and its consequences. Satellite remote sensing technology has great potential for applications in land condition assessment and can facilitate optimal planning in the agricultural sector. In this research work, the climate change of the last 22 years (2000-2022) in Durvoljin, Ugramal, and Erdenekhairkhan Sum areas of Zavkhan Province was determined and the state of desertification was evaluated based on satellite data. Within the scope of this research, among the vegetation indices, the Soil Adjusted Vegetation Index (SAVI) was calculated. When calculating SAVI using data from the Red and NIR channels of satellite MODIS data, values of SAVI from -0.4 to +0.5 as a result of image processing. The spatial heterogeneity of the land surface of the study area was characterized by SAVI-iin values ranging from -0.4 to +0.02for water, +0.02 to +0.08 for gravel and rock, +0.08 to +0.11 for sand, +0.11 to +0.16 for sparse soil, +0.16 From - to +0.23 with sparse vegetation and between +0.23 and +0.5 with good vegetation were mapped into 6 categories. As a result of the study, SAVI was proven to be more suitable for determining soil types in desert and semi-desert areas.

*Keywords:* Soil adjacent Vegetation Index (SAVI), desert, semi-desert zone, land degradation, monitoring.

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## Identifying groundwater site suitability of artificial recharge structures in Kalrayan hills, Tamil Nadu for tribal community using resistivity survey and geospatial technology

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#### ABSTRACT

Artificial recharge structures can improve water availability in regions with water scarcity, such as the Kalrayan hills in Tamil Nadu. The tribal communities in this region are particularly vulnerable to water scarcity effects, and thus mapping artificial recharge structures can significantly benefit them. One of the practical approaches to mapping these structures is using resistivity surveys and geospatial technology. Resistivity involves measuring the electrical resistance of the subsurface, which can help identify changes in the subsurface materials, including variations in water content. Geospatial technology can help to create accurate maps of the survey results, which can then be used to identify potential sites for artificial recharge structures. The present study focuses on potential groundwater zones in Kalrayan hills in Villupuram district, Tamil Nadu, India, with semi-arid climatic conditions. In this study the integrated GIS analysis, groundwater potential zones map of the study area was prepared qualitatively. For cross check in the field the Schlumberger Vertical Electrical Sounding review (VES) method have been done with the 10 sampling station in the hilly area of Kalrayan Hills. According to potential groundwater zones various recharge structures have been suggested for the research region based on the findings and potential groundwater zones. The outcome of Groundwater Potential Zones map is drawn from weighed overlay using AHP performed very well in predicting the groundwater surface and calibrated by using resistivity survey given accurate information of the area and hence this methodology proves to be a promising tool forfuture. Hence, groundwater management with an innovative method paves the way for sustainable water management.

**Keywords:** Groundwater, recharge structures, resistivity survey, semi-arid region, Remote Sensing and GIS.

### Novel operational strategy of anaerobic processes to recover volatile fatty acids from food wastes

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#### ABSTRACT

In order to determine the critical pH for acid failure and establish the optimal operating conditions for the VFA recovery reactor, the existing model was refined by incorporating a pH suppression equation. Through simulation of experimental data from other researchers, a range of pH parameters were identified that provide safety margins for efficient VFA recovery. For conservative calculations, low pH inhibition parameters ( $pH_{UL} = 6.41$ ,  $pH_{LL} = 5.47$  and n = 0.23) can be employed for plant operations and process design, providing a safety buffer to prevent acid failure. Alternatively, optimistic curves ( $pH_{UL} = 5.55$ ,  $pH_{LL} = 5.11$  and n = 0.24) can be utilized to subtract 0.4 d<sup>-1</sup> from the specific decay rate of acid-damaged methanogens, ensuring adequate acidification and maximizing VFA yield. Experimental results indicate that the optimal pH range for activity of acid-producing bacteria is between pH 5.5-6.2. This range is also beneficial for VFA recovery as the consumption of VFA by methanogenic bacteria is greatly reduced due to acid inhibition.

