

# Science Newsletter

2023 Volume 11 (Total 47) Website: <http://lib.jsut.edu.cn/2018/1015/c5474a113860/page.htm>  
December, 2023

---

## Contents

<b>INTRODUCTION:</b> .....	<b>2</b>
<b>I TOPICS</b> .....	<b>2</b>
<b>GRAPH MINING</b> .....	<b>2</b>
<b>CLUSTERING</b> .....	<b>5</b>
<b>MACHINE LEARNING</b> .....	<b>7</b>
<b>DEEP LEARNING</b> .....	<b>9</b>
<b>EMBEDDED SYSTEM</b> .....	<b>11</b>
<b>II CONCENTRATION</b> .....	<b>13</b>
<b>PHYSICS</b> .....	<b>13</b>
<b>MATERIALS</b> .....	<b>14</b>
<b>CHEMISTRY</b> .....	<b>16</b>
<b>BIOLOGY</b> .....	<b>17</b>
<b>III CALLING FOR PAPERS</b> .....	<b>19</b>
<b>ICCAE 2024</b> .....	<b>19</b>
<b>CSTE 2024</b> .....	<b>20</b>
<b>ICCCR 2024</b> .....	<b>21</b>
<b>ICICT 2024</b> .....	<b>23</b>
<b>ICCEE 2024</b> .....	<b>23</b>

# Introduction:

There are 3 main elements in the Science Newsletter which is composed. In the first part, we list the most up to date papers about central issues for each discipline in our university, and they are provided with 5 subjects for a time. In the second part, there are papers from the top journals last month, and most of them are from Nature and Science. In the third part, we post information about calling papers for international conferences. Hopefully, some of the information in this manuscript may be useful for those who are dedicating to scientific career. Besides, the journals are also posted on the website of our library, and they are available to be accessed any time at <https://lib.jsut.edu.cn/2018/1015/c5474a113860/page.htm> . If there are any questions or suggestions, please send e-mails to [ccy@jsut.edu.cn](mailto:ccy@jsut.edu.cn) in no hesitate.

## I Topics

The keywords of this month is **Computer Science**:

We post several papers which are related to the top concerned topics in researches on computer science. The papers are classified in 5 categories, and they are: **Graph Mining, Clustering, Machine learning, Deep Learning, and Embedded System**. Also, the listed papers are all arranged in a descending sort of JCR impact factor, and there are also accesses right after each abstract of papers.

### GRAPH MINING

Genome Med (impact factor: 12.3) 1 

#### **Personalized tumor combination therapy optimization using the single-cell transcriptome**

*Chen Tang, Shaliu Fu, et. al*

#### **Abstract:**

##### **Background**

The precise characterization of individual tumors and immune microenvironments using transcriptome sequencing has provided a great opportunity for successful personalized cancer treatment. However, the cancer treatment response is often characterized by in vitro assays or bulk transcriptomes that neglect the heterogeneity of

malignant tumors in vivo and the immune microenvironment, motivating the need to use single-cell transcriptomes for personalized cancer treatment.

### **Methods**

Here, we present comboSC, a computational proof-of-concept study to explore the feasibility of personalized cancer combination therapy optimization using single-cell transcriptomes. ComboSC provides a workable solution to stratify individual patient samples based on quantitative evaluation of their personalized immune microenvironment with single-cell RNA sequencing and maximize the translational potential of in vitro cellular response to unify the identification of synergistic drug/small molecule combinations or small molecules that can be paired with immune checkpoint inhibitors to boost immunotherapy from a large collection of small molecules and drugs, and finally prioritize them for personalized clinical use based on bipartition graph optimization.

### **Results**

We apply comboSC to publicly available 119 single-cell transcriptome data from a comprehensive set of 119 tumor samples from 15 cancer types and validate the predicted drug combination with literature evidence, mining clinical trial data, perturbation of patient-derived cell line data, and finally in-vivo samples.

### **Conclusions**

Overall, comboSC provides a feasible and one-stop computational prototype and a proof-of-concept study to predict potential drug combinations for further experimental validation and clinical usage using the single-cell transcriptome, which will facilitate and accelerate personalized tumor treatment by reducing screening time from a large drug combination space and saving valuable treatment time for individual patients. A user-friendly web server of comboSC for both clinical and research users is available at [www.combosc.top](http://www.combosc.top). The source code is also available on GitHub at <https://github.com/bm2-lab/comboSC>.

IEEE J Biomed Health Inform (impact factor: 7.7) 2 ☒

## **Semantic-enhanced Graph Contrastive Learning with Adaptive Denoising for Drug Repositioning.**

*Yu, Lu,, et. al*

### **Abstract:**

The traditional drug development process requires a significant investment in workforce and financial resources. Drug repositioning as an efficient alternative has attracted much attention during the last few years. Despite the wide application and success of the method, there are still many shortcomings in the existing model. For example, sparse datasets will seriously affect the existing methods' performance. Additionally, these methods do not pay attention to the noise in datasets. In response to the above defects, we propose a semantic-enriched augmented graph contrastive learning with an adaptive denoising method, called SGCD. This method enhances data

from the perspective of the embedding layer, deeply mines potential neighborhood relationships in semantic space, and combines similar drugs in the semantic neighborhoods into prototype comparison targets, thus effectively mitigating the impact of data sparsity on the model. Moreover, to enhance the model's robustness to noisy data, we use the adaptive denoising method, which can effectively identify noisy data in the training process. Exhaustive experiments on multiple real datasets show the effectiveness of the proposed model. The code implementation is available at <https://github.com/yuhuimin11/SGCD-master>.

J Chem Inf Model (impact factor: 5.6) 2 ☒

## **SiSGC: A Drug Repositioning Prediction Model Based on Heterogeneous Simplifying Graph Convolution.**

*Ren, Yu, et. al*

### **Abstract:**

Drug repositioning plays a key role in disease treatment. With the large-scale chemical data increasing, many computational methods are utilized for drug-disease association prediction. However, most of the existing models neglect the positive influence of non-Euclidean data and multisource information, and there is still a critical issue for graph neural networks regarding how to set the feature diffuse distance. To solve the problems, we proposed SiSGC, which makes full use of the biological knowledge information as initial features and learns the structure information from the constructed heterogeneous graph with the adaptive selection of the information diffuse distance. Then, the structural features are fused with the denoised similarity information and fed to the advanced classifier of CatBoost to make predictions. Three different data sets are used to confirm the robustness and generalization of SiSGC under two splitting strategies. Experiment results demonstrate that the proposed model achieves superior performance compared with the six leading methods and four variants. Our case study on breast neoplasms further indicates that SiSGC is trustworthy and robust yet simple. We also present four drugs for breast cancer treatment with high confidence and further give an explanation for demonstrating the rationality. There is no doubt that SiSGC can be used as a beneficial supplement for drug repositioning.

## CLUSTERING

Proc Natl Acad Sci U S A (impact factor: 11.1) 1 [☒](#) TOP

### **Drivers of the artiodactyl turnover in insular western Europe at the Eocene-Oligocene Transition.**

*Weppe, Condamine, et. al*

#### **Abstract:**

Simultaneously investigating the effects of abiotic and biotic factors on diversity dynamics is essential to understand the evolutionary history of clades. The Grande Coupure corresponds to a major faunal turnover at the Eocene-Oligocene transition (EOT) (~34.1 to 33.55 Mya) and is defined in western Europe as an extinction of insular European mammals coupled with the arrival of crown clades from Asia. Here, we focused on the species-rich group of endemic European artiodactyls to determine the drivers of the Grande Coupure during the major environmental disruptions at the EOT. Using Bayesian birth-death models, we analyzed an original high-resolution fossil dataset (90 species, >2,100 occurrences) from southwestern France (Quercy area) and estimated the regional diversification and diversity dynamics of endemic and immigrant artiodactyls. We show that the endemic artiodactyl radiation was mainly related to the Eocene tropical conditions, combined with biotic controls on speciation and clade-related diversity dependence. We further highlight that the major environmental changes at the transition (77% of species became extinct) and the concurrent increase in seasonality in Europe during the Oligocene were likely the main drivers of their decline. Surprisingly, our results do not support the widely-held hypothesis of active competition between endemic and immigrant artiodactyls but rather suggest a passive or opportunistic replacement by immigrants, which is further supported by morphological clustering of specific ecological traits across the Eocene-Oligocene transition. Our analyses provide insights into the evolutionary and ecological processes driving the diversification and decline of mammalian clades during a major biological and climatic crisis.

Proc Natl Acad Sci U S A (impact factor: 11.1) 1 [☒](#) TOP

### **Intrinsic circuitry of the rhombicbrain (central nervous system's intermediate sector) in a mammal.**

*Swanson, Hahn, et al*

#### **Abstract:**

The rhombicbrain (rhombencephalon or intermediate sector) is the vertebrate central nervous system part between the forebrain-midbrain (rostral sector) and spinal cord (caudal sector), and it has three main divisions: pons, cerebellum, and medulla. Using a data-driven approach, here we examine intrinsic rhombicbrain (intrarhombicbrain) network architecture that in rat consists of 52,670 possible axonal connections between

230 gray matter regions (115 bilaterally symmetrical pairs). Our analysis indicates that only 8,089 (15.4%) of these connections exist. Multiresolution consensus cluster analysis yields a nested hierarchy model of rhombicbrain subsystems that at the top level are associated with 1) the cerebellum and vestibular nuclei, 2) orofacial-pharyngeal-visceral integration, and 3) auditory connections; the bottom level has 68 clusters, ranging in size from 2 to 11 regions. The model provides a basis for functional hypothesis development and interrogation. More granular network analyses performed on the intrinsic connectivity of individual and combined main rhombicbrain divisions (pons, cerebellum, medulla, pons + cerebellum, and pons + medulla) demonstrate the mutability of network architecture in response to the addition or subtraction of connections. Clear differences between the structure-function network architecture of the rhombicbrain and forebrain-midbrain are discussed, with a stark comparison provided by the subsystem and small-world organization of the cerebellar cortex and cerebral cortex. Future analysis of the connections within and between the forebrain-midbrain and rhombicbrain will provide a model of brain neural network architecture in a mammal.

Plant Physiol (impact factor: 7.4) 2  TOP

### **Drying without Dying: a genome database for desiccation-tolerant plants and evolution of desiccation tolerance.**

*Gao, Li, et. al*

#### **Abstract:**

Desiccation is typically fatal, but a small number of land plants have evolved vegetative desiccation tolerance (VDT), allowing them to dry without dying through a process called anhydrobiosis. Advances in sequencing technologies have enabled the investigation of genomes for desiccation-tolerant plants over the past decade. However, a dedicated and integrated database for these valuable genomic resources has been lacking. Our prolonged interest in VDT plant genomes motivated us to create the "Drying without Dying" database, which contains a total of 16 VDT-related plant genomes (including ten mosses) and incorporates 10 genomes that are closely related to VDT plants. The database features bioinformatic tools, such as blast and homologous cluster search, sequence retrieval, GO term and metabolic pathway enrichment statistics, expression profiling, co-expression network extraction, and JBrowser exploration for each genome. To demonstrate its utility we conducted tailored PFAM family statistical analyses, and we discovered that the drought-responsive ABA transporter AWPM-19 family is significantly tandemly duplicated in all bryophytes but rarely so in tracheophytes. Transcriptomic investigations also revealed that response patterns following desiccation diverged between bryophytes and angiosperms. Combined, the analyses provided genomic and transcriptomic evidence supporting a possible divergence and lineage-specific evolution of VDT in plants. The database can be accessed at <http://desiccation.novogene.com>. We expect

this initial release of the "Drying without Dying" plant genome database will facilitate future discovery of VDT genetic resources.© The Author(s) 2023. Published by Oxford University Press on behalf of American Society of Plant Biologists. All rights reserved. For permissions, please e-mail: journals.permissions@oup.com.