*Keywords:* Anaerobic processes, food wastes, suppression of methanogens, VFA recovery.

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## Carbon footprint calculation of the University of Kitakyushu, Japan and Mongolian University of Science and Technology and ways to reduce the sources of greenhouse gas emissions

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#### ABSTRACT

Academic Research Institutions are highly influential organizations that work directly in the country's industry, the public, and the government. In this research, we report the first approximate carbon footprint calculation of emissions corresponding to scope 1, scope 2, and scope 3 emissions for the main urban campuses of The University of Kitakyushu and Mongolian University of Science and Technology, using the UNE-ISO 14064-1 and GHG Protocol Corporate standard. The carbon footprint in the UKK in 2021 was approximately 3081.56 tons CO<sub>2</sub> eq, and 0.432 tons CO<sub>2</sub> eq per person. In the MUST carbon footprint in 2021 was approximately 18766.66 tons CO<sub>2</sub> eq, and 0.831 tons CO<sub>2</sub> eq per person. Several reasons explain this behavior such as geographic location, cultural factors (consumption patterns and types of transportation), gross domestic product (GDP) of each country. Results cannot be extrapolated between the UKK and MUST cases and differences in the local conditions.

Keywords: University, Carbon footprint calculation, Reduction.

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## Runoff modeling using SCS-CN and GIS approach in the Chennai Tamil Nadu

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#### ABSTRACT

Runoff modelling is a critical component of water resources management and flood mitigation, we have employed the SCN- CN (Soil conservation services curve Number) and GIS (Geographic information system) approach to model the runoff potential of district Chennai, Tamil Nadu. We have created a land cover map and a soil map using remote sensing data and soil surveys, respectively. CN values have been assigned to each land cover and soil type, and the coverage CN value has been calculated for the study area. The SCSCN formula has been applied to estimate the runoff for a given rainfall event, taking into account rainfall intensity, duration and antecedent moisture condition. The GIS approach has been used to perform all the necessary calculations and mapping tasks. The findings of this study can be used to inform water resources management and land use planning in Chennai and other areas with similar characteristics. The SCN-CN and GIS approach can be a useful tool for assessing and managing the potential for surface runoff and infiltration in urban and rural areas. Modelling runoff is an integral part of water resources management and flood mitigation and analysis. This study models the discharge potential of Chennai, Tamil Nadu, using SCS-CN and GIS approach. Using data from satellite imagery and a soil survey, we have created a land cover map and a soil map, respectively. Each land cover and soil type has been assigned a CN value, and the average CN value for the study area has been calculated. Utilizing the rainfall event's intensity, duration, and antecedent moisture levels, the SCN-CN formula was implemented to estimate the discharge for a particular rainwater event. Using the Geographic Information Systems (GIS) method, all required calculations and mapping duties were completed. This study's findings can inform water resource management and land use planning in Chennai and other regions with similar features. The SCN-CN and GIS approach provide a useful tool for assessing and managing the potential for surface discharge and infiltration in urban and rural areas.

Keywords: SCS-CN; Runoff; Infiltration; GIS; Soil map, LULC.

## Time series analysis for the estimation of gross primary production using the satellite data

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#### ABSTRACT

Mongolian area is a dry, cold climate, and geographical features are associated with the fragility of natural ecosystems, also global climate change may have a strong impact on the Mongolian semi-desert zone. Understanding and monitoring Gross Primary Production (GPP) is a critical component of exploring the impact of desertification, and dust storms in the study area. The purpose of this study is to monitor GPP over the Mongolian semi-desert zone. We used MODIS GPP product and a machine-learning-based GPP (SVR-GPP) from 2000 to 2020. We applied a time series analysis to derive GPP over Mongolian across natural ecosystem zone semi-desert zones for years 2000-2020 and predict its future trends until 2030. The output GPP maps from the approach was validated by comparing them with the SVR GPP for the natural zone of semi-desert (r2=0.92). The results indicate that the GPP of the Mongolia values is high in range in semidesert can be between the range 0.01-1.3 gC m-2 day-1. The results of the research suggest that the proposed approach using SVR-GPP data is suitable for monitoring GPP over a semi-desert area and contributing to the control of the carbon cycle.