## MACHINE LEARNING

Water Res (impact factor: 12.8) 1  TOP

### **Machine learning-based prediction for settling velocity of microplastics with various shapes.**

*Qian, Qiao, et. al*

#### **Abstract:**

Microplastics can easily enter the aquatic environment and be transported between water bodies. The terminal settling velocity of microplastics, which affects their transport and distribution in the aquatic environment, is mainly influenced by their size, density, and shape. Due to the difficulty in accurately predicting the terminal settling velocity of microplastics with various shapes, this study focuses on establishing high-performance prediction models and understanding the importance and effect of each feature parameter using machine learning. Based on the number of principal dimensions, the shapes of microplastics are classified into fiber, film, and fragment, and their thresholds are identified. The microplastics of different shape categories have different optimal shape parameters for predicting the terminal settling velocity: Corey shape factor, flatness, elongation, and sphericity for the fragment, film, fiber, and mixed-shape MPs, respectively. By including the dimensionless diameter, relative density and optimal shape parameter in the input parameter combination, the machine learning models can well predict the terminal settling velocity for the microplastics of different shape categories and mixed-shape with  $R^2 > 0.867$ , achieving significantly higher performance than the existing theoretical and regression models. The interpretable analysis of machine learning reveals the highest importance of the microplastic size and its marginal effect when the dimensionless diameter  $D^* = dn(g/v^2)^{1/3} > 80$ , where  $dn$  is the equivalent diameter,  $g$  is the gravitational acceleration, and  $v$  is the fluid kinematic viscosity. The effect of shape is weak for small microplastics and becomes significant when  $D^*$  exceeds 65. Copyright © 2023 Elsevier Ltd. All rights reserved.

## **Real-time water quality prediction in water distribution networks using graph neural networks with sparse monitoring data.**

*Li, Liu, et. al*

### **Abstract:**

Ensuring the safety and reliability of drinking water supply requires accurate prediction of water quality in water distribution networks (WDNs). However, existing hydraulic model-based approaches for system state prediction face challenges in model calibration with limited sensor data and intensive computing requirements, while current machine learning models are lack of capacity to predict the system states at sites that are not monitored or included in model training. To address these gaps, this study proposes a novel gated graph neural network (GGNN) model for real-time water quality prediction in WDNs. The GGNN model integrates hydraulic flow directions and water quality data to represent the topology and system dynamics, and employs a masking operation for training to enhance prediction accuracy. Evaluation results from a real-world WDN demonstrate that the GGNN model is capable to achieve accurate water quality prediction across the entire WDN. Despite being trained with water quality data from a limited number of sensor sites, the model can achieve high predictive accuracies (Mean Absolute Error = 0.07 mg L<sup>-1</sup> and Mean Absolute Percentage Error = 10.0 %) across the entire network including those unmonitored sites. Furthermore, water quality-based sensor placement significantly improves predictive accuracy, emphasizing the importance of careful sensor location selection. This research advances water quality prediction in WDNs by offering a practical and effective machine learning solution to address challenges related to limited sensor data and network complexity. This study provides a first step towards developing machine learning models to replace hydraulic models in WDN modelling. Copyright © 2023. Published by Elsevier Ltd.

## **GCDN-Net: Garbage classifier deep neural network for recyclable urban waste management.**

*Hossen, Ashraf, et. al*

### **Abstract:**

The escalating waste volume due to urbanization and population growth has underscored the need for advanced waste sorting and recycling methods to ensure sustainable waste management. Deep learning models, adept at image recognition tasks, offer potential solutions for waste sorting applications. These models, trained on extensive waste image datasets, possess the ability to discern unique features of diverse waste types. Automating waste sorting hinges on robust deep learning models capable of accurately categorizing a wide range of waste types. In this study, a multi-stage



machine learning approach is proposed to classify different waste categories using the "Garbage In, Garbage Out" (GIGO) dataset of 25,000 images. The novel Garbage Classifier Deep Neural Network (GCDN-Net) is introduced as a comprehensive solution, adept in both single-label and multi-label classification tasks. Single-label classification distinguishes between garbage and non-garbage images, while multi-label classification identifies distinct garbage categories within single or multiple images. The performance of GCDN-Net is rigorously evaluated and compared against state-of-the-art waste classification methods. Results demonstrate GCDN-Net's excellence, achieving 95.77% accuracy, 95.78% precision, 95.77% recall, 95.77% F1-score, and 95.54% specificity when classifying waste images, outperforming existing models in single-label classification. In multi-label classification, GCDN-Net attains an overall Mean Average Precision (mAP) of 0.69 and an F1-score of 75.01%. The reliability of network performance is affirmed through saliency map-based visualization generated by Score-CAM (class activation mapping). In conclusion, deep learning-based models exhibit efficacy in categorizing diverse waste types, paving the way for automated waste sorting and recycling systems that can mitigate costs and processing times. Copyright © 2023 Elsevier Ltd. All rights reserved.

## DEEP LEARNING

Med Image Anal (impact factor: 10.9) 1 ☒

### **Learning image representations for anomaly detection: Application to discovery of histological alterations in drug development.**

*Zingman, Stierstorfer, et. al*

#### **Abstract**

We present a system for anomaly detection in histopathological images. In histology, normal samples are usually abundant, whereas anomalous (pathological) cases are scarce or not available. Under such settings, one-class classifiers trained on healthy data can detect out-of-distribution anomalous samples. Such approaches combined with pre-trained Convolutional Neural Network (CNN) representations of images were previously employed for anomaly detection (AD). However, pre-trained off-the-shelf CNN representations may not be sensitive to abnormal conditions in tissues, while natural variations of healthy tissue may result in distant representations. To adapt representations to relevant details in healthy tissue we propose training a CNN on an auxiliary task that discriminates healthy tissue of different species, organs, and staining reagents. Almost no additional labeling workload is required, since healthy samples come automatically with aforementioned labels. During training we enforce compact image representations with a center-loss term, which further improves

representations for AD. The proposed system outperforms established AD methods on a published dataset of liver anomalies. Moreover, it provided comparable results to conventional methods specifically tailored for quantification of liver anomalies. We show that our approach can be used for toxicity assessment of candidate drugs at early development stages and thereby may reduce expensive late-stage drug attrition. Copyright © 2023 Elsevier B.V. All rights reserved.

Sci Total Environ (impact factor: 9.8) 2 [✕](#) TOP

### **A timely and accurate approach to nearshore oil spill monitoring using deep learning and GIS.**

*Lau, Huang, et. al*

#### **Abstract**

Oil spill accidents are a key contributor to marine pollution worldwide. Therefore, timely and effective oil spill detection is crucial for reducing marine pollution and enhancing environmental protection. Against this backdrop, this study explored two methods for performing nearshore on-site oil spill detection and segmentation, namely the U-net and Mask region-based convolutional neural network (R-CNN) methods. The U-net and Mask R-CNN models were revealed to exhibit acceptable and favorable performance, achieving overall accuracy of 77.01 % and 89.02 %, respectively. Subsequently, a verification system based on the Geographic Information System (GIS) was developed to improve the performance of the deep-learning model. With the integration of the verification system, the Mask R-CNN model achieved higher overall accuracy of 90.78 %. The feasibility of applying deep-learning methods to nearshore on-site oil spill monitoring was demonstrated through this study. In addition, the integration of the GIS not only assisted in the provision of oil spill information but also in the improvement of the deep-learning models. The timely, accurate, and effective method for nearshore on-site oil spill monitoring that this study explored can be applied to considerably improve traditional on-site oil spill monitoring, which has received limited academic attention in the last two decades. Copyright © 2023. Published by Elsevier B.V.

Curr Biol (impact factor: 9.2) 1 [✕](#) TOP

### **Neurophysiological and behavioral synchronization in group-living and sleeping mice.**

*Sotelo, Markunas, et. al*

#### **Abstract**

Social interactions profoundly influence animal development, physiology, and behavior. Yet, how sleep—a central behavioral and neurophysiological process—is modulated by social interactions is poorly understood. Here, we characterized sleep behavior and

neurophysiology in freely moving and co-living mice under different social conditions. We utilized wireless neurophysiological devices to simultaneously record multiple individuals within a group for 24 h, alongside video acquisition. We first demonstrated that mice seek physical contact before sleep initiation and sleep while in close proximity to each other (hereafter, "huddling"). To determine whether huddling during sleep is a motivated behavior, we devised a novel behavioral apparatus allowing mice to choose whether to sleep in close proximity to a conspecific or in solitude, under different environmental conditions. We also applied a deep-learning-based approach to classify huddling behavior. We demonstrate that mice are willing to forgo their preferred sleep location, even under thermoneutral conditions, to gain access to social contact during sleep. This strongly suggests that the motivation for prolonged physical contact-which we term somatolonging-drives huddling behavior. We then characterized sleep architecture under different social conditions and uncovered a social-dependent modulation of sleep. We also revealed coordination in multiple neurophysiological features among co-sleeping individuals, including in the timing of falling asleep and waking up and non-rapid eye movement sleep (NREMS) intensity. Notably, the timing of rapid eye movement sleep (REMS) was synchronized among co-sleeping male siblings but not co-sleeping female or unfamiliar mice. Our findings provide novel insights into the motivation for physical contact and the extent of social-dependent plasticity in sleep. Copyright © 2023 Elsevier Inc. All rights reserved.

## EMBEDDED SYSTEM

Phys Rev Lett (impact factor: 8.6) 1 [☒](#) TOP

### **Heterogeneous Mean First-Passage Time Scaling in Fractal Media.**

*Chun, Hwang, et. al*

#### **Abstract**

The mean first passage time (MFPT) of random walks is a key quantity characterizing dynamic processes on disordered media. In a random fractal embedded in the Euclidean space, the MFPT is known to obey the power law scaling with the distance between a source and a target site with a universal exponent. We find that the scaling law for the MFPT is not determined solely by the distance between a source and a target but also by their locations. The role of a site in the first passage processes is quantified by the random walk centrality. It turns out that the site of highest random walk centrality, dubbed as a hub, intervenes in first passage processes. We show that the MFPT from a departure site to a target site is determined by a competition between direct paths and indirect paths detouring via the hub. Consequently, the MFPT displays a crossover scaling between a short distance regime, where direct paths are dominant, and a long

distance regime, where indirect paths are dominant. The two regimes are characterized by power laws with different scaling exponents. The crossover scaling behavior is confirmed by extensive numerical calculations of the MFPTs on the critical percolation cluster in two dimensional square lattices.

Phys Rev Lett (impact factor: 8.6) 1 [☒](#) [TOP](#)

### **Molecules in Environments: Toward Systematic Quantum Embedding of Electrons and Drude Oscillators.**

*Ditte, Barborini, et. al*

#### **Abstract:**

We develop a quantum embedding method that enables accurate and efficient treatment of interactions between molecules and an environment, while explicitly including many-body correlations. The molecule is composed of classical nuclei and quantum electrons, whereas the environment is modeled via charged quantum harmonic oscillators. We construct a general Hamiltonian and introduce a variational Ansatz for the correlated ground state of the fully interacting molecule-environment system. This wave function is optimized via the variational Monte Carlo method and the ground state energy is subsequently estimated through the diffusion Monte Carlo method. The proposed scheme allows an explicit many-body treatment of electrostatic, polarization, and dispersion interactions between the molecule and the environment. We study solvation energies and excitation energies of benzene derivatives, obtaining excellent agreement with explicit ab initio calculations and experiments.