Keywords: Gross Primary Productivity (GPP), Support Vector Regression (SVR).

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### Changes of the land surface of Ogii lake basin

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#### ABSTRACT

Located in Arkhangai Province in the central part of Mongolia, Lake Ugii is a freshwater lake included in the Ramsar Convention for the Protection of International Wetlands. In addition to climate change, there is also severe degradation of soils in the Lake Ugii watershed due to human activities. The objective of this study is to determine the conditions for good vegetation by using the relationship between vegetation cover, surface temperature, and climate factors that represent the outer limits of the basin geological environment for 2000-2021. Land surface temperature in the Lake Ugii basin was determined over a long period of time. The mean surface temperature (LST) of channels 31 and 32 of MODIS satellite data for the period August 2000-2021 was used. The results were summarised with NDVI, which represents the state of vegetation for 2000-2021, data from meteorological stations, and maps of man-made systems in the basin, and verified by comparison with the results of ground measurements. It was determined that favourable conditions for vegetation exist in the basin when the following two conditions are met. First, precipitation is about 100 mm above the long-term average, and second, land surface temperature is  $24.9^{\circ}C - 30.7^{\circ}C$ . Since surface temperature and vegetation density determine soil erosion, it is important to improve the planning of measures against soil degradation and climate change for the basin.

*Keywords: MODIS data*, *normalized vegetation index NDVI*, *land surface temperature LST*, *basin*.

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## Comparative study on legal environment for management of end-of-life electric vehicles and lithium-ion batteries in Mongolia vs. other countries

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#### ABSTRACT

The increasing volume of cars for our daily necessities poses serious risks to the environment and public health. The use of electric and combined engine hybrid cars, which have lower running costs, has been more popular in recent years than gasoline cars. The amount of imported hybrid vehicles in Mongolia has tripled from 2012 to 2016. Plug-in hybrid electric vehicles (PHEVs) and hybrid electric vehicles (HEVs), use lithium-ion batteries (LIBs). However, LIBs have numerous advantages such as energy saving, fast charging, and low maintenance, they can be toxic to the environment and human health if handled or disposed inappropriately. Due to the presence of toxic components (e.g cathodes and electrolytes) in end-of-life (EoL) LIBs, it is fundamental to find optimal solutions to manage this type of waste. The main objective is to study and assess the Mongolian laws and regulations regarding this type of waste and compare them with the laws and regulations of other countries. In this study, a literature review on the legal environment for LIB is conducted and its comparison is done. As a result of the research, it was found that there is not enough detailed legal environments related to the management of the EoL LIBs in Mongolia. Therefore, in order to properly manage this type of hazardous waste, the country needs to develop an appropriate legal environment for a proper solution.

Keywords: LIB, EoL EV, Legislation, Waste management chain, Mongolia, Europe.

## A numerical method for solving time dependent Hartree-Fock equations of helium atom using CWDVR approach

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#### ABSTRACT

In this work, the atomic structure of the helium atom is determined by solving Hartree-Fock equations approximated by a Slater determinant. The time-dependent Hartree-Fock equations are calculated by the Coulomb Wave Function Discrete Variable Representation (CWDVR) approach. Self-consistent integro-differential equations were solved using the discrete variable method for the uniform and optimal spatial grid discretization. The time-dependent variational principle was used to derive the time-dependent Hartree-Fock equation. We illustrate that the calculated electronic energies for the helium atom are in good agreement with other best available values.

*Keywords:* Self-consistent field, atomic structure, Hartree-Fock equations, exchange potential.

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# Scanning probe microscopy observation of molybdenum disulfide surface

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#### ABSTRACT

The surface structure of  $MoS_2$  was studied by scanning probe microscopy. Few layers of  $MoS_2$  flakes were revealed by AFM measurements. The exfoliation method in an ultrahigh vacuum chamber is used to obtain a clean surface of  $MoS_2$  samples with atomically smooth terraces and multilayered steps. Atomically resolved images revealed of atomic defects on the surface or near the surface.