Plant Biotechnol J (impact factor: 13.8) 1 [☒](#) [TOP](#)

### **Robust Zero Modes in Non-Hermitian Systems without Global Symmetries.**

*Rivero, Fleming, et. al*

#### **Abstract:**

We present an approach to achieve zero modes in lattice models that do not rely on any symmetry or topology of the bulk, which are robust against disorder in the bulk of any type and strength. Such symmetry-free zero modes (SFZMs) are formed by attaching a single site or small cluster with zero mode(s) to the bulk, which serves as the "nucleus" that expands to the entire lattice. We identify the requirements on the couplings between this boundary and the bulk, which reveals that this approach is intrinsically non-Hermitian. We then provide several examples with either an arbitrary or structured bulk, forming spectrally embedded zero modes in the bulk continuum, midgap zero modes, and even restoring the "zerness" of coupling or disorder-shifted topological corner states. Focusing on viable realizations using photonic lattices, we show that the resulting SFZM can be observed as the single lasing mode when optical gain is applied to the boundary.

# II Concentration

## PHYSICS

### **On-demand entanglement of molecules in a reconfigurable optical tweezer array**

*Connor M. Holland, Yukai Lu, et al.*

#### **Abstract**

Entanglement is crucial to many quantum applications, including quantum information processing, quantum simulation, and quantum-enhanced sensing. Because of their rich internal structure and interactions, molecules have been proposed as a promising platform for quantum science. Deterministic entanglement of individually controlled molecules has nevertheless been a long-standing experimental challenge. We demonstrate on-demand entanglement of individually prepared molecules. Using the electric dipolar interaction between pairs of molecules prepared by using a reconfigurable optical tweezer array, we deterministically created Bell pairs of molecules. Our results demonstrate the key building blocks needed for quantum applications and may advance quantum-enhanced fundamental physics tests that use trapped molecules.

### **Dipolar spin-exchange and entanglement between molecules in an optical tweezer array**

*Yicheng Bao, Scarlett S. Yu, et al.*

#### **Abstract**

Ultracold polar molecules are promising candidate qubits for quantum computing and quantum simulations. Their long-lived molecular rotational states form robust qubits, and the long-range dipolar interaction between molecules provides quantum entanglement. In this work, we demonstrate dipolar spin-exchange interactions between single calcium monofluoride (CaF) molecules trapped in an optical tweezer array. We realized the spin-12 quantum XY model by encoding an effective spin-12 system into the rotational states of the molecules and used it to generate a Bell state through an iSWAP operation. Conditioned on the verified existence of molecules in both tweezers at the end of the measurement, we obtained a Bell state fidelity of 0.89(6). Using interleaved tweezer arrays, we demonstrate single-site molecular addressability.

# Self-enhancing sono-inks enable deep-penetration acoustic volumetric printing

*Xiao Kuang, Qiangzhou Rong, et al.*

## Abstract

Volumetric printing, an emerging additive manufacturing technique, builds objects with enhanced printing speed and surface quality by forgoing the stepwise ink-renewal step. Existing volumetric printing techniques almost exclusively rely on light energy to trigger photopolymerization in transparent inks, limiting material choices and build sizes. We report a self-enhancing sonicated ink (or sono-ink) design and corresponding focused-ultrasound writing technique for deep-penetration acoustic volumetric printing (DAVP). We used experiments and acoustic modeling to study the frequency and scanning rate-dependent acoustic printing behaviors. DAVP achieves the key features of low acoustic streaming, rapid sonothermal polymerization, and large printing depth, enabling the printing of volumetric hydrogels and nanocomposites with various shapes regardless of their optical properties. DAVP also allows printing at centimeter depths through biological tissues, paving the way toward minimally invasive medicine.

## MATERIALS

### Low voltage-driven high-performance thermal switching in antiferroelectric PbZrO<sub>3</sub> thin films

*Chenhan Liu, Yangyang Si, et al.*

## Abstract

Effective control of heat transfer is vital for energy saving and carbon emission reduction. In contrast to achievements in electrical conduction, active control of heat transfer is much more challenging. Ferroelectrics are promising candidates for thermal switching as a result of their tunable domain structures. However, switching ratios in ferroelectrics are low (<1.2). We report that high-quality antiferroelectric PbZrO<sub>3</sub> epitaxial thin films exhibit high-contrast (>2.2), fast-speed (<150 nanoseconds), and long-lifetime (>10<sup>7</sup>) thermal switching under a small voltage (<10 V). In situ reciprocal space mapping and atomistic modelings reveal that the field-driven antiferroelectric-ferroelectric phase transition induces a substantial change of primitive cell size, which modulates phonon-phonon scattering phase space drastically and results in high switching ratio. These results advance the concept of thermal transport control in ferroic materials.

## Emission and coherent control of Levitons in graphene

*A. Assouline, L. Pugliese, et al.*

### Abstract

Flying qubits encode quantum information in propagating modes instead of stationary discrete states. Although photonic flying qubits are available, the weak interaction between photons limits the efficiency of conditional quantum gates. Conversely, electronic flying qubits can use Coulomb interactions, but the weaker quantum coherence in conventional semiconductors has hindered their realization. In this work, we engineered on-demand injection of a single electronic flying qubit state and its manipulation over the Bloch sphere. The flying qubit is a Leviton propagating in quantum Hall edge channels of a high-mobility graphene monolayer. Although single-shot qubit readout and two-qubit operations are still needed for a viable manipulation of flying qubits, the coherent manipulation of an itinerant electronic state at the single-electron level presents a highly promising alternative to conventional qubits.

## Self-sustaining personal all-day thermoregulatory clothing using only sunlight

*Ziyuan Wang, Yiwen Bo, et al.*

### Abstract

The human body must stay within a certain temperature range for comfort and safety. However, challenges for thermoregulatory clothing exist for harsh application scenarios, such as full day/night cycles, frigid polar regions, and space travel. We developed a flexible and sustainable personal thermoregulatory clothing system by integrating a flexible organic photovoltaic (OPV) module to directly acquire energy from sunlight and bidirectional electrocaloric (EC) devices. The flexible OPV-EC thermoregulatory clothing (OETC) can extend the human thermal comfort zone from 22°–28°C to 12.5°–37.6°C with a fast thermoregulation rate. The low energy consumption and high efficiency of the EC device allows for 24 hours of controllable and dual-mode thermoregulation with 12 hours of sunlight energy input. This self-powered wearable thermoregulatory platform has a simple structure, compact design, high efficiency, and strong self-adaptability with sunlight as the sole energy source.

## CHEMISTRY

### **Kinetic and thermodynamic control of C(sp<sup>2</sup>)-H activation enables site-selective borylation**

*Jose B. Roque, Alex M. Shimozone, et. al*

#### **Abstract**

Catalysts that distinguish between electronically distinct carbon-hydrogen (C-H) bonds without relying on steric effects or directing groups are challenging to design. In this work, cobalt precatalysts supported by N-alkyl-imidazole-substituted pyridine dicarbene (ACNC) pincer ligands are described that enable undirected, remote borylation of fluoroaromatics and expansion of scope to include electron-rich arenes, pyridines, and tri- and difluoromethoxylated arenes, thereby addressing one of the major limitations of first-row transition metal C-H functionalization catalysts. Mechanistic studies established a kinetic preference for C-H bond activation at the meta-position despite cobalt-aryl complexes resulting from ortho C-H activation being thermodynamically preferred. Switchable site selectivity in C-H borylation as a function of the boron reagent was thereby preliminarily demonstrated using a single precatalyst.

### **Element abundance patterns in stars indicate fission of nuclei heavier than uranium**

*Ian U. Roederer, Nicole Vassh, et. al*

#### **Abstract**

The heaviest chemical elements are naturally produced by the rapid neutron-capture process (r-process) during neutron star mergers or supernovae. The r-process production of elements heavier than uranium (transuranic nuclei) is poorly understood and inaccessible to experiments so must be extrapolated by using nucleosynthesis models. We examined element abundances in a sample of stars that are enhanced in r-process elements. The abundances of elements ruthenium, rhodium, palladium, and silver (atomic numbers  $Z = 44$  to  $47$ ; mass numbers  $A = 99$  to  $110$ ) correlate with those of heavier elements ( $63 \leq Z \leq 78, A > 150$ ). There is no correlation for neighboring elements ( $34 \leq Z \leq 42$  and  $48 \leq Z \leq 62$ ). We interpret this as evidence that fission fragments of transuranic nuclei contribute to the abundances. Our results indicate that neutron-rich nuclei with mass numbers  $>260$  are produced in r-process events.



## **Boryl radical catalysis enables asymmetric radical cycloisomerization reactions**

*Chang-Ling Wang, Jie Wang, et. al*

### **Abstract**

The development of functionally distinct catalysts for enantioselective synthesis is a prominent yet challenging goal of synthetic chemistry. In this work, we report a family of chiral N-heterocyclic carbene (NHC)-ligated boryl radicals as catalysts that enable catalytic asymmetric radical cycloisomerization reactions. The radical catalysts can be generated from easily prepared NHC-borane complexes, and the broad availability of the chiral NHC component provides substantial benefits for stereochemical control. Mechanistic studies support a catalytic cycle comprising a sequence of boryl radical addition, hydrogen atom transfer, cyclization, and elimination of the boryl radical catalyst, wherein the chiral NHC subunit determines the enantioselectivity of the radical cyclization. This catalysis allows asymmetric construction of valuable chiral heterocyclic products from simple starting materials.

## **BIOLOGY**

### **Multifaceted SOX2-chromatin interaction underpins pluripotency progression in early embryos**

*Lijia Li, Fangnong Lai, et al.*

### **Abstract**

Pioneer transcription factors (TFs), such as OCT4 and SOX2, play crucial roles in pluripotency regulation. However, the master TF-governed pluripotency regulatory circuitry was largely inferred from cultured cells. In this work, we investigated SOX2 binding from embryonic day 3.5 (E3.5) to E7.5 in the mouse. In E3.5 inner cell mass (ICM), SOX2 regulates the ICM-trophectoderm program but is dispensable for opening global enhancers. Instead, SOX2 occupies preaccessible enhancers in part opened by early-stage expressing TFs TFAP2C and NR5A2. SOX2 then widely redistributes when cells adopt naive and formative pluripotency by opening enhancers or poisoning them for rapid future activation. Hence, multifaceted pioneer TF-enhancer interaction underpins pluripotency progression in embryos, including a distinctive state in E3.5 ICM that bridges totipotency and pluripotency.

## **Microbiome diversity protects against pathogens by nutrient blocking**

*Frances Spragge, Erik Bakkeren, et. al*

### **Abstract**

The human gut microbiome plays an important role in resisting colonization of the host by pathogens, but we lack the ability to predict which communities will be protective. We studied how human gut bacteria influence colonization of two major bacterial pathogens, both in vitro and in gnotobiotic mice. Whereas single species alone had negligible effects, colonization resistance greatly increased with community diversity. Moreover, this community-level resistance rested critically upon certain species being present. We explained these ecological patterns through the collective ability of resistant communities to consume nutrients that overlap with those used by the pathogen. Furthermore, we applied our findings to successfully predict communities that resist a novel target strain. Our work provides a reason why microbiome diversity is beneficial and suggests a route for the rational design of pathogen-resistant communities.