*Keywords:* Surface defects, impurities, transition metal dichalcogenides, a few layers.

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# System dynamic modelling and financial analysis of solid waste management in Ulaanbaatar, Mongolia

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#### ABSTRACT

Due to population growth, urbanization and industrialization, the amount of waste in Mongolia has increased dramatically in recent years. This leads to environmental degradation and climate change, and risks further damage.

To improve the capacity of waste management, the legal framework and inter sectorial coordination must be ensured. Establishing a stable and reliable infrastructure, creating a mechanism for optimal technical and financial resource allocation, and responsible execution are therefore required. This research has resulted in a model that can be recommended the waste managers in decision making regarding waste management.

In this research, a possible option for payment of service fee for domestic waste generated by households in Ulaanbaatar was developed depending on the amount of waste generated. Based on the research, a dynamic model of the system depending on the factors affecting the amount of waste is developed, and as a result of the experiment and simulation, the possible options for optimal management are proposed.

Keywords: Municipal solid waste management, System dynamic, Simulation

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# Calculation of the entropy for hard-sphere from integral equation method

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#### ABSTRACT

The Orsntein-Zernike integral equation method has been employed for a single-component hard sphere fluid in terms of the Percus-Yevick (PY) and Martynov-Sarkisov (MS) approximations. The virial equation of state has been computed in both approximations. An excess chemical potential has been calculated with an analytical expression based on correlation functions, and the entropy has been computed with a thermodynamical expression. Calculations have been carried out for reduced densities of 0.1 to 1.0. It has been shown that the MS approximation gives better values than those from the PY approximation, especially for higher densities, and presents a reasonable comparison with available data in the literature.

**Keywords:** Ornstein-Zernike equation, integral equation, closure relation, hardsphere potential, excess chemical potential, entropy.

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## Photoelectron distributions of some inert gas atoms

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#### ABSTRACT

In this work, when a linearly polarized laser pulse interacts with an atom, the wave function of the photoelectron ejected from the atom was calculated by solving the time-dependent Schrödinger equation (TDSE) for some inert gas atoms such that He, Ne, and Ar. The solution of the TDSE was performed by assuming that the active electron of an atom is moves in the mean field created by the other electrons and the nucleus. From the numerical solution of the time-dependent Schrödinger equation, it was observed that the distribution of the photoelectron in coordinate's space, represented by the square of the modulus of the electron wave function is similar to the probability distribution of the photoelectron in momentum space.

Keywords: Hydrogen, Helium, Argon, Neon, PMD, laser pulse

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## Investigation of distribution residual strain in austenite sample using the TOF neutron diffraction

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#### ABSTRACT

The tensional residual strain distributions investigation on austenite steel samples manufactured by a thermo-mechanical (Tempcore) process has been performed. That the investigation has been carried out using in-situ stress experiments with the time-of-flight (TOF) neutron diffraction method. Concerning the fatigue resistance, it was aimed at measuring the longitudinal (axial) residual strain. The strain were assessed by deformation measurements during and after the slitting processes. Additional investigations of structural texture, compression and tensional strain scanning by step of 5 mm were carried out. The main result was that contrary to the former assumption compression strain exists in the inner cross-section part and tensile strain near or even at the surface.

*Keywords: Time-of-flight (TOF), neutron diffraction, compression, tensional residual strain, texture.* 

## Influence of ultrasound activation on corrosion rate of porous Ni-Ti shape memory alloys by SHS

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#### ABSTRACT

Near equiatomic Ni-Ti shape memory alloy is considered of the best biomaterials. Then, the porous Ni-Ti alloy obtained were synthesized by self-propagating high temperature synthesis (SHS) at preheating temperature 3000C. In this study, effect of the ultrasound activation for different periods (t=0, 15, 30, 60, 120min) were corrosion rate porous Ni-Ti shape memory alloys. The corrosion rate of the synthesized samples was in the range 0.872125-0.718250µm/y.