## **Ancient chicken remains reveal the origins of virulence in Marek's disease virus**

*Steven R. Fiddaman, Evangelos A. Dimopoulos, et. al*

### **Abstract**

The pronounced growth in livestock populations since the 1950s has altered the epidemiological and evolutionary trajectory of their associated pathogens. For example, Marek's disease virus (MDV), which causes lymphoid tumors in chickens, has experienced a marked increase in virulence over the past century. Today, MDV infections kill >90% of unvaccinated birds, and controlling it costs more than US\$1 billion annually. By sequencing MDV genomes derived from archeological chickens, we demonstrate that it has been circulating for at least 1000 years. We functionally tested the Meq oncogene, one of 49 viral genes positively selected in modern strains, demonstrating that ancient MDV was likely incapable of driving tumor formation. Our results demonstrate the power of ancient DNA approaches to trace the molecular basis of virulence in economically relevant pathogens.

# III Calling for papers

## ICCAE 2024

**Submission deadline:** Jan 5, 2024  
**Conference date:** Mar 14, 2024 - Mar 16, 2024  
**Full name:** International Conference on Computer and Automation Engineering  
**Location:** Melbourne, Australia  
**Website:** <http://www.iccae.org/>

As we stand on the brink of the fourth industrial revolution, the field of Computer and Automation Engineering continues to evolve at an unprecedented pace, playing a crucial role in shaping our technological future. Advances in this discipline are key drivers of Industry 4.0, underpinning the design, development, application, and integration of intelligent systems in a wide range of sectors.

Automation, driven by machine learning and artificial intelligence, is transforming traditional industries by improving productivity, enhancing safety, reducing human error, and enabling more sophisticated data analysis. Developments in this area have led to innovations such as autonomous vehicles, smart homes, automated manufacturing systems, and medical robotics.

In parallel, Computer Engineering is at the heart of this technological revolution, developing hardware and software solutions that allow the seamless integration of physical systems and digital technologies. Pioneering work in areas such as embedded systems, cloud computing, cybersecurity, and IoT has allowed for the creation of more efficient and robust automated systems.

In this context, the International Conference on Computer and Automation Engineering (ICCAE) offers an ideal platform to keep pace with these rapid advancements. After the successes of ICCAE 2009 (Bangkok, Thailand), ICCAE 2010 (Singapore), ICCAE 2011 (Chongqing, China), ICCAE 2012 (Mumbai, India), ICCAE 2013 (Bruxelles, Belgium), ICCAE 2014 (Melbourne, Australia), ICCAE 2015 (Bali, Indonesia), ICCAE 2016 (Melbourne, Australia), ICCAE 2017 (Sydney, Australia), ICCAE 2018 (Brisbane, Australia), ICCAE 2019 (Perth, Australia), ICCAE 2020 (Sydney, Australia), ICCAE 2021 (virtual conference), and ICCAE 2022 (virtual conference), ICCAE 2023 (Sydney, Australia), the 16th International Conference on Computer and Automation Engineering (ICCAE 2024) is going to take place in Melbourne, Australia during March 14-16, 2024.

The conference aims to bring together global experts, researchers, practitioners, and industry leaders to share their latest research results, explore new areas of research and development, and discuss the challenges and practical solutions in Computer and Automation Engineering. Through collaborative discussion and knowledge sharing, the conference aims to contribute to shaping the future of this exciting and rapidly evolving field.

### Call for papers:

Topics of interest for submission include, but are not limited to:

T1: Modern and Advanced Control Strategies . Fuzzy Logic Control  
Neural Networks Control . Genetic Algorithms & Evolutionary Control

. Model-Predictive Control

T2: Human-Machine Systems

. Man-Machine Systems

. Human Computer Interaction

. Human Factors in system Design

T3: Multimedia and Communication Systems

. Multimedia and New Media

. High Speed Communication

. Hyper Network Communication

T4: Hybrid Systems

. Fuzzy Evolutionary Systems

. Fuzzy Expert Systems

. Fuzzy Neural Systems

. Neural Genetic Systems

T5: Robotics and Automation

. Robot Dynamics and Control

. Human-robot Systems

. Intelligent Robots

. Autonomous Robots

T6: Decision Making and Information Retrieval

. Case-Based Reasoning

. Decision Analysis

. Intelligent Databases & Information Retrieval

. Dynamic Systems Modeling

T7: Data Analysis, Prediction and Model Identification

. Signal Processing

. Prediction and Time Series Analysis

. System Identification

. Data Fusion and Mining

T8: Control System Applications

. Manufacturing Systems

. Transportation Systems

. Medical and Health Care Systems

. Medical Decision Making

More details, please view:

<http://www.iccae.org/cfp.html>

## CSTE 2024

**Submission deadline:**

**Jan 5, 2024**

**Conference date:**

**Apr 19, 2024 - Apr 21, 2024**

**Full name:**

**International Conference on Computer Science and Technologies in Education**

**Location:**

**Xi'an, China**

**Website:**

<http://cste.net/>

The 6th International Conference on Computer Science and Technologies in Education (CSTE 2024) will be held in Xi'an, China during April 19-21, 2024. CSTE 2024 is organized by Shaanxi Normal University, China, hosted by Faculty of Education, Shaanxi Normal University, China, and assisted by Research Center for AI & STEM Education of Shaanxi Normal University, China.

At CSTE 2024, participants will have the opportunity to engage with leading experts in education technology, and to gain insights into the latest research and best practices in the field.

**20 / 24**

**Editor: Chaoyi Chu (褚朝奕)**

**TEL: 3548**

**Email: ccy@jsut.edu.cn**

The conference will also provide a platform for networking and collaboration, enabling participants to build valuable connections with colleagues from around the world.