Keywords: Corrosion rate, nickel-titanium, shape memory alloy, porous.

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## Theoretical and Experimental studies of structural and optical properties of pr-doped LiYF4 compounds

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#### ABSTRACT

In this study, the LiYF4 compounds doped with rare earth Pr3+ ions are synthesized by environmentally friendly and solid-state reaction methods. The outcomes of XRD, optical absorption, and emission measurements show that the doped sample is successfully synthesized. The optical properties of Pr-doped LiYF4 were investigated by comparing theoretical and experimental methods. Our results of the optical properties of the Pr-doped LiYF4 are demonstrated.

Optical absorption and emission results of Pr-doped LiYF4 obtain that this material can emit radiation with several wavelengths in visible ranges.

Acknowledgement: The work was supported by Mongolian Science and Technology Foundation under project ShuSS\_2020/61.

Keywords: Visible laser, solid-state reaction, optical absorption, and emission, DFT

### **Bi Doped Barium Hexaferrite: Preparation and Characterization**

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#### ABSTRACT

Nowadays, electromagnetic interference (EMI) pollution is arising due to the excessive and continuous use of electronic devices. This pollution has led to an increase in severe health problems and the failure of instruments. To diminish such effect, a variety of electromagnetic wave absorbing materials have been developed to date.

Among these materials, M-type ferrite hexagonal barium ferrite (BaFe12O19, BFO) is considered to be an outstanding EMI absorbing material owing to its excellent magnetic properties with high coercivity, magnetic resonance frequency, and large magnetocrystalline anisotropy. The BFO is hexagonal closed packed with lattice constants a = 5.89Å and c = 23.19Å6. The iron (Fe) atoms are connected with oxygen (O) and barium (Ba) atoms in the five different sites such as octahedral (12k, 4f2, and 2a), tetrahedral (4f1), and trigonal bipyramidal/hexahedral (2b). The Fe cations are the sole source of magnetic properties: the 12 k, 2a, and 2b sites are spin up and 4f1 and 4f2 sites are spin down, where the numbers in the site designations show total number of such sites in the unit cell.

In the present work, we synthesized bismuth (Bi) doped BFO with different concentrations (x=0.1 - 0.5) using the sol-gel method for purpose of EMI shielding material. The influence of doping element on phase purity, crystal structures, and heat generation ability is explored.

Keywords: Barium ferrite, Bi-dope, EMI sheilding.

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### Theoretical study of interaction fullerene molecules with and without oxygen atoms

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#### ABSTRACT

Fullerene  $C_{60}$  is an organic macromolecule with a size of 1 nm consisting of 60 single carbon atoms. Fullerenes are used in a variety of advanced materials research using their remarkable electrical, magnetic, and elastic properties. In addition, its solubility in various solvents is better than that of other carbon compounds such as nanotubes, graphite sheets, and diamonds. Therefore, the properties of fullerene in solutions have attracted much attention of researchers in recent years. Fullerene is soluble in more than 120 organic and inorganic solvents. The kinetic processes in solution depends on the nature of the solvent. Usually, stable large clusters (< 500 nm) are formed in polar solvents (NMP, Pyridine), while smaller (> 100 nm) clusters are formed in less polar solvents such as benzene, toluene, and chlorobenzene. On the other hand, observed that the cluster growth in low polar solvents is activated by light, and hypothesized that oxygen atoms in the solution influence this process.

In this work, the interaction between fullerene molecules bonded with and without oxygen atoms were determined by density functional theory method at different distances between molecules. From the results of theoretical calculations, the minimum value of the interaction potential between fullerenes bonded to oxygen was determined at a distance smaller than the minimum value of the interaction potential between single fullerenes, which shows that oxygen acts as a bridge of attraction between fullerene molecules and also supports the process of cluster formation. The obtained interaction energies of fullerene and oxygen atoms compared with molecular dynamic simulation results.

Keywords: DFT, Molecular dynamics, fullerene, potential energy.