**Topics of Interest :**

Topics of interest for submission include, but are not limited to:

Track 1: Educational Technologies and Systems

- E-learning platforms and tools
- Computer-supported collaborative learning
- Mobile and ubiquitous learning

Track 2: Computer-supported Collaborative Learning and Social Computing

- Collaborative learning theories and models
- Social computing and learning
- Online communities and networks in education

Track 3: Artificial Intelligence in Education

- Intelligent tutoring systems
- Natural language processing in education
- Knowledge representation and reasoning in education

Track 4: STEM Education and Computational Thinking

- STEM education and pedagogy
- Computational thinking and coding education
- Robotics and automation in STEM education

Track 5: Educational Data Mining and Learning Analytics

- Data-driven approaches to education
- Learning analytics and visualization
- Educational data mining and machine learning

Track 6: Innovative Technologies for Teaching and Learning

- Wearable technology in education
- Gamification and game-based learning
- Personalized and adaptive learning

For more topics, please visit: <http://cste.net/cfp.html>

## ICCCR 2024

<b>Submission deadline:</b>	<b>Jan 5, 2024</b>
<b>Conference date:</b>	<b>Apr 19, 2024 - Apr 21, 2024</b>
<b>Full name:</b>	<b>International Conference on Computer, Control and Robotics</b>
<b>Location:</b>	<b>Shanghai, China</b>
<b>Website:</b>	<a href="http://www.iccr.org/">http://www.iccr.org/</a>

2024 the 4th International Conference on Computer, Control and Robotics (ICCCR 2024-[www.iccr.org](http://www.iccr.org)) will be held during the period April 19-21, 2024 in Shanghai, China. It's sponsored by Shanghai University, hosted by School of Mechatronic Engineering and Automation, Shanghai University. ICCCR focuses on the synergetic interaction of computing technologies, control technologies and robotic technologies, and provide an excellent platform to all researchers share latest ideas. The mutual benefit make it possible to build and evolve new robotic systems, to reduce the development cost, and to enhance the quality.

**Call for Papers:**

Please check the topics of ICCCR 2024. The topics are not limited to those as below:

★Control Systems and Optimization

- \* Genetic Algorithms
- \* Fuzzy Control
- \* Decision Support Systems
- \* Machine Learning in Control Applications
- \* Knowledge-based Systems Applications

★Robotics

- \* RAMS abilities of robotic systems
- \* Hardware modeling and abstraction
- \* Resource awareness
- \* Sensor fusion, integration
- \* Place recognition, localization
- \* Image Processing

★Computer Science

- \* Formal methods for analysis and design
- \* Software architectures
- \* Middleware infrastructures
- \* Model-driven engineering
- \* Component-based engineering
- \* Natural language understanding
- \* Machine learning
- \* Reasoning
- \* Multi agent system

More details, please view: <http://www.iccr.org/cfp.html>

## ICICT 2024

**Submission deadline:** Jan 10, 2024  
**Conference date:** Mar 15, 2024 - Mar 17, 2024  
**Full name:** International Conference on Information and Computer Technologies  
**Location:** Honolulu, Hawaii, USA  
**Website:** <http://icict.org/>

ICICT is an annual conference hold each year in United States and 2024 The 7th International Conference on Information and Computer Technologies will be held at Honolulu, Hawaii during March 15-17, 2024. It is an international forum for academia and industries to exchange visions and ideas in the state of the art and practice of information and computer technologies.

**\*Call for papers:**

Include but not limited:

- \* Algorithms
- \* Artificial Intelligence
- \* Automated Software Engineering
- \* Bioinformatics & Scientific Computing
- \* Biomedical Engineering
- \* Bio-informatics
- \* Compilers & Interpreters
- \* Computational Intelligence
- \* Computer Animation
- \* Computer Architecture & VLSI
- \* Information Systems

.....

more please click: <http://icict.org/cfp.html>

## ICCEE 2024

**Submission deadline:** Jan 10, 2024  
**Conference date:** Jun 28, 2024 - Jun 30, 2024  
**Full name:** International Conference on Computer and Electrical Engineering  
**Location:** Shenzhen, China  
**Website:** <http://iccee.org>

Welcome to the official website of the 2024 The 17th International Conference on Computer and

Electrical Engineering (ICCEE 2024). The conference will be held in Shenzhen University, Shenzhen, China on June 28-30, 2024.

Computer engineering programs largely developed in engineering departments strong in electrical engineering. Nowadays, the influence of computers has been more revolutionary than in electrical engineering. The design, analysis, and operation of electrical and electronic systems are now dominated by computers, driven by a natural and convenient interface between computers and electrical systems, as well as significant improvements in speed and efficiency.

ICCEE was started in Phuket Island, Thailand in the year of 2008, and after the success of the first edition, it has been held annually from 2009 to 2019 in Dubai(UAE), Chengdu(China), Singapore, Hong Kong, Paris(France), Geneva(Switzerland), Paris(France), Barcelona(Spain), Edmonton(Canada), Tokyo(Japan), TU Delft, Netherlands. Due to the impact of COVID19, ICCEE2020~2022 were held as a virtual conference. 2023 witnessed the 16th edition of ICCEE held onsite in Xi'an.

The objective of ICCEE is to present the latest research and results of scientists (preferred students, PhD Students, and post-doc scientists) related to Computer and Electrical Engineering topics. This conference provides opportunities for the different areas delegates to exchange new ideas and application experiences face to face, to establish business or research relations and to find global partners for future collaboration. We hope that the conference results constituted significant contribution to the knowledge in these up to date scientific fields.

Now, the platform is ready, what we need is for you all to come up here one by one to seize this opportunity to join us and express your thoughts and opinions confidently. Your full paper or abstract submission is highly welcome. New ideas and innovation will be 100 percent respected in our conferences.

Look forward to seeing you in Shenzhen!

### Topics of interest

\*\*\*Computer Engineering

- Algorithm
- Bioinformatics and Biosciences
- Computational and Artificial Intelligence
- Computer Architecture
- Computer Graphics and Virtual Reality

\*\*\*Electrical Engineering

- Advanced Power Semiconductors
- Analogue and Digital Signal Processing
- Biomedical Engineering
- Computation Intelligence in Electrical Engineering
- Computer and AI Applications in Power Industry
- Control Science and Control

\*For more topics, please visit at:

<http://iccee.org/call-for-papers.html>